Formal Verification of Machine Learning

MPRI 2-6: Abstract Interpretation, Application to Verification and Static Analysis



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Machine Learning Revolution

Computer software able to efficiently and **autonomously perform tasks** that are difficult or even *impossible* to design using explicit programming



Examples: object recognition, image classification, speech recognition, etc.

Lesson 15

ML in Safety-Critical Applications

Enables new functions that could not be envisioned before



Self-Driving Cars



Image-Based Taxiing, Takeoff, Landing

Aircraft Voice Control

ML in Safety-Critical Applications

Approximates complex systems and automates decision-making



Diagnosis and Drug Discovery



AIRBUS A380

.....

floating point storage. A simple technique to reduce the size of the score table is to downsample the table after dynamic programming. To minimize the degradation in decision quality, states are removed in areas where the variation between values in the table are smooth. The downsampling reduces the size of the table by a factor of 180 from that produced by dynamic programming. For the rest of this paper, the downsampled ACAS Xu horizontal table is referred to as the baseline, original table.

the current table requires over

an aircraft collision avoidance system frames the problem as a

Abstract—One approach to designing decision making logic for

Markov decision process and optimizes the system using dynamic programming. The resulting collision avoidance strategy can be represented as a numeric table. This methodology has been used in the development of the Airborne Collision Avoidance System X (ACAS X) family of collision avoidance systems for manned and unmanned aircraft, but the high dimensionality of the state space ables To improve storage efficiency, a deep

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Lesson 15

Formal Verification of Machine Learning

Aircraft Collision Avoidance

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ML in Safety-Critical Applications

STAT+2 IBM's Watson supercomputer recommended 'unsafe and incorrect' cancer treatments, internal documents show

By Casey Ross³ @caseymross⁴ and Ike Swetlitz

July 25, 2018

A self-driving Uber ran a red light last December, contrary to company claims

Internal documents reveal that the car was at fault

By Andrew Liptak | @AndrewLiptak | Feb 25, 2017, 11:08am EST

Feds Say Self-Driving Uber SUV Did Not Recognize Jaywalking Pedestrian In Fatal Crash

Richard Gonzales November 7, 201910:57 PM ET



Machine Learning Pipeline





data preparation



model training



model deployment



predictions

Machine Learning Pipeline

Model Training is Highly Non-Deterministic





Formal Methods Mathematical Guarantees of Safety



Deductive Verification

- extremely expressive ٠
- relies on the user to guide the proof •







Model Checking

- analysis of a **model** of the software
- with respect to the model

Static Analysis

- analysis of the software at some level of abstraction
- fully automatic and sound by construction
- generally not complete



Formal Methods for Trained Models

Neural Networks

Neural Networks

Feed-Forward Fully-Connected Neural Networks with ReLU Activation Functions



Rectified Linear Unit (ReLU)

Feed-Forward Fully-Connected ReLU Networks as Programs



x00 = input() x01 = input() x10 = -0.31 * x00 + 0.99 * x01 + (-0.63)

x11 = -1.25 * x00 + (-0.64) * x01 + 1.88 x10 = 0 if x10 < 0 else x10 x11 = 0 if x11 < 0 else x11 x20 = 0.40 * x10 + 1.21 * x11 + 0.00x21 = 0.64 * x10 + 0.69 * x11 + (-0.39)



Maximal Trace Semantics



Neural Network Verification

Lesson 15





Goal G3 in [Kurd03]



Safety Goal G4 in [Kurd03]

Fairness

Stability

Goal G3 in [Kurd03]

Safety

Goal G4 in [Kurd03]









Local Stability

The classification is unaffected by small input perturbations



Local Stability

Distance-Based Perturbations

 $P_{\delta,\epsilon}(\mathbf{x}) \stackrel{\mathsf{def}}{=} \{ \mathbf{x}' \in \mathscr{R}^{|L_0|} \mid \delta(\mathbf{x}, \mathbf{x}') \le \epsilon \}$

Example (L_{∞} distance): $P_{\infty,\epsilon}(\mathbf{x}) \stackrel{\text{def}}{=} \{\mathbf{x}' \in \mathscr{R}^{|L_0|} \mid \max_i |\mathbf{x}_i - \mathbf{x}'_i| \le \epsilon\}$

$\mathscr{R}_{\mathbf{x}}^{\delta,\epsilon} \stackrel{\mathsf{def}}{=} \{\llbracket M \rrbracket \in \mathscr{P}(\Sigma^*) \mid \mathsf{STABLE}_{\mathbf{x}}^{\delta,\epsilon}(\llbracket M \rrbracket)\}$

 $\mathscr{R}^{\delta,\epsilon}_{\mathbf{x}}$ is the set of all neural networks M (or, rather, their semantics [[M]]) that are **stable** in the neighborhood $P_{\delta,\epsilon}(\mathbf{x})$ of a given input \mathbf{x}

$$\begin{aligned} \mathsf{STABLE}_{\mathbf{x}}^{\delta,\epsilon}(\llbracket M \rrbracket) \stackrel{\text{def}}{=} \forall t \in \llbracket M \rrbracket : (\exists t' \in \llbracket M \rrbracket : \forall 0 \le i \le |L_0| : t'_0(x_{0,i}) = \mathbf{x}_i) \\ & \wedge (\exists \mathbf{x}' \in P_{\delta,\epsilon}(\mathbf{x}) : \forall 0 \le i \le |L_0| : t_0(x_{0,i}) = \mathbf{x}'_i) \\ & \Rightarrow \max_j t_{\omega}(x_{N,j}) = \max_j t'_{\omega}(x_{N,j}) \end{aligned}$$





Static Analysis Methods

Forward Analysis



 proceed forwards from an abstraction of all possible perturbations





 $P(\langle 0.5, 0.75 \rangle) \stackrel{\mathsf{def}}{=} \{ \mathbf{x} \in \mathcal{R} \times \mathcal{R} \mid 0 \leq \mathbf{x}_0 \leq 1 \land 0 \leq \mathbf{x}_1 \leq 1 \}$

 $x_{i,j} \mapsto [a,b]$ $a,b \in \mathcal{R}$



each neuron as a linear combination of the inputs and the previous ReLUs

with Symbolic Constant Propagation [Li19]

$$x_{i,j} \mapsto \begin{cases} \sum_{k=0}^{i-1} \mathbf{c}_k \cdot \mathbf{x}_k + \mathbf{c} & \mathbf{c}_k, \mathbf{c} \in \mathscr{R}^{|\mathbf{X}_k|} \\ [a, b] & a, b \in \mathscr{R} \end{cases}$$



J. Li et al. - Analyzing Deep Neural Networks with Symbolic Propagation (SAS 2019)

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with Symbolic Constant Propagation [Li19]



with Symbolic Constant Propagation [Li19]





G. Singh, T. Gehr, M. Püschel, and M. Vechev - An Abstract Domain for Certifying Neural Networks (POPL 2019)









$$\begin{aligned} x_{00} \mapsto \begin{cases} [x_{00}, x_{00}] \\ [0, 1] \end{cases} & x_{01} \mapsto \begin{cases} [x_{01}, x_{01}] \\ [0, 1] \end{cases} \\ x_{10} \mapsto \begin{cases} [x_{00} + x_{01} + 4, x_{00} + x_{01} + 4] \\ [4, 6] \end{cases} & x_{11} \mapsto \begin{cases} [0.5 \cdot x_{00} + 0.5 \cdot x_{01} + 3, 0.5 \cdot x_{00} + 0.5 \cdot x_{01} + 3] \\ [3, 4] \end{cases} \\ x_{20} \mapsto \begin{cases} [2 \cdot x_{10} + 3 \cdot x_{11}, 2 \cdot x_{10} + 3 \cdot x_{11}] \\ [17, 24] \end{cases} & x_{21} \mapsto \begin{cases} [x_{10} - x_{11}, x_{10} - x_{11}] \\ [1, 2] \end{cases} \\ x_{30} \mapsto \begin{cases} [x_{20} - x_{21} - 14, x_{20} - x_{21} - 14] \\ [2, 8] \end{cases} & x_{31} \mapsto \begin{cases} [0, 0.5 \cdot (0.5 \cdot x_{20} - 1.5 \cdot x_{21} - 8) + 0.5] \\ [0, 1] \end{cases} \\ x_{40} \mapsto \begin{cases} [x_{10} - x_{11} + 1, 0.5 \cdot x_{30} - 2 \cdot x_{31} + 1] \\ \mapsto \begin{cases} [x_{10} - x_{11} + 1, 0.5 \cdot x_{10} + 2 \cdot x_{11} - 6] \\ \mapsto \begin{cases} [x_{10} - x_{11} + 1, 0.5 \cdot x_{01} + 2, 1.5 \cdot x_{00} + 1.5 \cdot x_{11} + 2] \\ [2, 5] \end{cases} \end{aligned}$$



$$\begin{aligned} x_{00} \mapsto \begin{cases} [x_{00}, x_{00}] \\ [0, 1] \end{cases} & x_{01} \mapsto \begin{cases} [x_{01}, x_{01}] \\ [0, 1] \end{cases} \\ x_{10} \mapsto \begin{cases} [x_{00} + x_{01} + 4, x_{00} + x_{01} + 4] \\ [4, 6] \end{cases} & x_{11} \mapsto \begin{cases} [0.5 \cdot x_{00} + 0.5 \cdot x_{01} + 3, 0.5 \cdot x_{00} + 0.5 \cdot x_{01} + 3] \\ [3, 4] \end{cases} \\ x_{20} \mapsto \begin{cases} [2 \cdot x_{10} + 3 \cdot x_{11}, 2 \cdot x_{10} + 3 \cdot x_{11}] \\ [17, 24] \end{cases} & x_{21} \mapsto \begin{cases} [x_{10} - x_{11}, x_{10} - x_{11}] \\ [1, 2] \end{cases} \\ x_{30} \mapsto \begin{cases} [x_{20} - x_{21} - 14, x_{20} - x_{21} - 14] \\ [2, 8] \end{cases} & x_{31} \mapsto \begin{cases} [0, 0.5 \cdot (0.5 \cdot x_{20} - 1.5 \cdot x_{21} - 8) + 0.5] \\ [0, 1] \end{cases} \\ x_{41} \mapsto \begin{cases} [x_{31}, x_{31}] \\ \Rightarrow \begin{cases} [0, -0.25 \cdot x_{20} - 0.75 \cdot x_{21} - 3.5] \\ \Rightarrow \end{cases} \\ [0, -0.25 \cdot x_{10} + 1.5 \cdot x_{11} - 3.5] \\ \Rightarrow \begin{cases} [0, 0.5 \cdot x_{00} + 0.5 \cdot x_{01}] \\ [0, 1] \end{cases} \end{aligned} \end{aligned}$$


Other Static Analysis Methods

- T. Gehr, M. Mirman, D. Drachsler-Cohen, P. Tsankov, S. Chaudhuri, and M. Vechev. Al2: Safety and Robustness Certification of Neural Networks with Abstract Interpretation. In S&P, 2018.
 the first use of abstract interpretation for verifying neural networks
- G. Singh, T. Gehr, M. Mirman, M. Püschel, and M. Vechev. Fast and Effective Robustness Certification. In NeurIPS, 2018.
 a custom zonotope domain for certifying neural networks
- G. Singh, R. Ganvir, M. Püschel, and M. Vechev. Beyond the Single Neuron Convex Barrier for Neural Network Certification. In NeurIPS, 2019.
 a framework to jointly approximate k ReLU activations
- M. N. Müller, G. Makarchuk, G. Singh, M. Püschel, and M. Vechev. PRIMA: General and Precise Neural Network Certification via Scalable Convex Hull Approximations. In POPL, 2022.
 a multi-neuron abstraction via a convex-hull approximation algorithm



Goal G3 in [Kurd03]

Safety

Goal G4 in [Kurd03]













ACAS Xu [Julian16][Katz17]

Airborne Collision Avoidance System for Unmanned Aircraft implemented using 45 feed-forward fully-connected ReLU networks



5 0 -5 COC -5 0 SR SR WL WL WL -5 0 5 10 15

5 input sensor measurements

- ρ : distance from ownship to intruder
- θ : angle to intruder relative to ownship heading direction
- ψ : heading angle to intruder relative to ownship heading direction
- v_{own}: speed of ownship
- *v_{int}*: speed of intruder

5 output horizontal advisories

- Strong Left
- Weak Left
- Clear of Conflict
- Weak Right
- Strong Right

ACAS Xu Properties [Katz17]

Example: "if intruder is near and approaching from the left, go Strong Right"





Input-Output Properties

- I: input specification
- O: output specification

$$\mathcal{S}_{\mathbf{O}}^{\mathbf{I}} \stackrel{\mathsf{def}}{=} \{\llbracket M \rrbracket \in \mathscr{P}(\Sigma^*) \mid \mathsf{SAFE}_{\mathbf{O}}^{\mathbf{I}}(\llbracket M \rrbracket)\}$$

 $\mathscr{S}^{\mathbf{I}}_{\mathbf{O}}$ is the set of all neural networks M (or, rather, their semantics [[M]]) that **satisfy** the input and output specification **I** and **O** SAFE_{\mathbf{O}}^{\mathbf{I}}([[M]]) \stackrel{\text{def}}{=} \forall t \in [[M]]: t_0 \models \mathbf{I} \Rightarrow t_{\omega} \models \mathbf{O}

Theorem

 $M \models \mathcal{S}_{\mathbf{O}}^{\mathbf{I}} \Leftrightarrow \{\llbracket M \rrbracket\} \subseteq \mathcal{S}_{\mathbf{O}}^{\mathbf{I}}$

Corollary

$$M \models \mathcal{S}_{\mathbf{0}}^{\mathbf{I}} \Leftrightarrow \llbracket M \rrbracket \subseteq \bigcup \mathcal{S}_{\mathbf{0}}^{\mathbf{I}}$$



Model Checking Methods





SMT-Based Methods

Verification Reduced to Constraint Satisfiability

 $l_j \leq x_{0,j} \leq u_j$

 $j \in \{0, ..., |\mathbf{X}_0|\}$

input specification



$$i \in \{0, ..., n-1\}$$

 $i \in \{1, ..., n-1\},$
 $j \in \{0, ..., |\mathbf{X}_i|\}$



(negation of) output specification



 $\mathbf{x}_{N} \leq \mathbf{0}$

Planet

use approximations to reduce the solution search space



R. Ehlers - Formal Verification of Piece-Wise Linear Feed-Forward Neural Networks (ATVA 2017)

Formal Verification of Machine Learning

Reluplex

based on the simplex algorithm extended to support ReLUs

Variable	Value
X 00	v_{00}
• • •	• • •
x _{ij}	\hat{v}'_{ij}
X _{ij}	\hat{v}'_{ij}
• • •	• • •
X _N	v_N

Variable	Value
X 00	v_{00}
• • •	• • •
Âx _{ij}	\hat{v}'_{ij}
X _{ij}	0
• • •	• • •
X _N	v_N

Variable	Value
X 00	v_{00}
• • •	• • •
$\hat{\mathbf{x}}_{\mathbf{ij}}$	\hat{v}_{ij}
X _{ij}	V _{ij}
• • •	• • •
X _N	v_N

Variable	Value
X ₀₀	v_{00}
• • •	• • •
$\hat{\mathbf{x}}_{\mathbf{ij}}$	$\hat{\mathcal{V}}'_{ij}$
X _{ij}	V _{ij}
• • •	• • •
x _N	v_N

G. Katz et al. - Reluplex: An Efficient SMT Solver for Verifying Deep Neural Networks (CAV 2017)

Reluplex

Follow-up Work

G. Katz et al. - The Marabou Framework for Verification and Analysis of Deep Neural Networks (CAV 2019)

X ₀₀	v_{00}
• • •	• • •
$\hat{\mathbf{x}}_{\mathbf{ij}}$	\hat{v}'_{ij}
X _{ij}	$\hat{\mathcal{V}}'_{ij}$
• • •	• • •
X _N	v_N

Variable

Variable	Value
x ₀₀	v_{00}
•••	• • •
$\hat{\mathbf{x}}_{\mathbf{ij}}$	\hat{v}'_{ij}
X _{ij}	0
•••	• • •
X _N	v_N

Variable	Value
X ₀₀	v_{00}
• • •	• • •
$\hat{\mathbf{x}}_{\mathbf{ij}}$	\hat{v}_{ij}
X _{ij}	V _{ij}
• • •	• • •
X _N	v_N

Variable	Value
X 00	v_{00}
• • •	• • •
$\hat{\mathbf{x}}_{\mathbf{ij}}$	$\hat{\mathcal{V}}'_{ij}$
X _{ij}	V _{ij}
• • •	• • •
x _N	v_N

G. Katz et al. - Reluplex: An Efficient SMT Solver for Verifying Deep Neural Networks (CAV 2017)

Other SMT-Based Methods

- L. Pulina and A. Tacchella. An Abstraction-Refinement Approach to Verification of Artificial Neural Networks. In CAV, 2010.
 the first formal verification method for neural networks
- O. Bastani, Y. Ioannou, L. Lampropoulos, D. Vytiniotis, A. Nori, and A. Criminisi. Measuring Neural Net Robustness with Constraints. In NeurIPS, 2016.
 an approach for finding the nearest adversarial example according to the L∞ distance
- X. Huang, M. Kwiatkowska, S. Wang, and M. Wu. Safety Verification of Deep Neural Networks. In CAV, 2017.
 an approach for proving local robustness to adversarial perturbations
- N. Narodytska, S. Kasiviswanathan, L. Ryzhyk, M. Sagiv, and T. Walsh. Verifying Properties of Binarized Deep Neural Networks. In AAAI, 2018.
 C. H. Cheng, G. Nührenberg, C. H. Huang, and H. Ruess. Verification of Binarized Neural Networks via Inter-Neuron Factoring. In VSTTE, 2018.
 approaches focusing on binarized neural networks

MILP-Based Methods

Verification Reduced to Mixed Integer Linear Program

 $l_i \leq x_{0,i} \leq u_i$

 $j \in \{0, ..., |\mathbf{X}_0|\}$

input specification

- $\hat{x}_{i+1,j} = \sum_{j=1}^{|\mathbf{X}_i|} w_{j,k}^i \cdot x_{i,k} + b_{i,j} \qquad i \in \{0, \dots, n-1\}$ k=0 $x_{i,i} = \delta_{i,i} \cdot \hat{x}_{i,i}$ $\delta_{\mathbf{i},\mathbf{i}} = 1 \Rightarrow \hat{x}_{i,i} \ge 0$
- $\delta_{\mathbf{i},\mathbf{i}} = 0 \Rightarrow \hat{x}_{i,i} < 0$

 $\delta_{\mathbf{i},\mathbf{i}} \in \{\mathbf{0},\mathbf{1}\}$ $i \in \{1, ..., n-1\}$

 $j \in \{0, ..., |\mathbf{X}_i|\}$



objective function

min X_N



MILP-Based Methods

Bounded Encoding with Symmetric Bounds

$$\begin{aligned} \hat{x}_{i+1,j} &= \sum_{k=0}^{|\mathbf{X}_i|} w_{j,k}^i \cdot x_{i,k} + b_{i,j} & i \in \{0, \dots, n-1\} \\ 0 &\leq x_{i,j} \leq \mathbf{M}_{\mathbf{i},\mathbf{j}} \cdot \delta_{i,j} & \delta_{\mathbf{i},\mathbf{j}} \in \{\mathbf{0}, \mathbf{1}\} \\ \hat{x}_{i,j} &\leq x_{i,j} \leq \hat{x}_{i,j} - \mathbf{M}_{\mathbf{i},\mathbf{j}} \cdot (1 - \delta_{i,j}) & i \in \{1, \dots, n-1\} \\ \mathbf{M}_{\mathbf{i},\mathbf{j}} &= \max\{-\mathbf{l}_{\mathbf{i}}, \mathbf{u}_{\mathbf{i}}\} & j \in \{0, \dots, |\mathbf{X}_i|\} \end{aligned}$$



Output Range Analysis

 $l_j \leq x_{0,j} \leq u_j$

$$\hat{x}_{i+1,j} = \sum_{k=0}^{|\mathbf{X}_i|} w_{j,k}^i \cdot x_{i,k} + b_{i,j}$$
$$0 \le x_{i,j} \le \mathbf{M}_{\mathbf{i},\mathbf{j}} \cdot \delta_{i,j}$$
$$\hat{x}_{i,j} \le x_{i,j} \le \hat{x}_{i,j} - \mathbf{M}_{\mathbf{i},\mathbf{j}} \cdot (1 - \delta_{i,j})$$
$$\mathbf{M}_{\mathbf{i},\mathbf{j}} = \max\{-\mathbf{l}_{\mathbf{i}}, \mathbf{u}_{\mathbf{i}}\}$$

 $min \ x_N \\$

use local search to

speed up the MILP solver

S. Dutta et al. - Output Range Analysis for Deep Feedforward Neural Networks (NFM 2018)

Output Range Analysis

 $l_j \leq x_{0,j} \leq u_j$

$$\hat{x}_{i+1,j} = \sum_{k=0}^{|\mathbf{X}_i|} w_{j,k}^i \cdot x_{i,k} + b_{i,j}$$

$$0 \le x_{i,j} \le \mathbf{M}_{\mathbf{i},\mathbf{j}} \cdot \delta_{i,j}$$
$$\hat{x}_{i,j} \le x_{i,j} \le \hat{x}_{i,j} - \mathbf{M}_{\mathbf{i},\mathbf{j}} \cdot (1 - \delta_{i,j})$$
$$\mathbf{M}_{\mathbf{i},\mathbf{j}} = \max\{-\mathbf{l}_{\mathbf{i}}, \mathbf{u}_{\mathbf{i}}\}$$

 $x_N < L$



S. Dutta et al. - Output Range Analysis for Deep Feedforward Neural Networks (NFM 2018)

use local search to speed up the MILP solver

 $\begin{array}{l} \text{sample } \text{random input } X \\ \text{and evaluate output } L \end{array}$

use local search to speed up the MILP solver

Output Range Analysis

$$\begin{split} \mathbf{l_j} &\leq \mathbf{x_{0,j}} \leq \mathbf{u_j} \\ \hat{x}_{i+1,j} &= \sum_{k=0}^{|\mathbf{X}_i|} w_{j,k}^i \cdot x_{i,k} + b_{i,j} \\ 0 &\leq x_{i,j} \leq \mathbf{M_{i,j}} \cdot \delta_{i,j} \\ \hat{x}_{i,j} &\leq x_{i,j} \leq \hat{x}_{i,j} - \mathbf{M_{i,j}} \cdot (1 - \delta_{i,j}) \\ \mathbf{M_{i,j}} &= \max\{-\mathbf{l_i}, \mathbf{u_i}\} \end{split}$$

find another input \hat{X} such that $\hat{L} \leq x_N$

 $x_N < L$

S. Dutta et al. - Output Range Analysis for Deep Feedforward Neural Networks (NFM 2018)

use local search to speed up the MILP solver

Output Range Analysis





S. Dutta et al. - Output Range Analysis for Deep Feedforward Neural Networks (NFM 2018)

MILP-Based Methods

Bounded Encoding with Asymmetric Bounds

$$\hat{x}_{i+1,j} = \sum_{k=0}^{|\mathbf{X}_i|} w_{j,k}^i \cdot x_{i,k} + b_{i,j} \qquad i \in \{0, \dots, n-1\}$$

$$0 \le x_{i,j} \le \mathbf{u}_{\mathbf{i},\mathbf{j}} \cdot \delta_{i,j} \qquad \qquad \delta_{\mathbf{i},\mathbf{j}} \in \{\mathbf{0}, \mathbf{1}\}$$

$$\hat{x}_{i,j} \le x_{i,j} \le \hat{x}_{i,j} - \mathbf{l}_{\mathbf{i},\mathbf{j}} \cdot (1 - \delta_{i,j}) \qquad \qquad i \in \{1, \dots, n-1\}$$

$$j \in \{0, \dots, |\mathbf{X}_i|\}$$



MIPVerify

Finding Nearest Adversarial Example

$\mathsf{min}_{X'} \; d(X,X')$

$$\hat{x}_{i+1,j} = \sum_{k=0}^{|\mathbf{X}_i|} w_{j,k}^i \cdot x_{i,k} + b_{i,j} \qquad i \in \{0, \dots, n-1\}$$

$$0 \le x_{i,j} \le \mathbf{u}_{\mathbf{i},\mathbf{j}} \cdot \delta_{i,j} \qquad \delta_{\mathbf{i},\mathbf{j}} \in \{\mathbf{0}, \mathbf{1}\}$$

$$\hat{x}_{i,j} \le x_{i,j} \le \hat{x}_{i,j} - \mathbf{l}_{\mathbf{i},\mathbf{j}} \cdot (1 - \delta_{i,j}) \qquad i \in \{1, \dots, n-1\}$$

$$j \in \{0, \dots, |\mathbf{X}_i|\}$$



 $\boldsymbol{x_N \neq 0}$

V. Tjeng et al. - Evaluating Robustness of Neural Networks with Mixed Integer Programming (ICLR 2019)

Other MILP-Based Methods

- R. Bunel, I. Turkaslan, P. H. S. Torr, P. Kohli, and M. P. Kumar. A Unified View of Piecewise Linear Neural Network Verification. In NeurIPS, 2018.
 a unifying verification framework for piecewise-linear ReLU neural networks
- C.-H. Cheng, G. Nührenberg, and H. Ruess. Maximum Resilience of Artificial Neural Networks. In ATVA, 2017.
 an approach for finding a lower bound on robustness to adversarial perturbations
- M. Fischetti and J. Jo. Deep Neural Networks and Mixed Integer Linear Optimization. 2018.
 an approach for feature visualization and building adversarial examples



Static Analysis Methods

Forward Analysis



 proceed forwards from an abstraction of the input specification I

Lesson 15







DeepPoly Domain [Singh19]



DeepPoly Domain [Singh19]



Interval Domain

with Symbolic Constant Propagation [Li19]



Interval Domain

with Symbolic Constant Propagation [Li19]



Interval Domain

with Symbolic Constant Propagation [Li19]



DeepPoly with Symbolic Constant Propagation











Other Complete Methods

Lesson 15

Formal Verification of Machine Learning



use union of efficient representations of bounded convex polyhedra

Exact Static Analysis Method

$$\Theta \stackrel{\text{def}}{=} \langle c, V, P \rangle \qquad \qquad c \in \mathscr{R}^n: \text{ center} \\ V = \{v_1, \dots, v_m\}: \text{ basis vectors in } \mathscr{R}^n \\ P: \mathscr{R}^m \to \{ \bot, T \}: \text{ predicate} \end{cases}$$

$$[\![\Theta]\!] = \{x \mid x = c + \sum_{i=1}^{m} \alpha_i v_i \text{ such that } P(\alpha_1, ..., \alpha_m) = \mathsf{T} \}$$

- fast and cheap **affine mapping operations** \rightarrow neural network layers
- inexpensive intersections with half-spaces \rightarrow ReLU activations

H.-D. Tran et al. - Star-Based Reachability Analysis of Deep Neural Networks (FM 2018)
Star Sets

 $\Theta \stackrel{\text{def}}{=} \langle c, V, P \rangle$

Exact Static Analysis Method

H.-D. Tran et al. -Verification of Deep Convolutional Neural Networks Using ImageStars (CAV 2020)

Follow-up Work

US

efficient

of bounded

 $c \in \mathscr{R}^n$: center $V = \{v_1, ..., v_m\}$: basis vectors in \mathscr{R}^n $P: \mathscr{R}^m \to \{ \bot, T \}$: predicate

$$\llbracket \Theta \rrbracket = \{ x \mid x = c + \sum_{i=1}^{m} \alpha_{i} v_{i} \text{ such that } P(\alpha_{1}, \dots, \alpha_{m}) = \mathsf{T} \}$$

• inexpensive intersections with half-spaces
$$\rightarrow$$
 ReLU activations



H.-D. Tran et al. - Star-Based Reachability Analysis of Deep Neural Networks (FM 2018)





Asymptotically Complete Method



S. Wang et al. - Formal Security Analysis of Neural Networks Using Symbolic Intervals (USENIX Security 2018)



use symbolic propagation + convex ReLU approximation + iterative input/ReLU refinement

Asymptotically Complete Method



S. Wang et al. - Formal Security Analysis of Neural Networks Using Symbolic Intervals (USENIX Security 2018)

Further Complete Methods

- W. Ruan, X. Huang, and M. Kwiatkowska. Reachability Analysis of Deep Neural Networks with Provable Guarantees. In IJCAI, 2018.
 a global optimization-based approach for verifying Lipschitz continuous neural networks
- G. Singh, T. Gehr, M. Püschel, and M. Vechev. Boosting Robustness Certification of Neural Networks. In ICLR, 2019.
 an approach combining abstract interpretation and (mixed integer) linear programming



Other Incomplete Methods

Lesson 15

Formal Verification of Machine Learning

Interval Neural Networks

Abstraction-Based Method

Related Work

Y. Y. Elboher et al. - An Abstraction-Based Framework for Neural Network Verification (CAV 2020)



Further Incomplete Methods

- W. Xiang, H.-D. Tran, and T. T. Johnson. Output Reachable Set Estimation and Verification for Multi-Layer Neural Networks. 2018.
 an approach combining simulation and linear programming
- K. Dvijotham, R. Stanforth, S. Gowal, T. Mann, and P. Kohli. A Dual Approach to Scalable Verification of Deep Networks. In UAI, 2018.
 an approach based on duality for verifying neural networks

Further Incomplete Methods

• E. Wong and Z. Kolter. Provable Defenses Against Adversarial Examples via the Convex Outer Adversarial Polytope. In ICML, 2018.

A. Raghunathan, J. Steinhardt, and P. Liang. *Certified Defenses against Adversarial Examples*. In ICML, 2018.

T.-W. Weng, H. Zhang, H. Chen, Z. Song, C.-J. Hsieh, L. Daniel, D. Boning, and I. Dhillon. *Towards Fast Computation of Certified Robustness for ReLU Networks*. In ICML, 2018.

H. Zhang, T.-W. Weng, P.-Y. Chen, C.-J. Hsieh, and L. Daniel. Efficient *Neural Network Robustness Certification with General Activation Functions*. In NeurIPS, 2018.

approaches for finding a lower bound on robustness to adversarial perturbations

Further Incomplete Methods

- A. Boopathy, T.-W. Weng, P.-Y. Chen, S. Liu, and L. Daniel. CNN-Cert: An Efficient Framework for Certifying Robustness of Convolutional Neural Networks. In AAAI, 2019.
 approach focusing on convolutional neural networks
- C.-Y. Ko, Z. Lyu, T.-W. Weng, L. Daniel, N. Wong, and D. Lin. POPQORN: Quantifying Robustness of Recurrent Neural Networks. In ICML, 2019.
 H. Zhang, M. Shinn, A. Gupta, A. Gurfinkel, N. Le, and N. Narodytska. Verification of Recurrent Neural Networks for Cognitive Tasks via Reachability Analysis. In ECAI, 2020.
 approaches focusing on recurrent neural networks
- D. Gopinath, H. Converse, C. S. Pasareanu, and A. Taly. Property Inference for Deep Neural Networks. In ASE, 2019.
 an approach for inferring safety properties of neural networks

Complete Methods

Advantages

sound and complete

Disadvantages

soundness not typically guaranteed with respect to floating-point arithmetic

do not scale to large models

often limited to certain model architectures

suffer from false positives

Disadvantages

able to scale to large models

sound often also with respect to floating-point arithmetic

less limited to certain model architectures

Advantages

Incomplete Methods



Goal G3 in [Kurd03]





Fairness





Lesson 15

Formal Verification of Machine Learning



Dependency Fairness [Galhotra17]

The classification is independent of the values of the sensitive inputs



Dependency Fairness

 $\mathcal{F}_i \stackrel{\mathsf{def}}{=} \{\llbracket M \rrbracket \in \mathscr{P}(\Sigma^*) \mid \mathsf{UNUSED}_i(\llbracket M \rrbracket)\}$

 \mathcal{F}_i is the set of all neural networks M (or, rather, their semantics [[M]]) that **do not use** the value of the sensitive input node $x_{0,i}$ for classification

$$\begin{aligned} \mathsf{UNUSED}_{i}(\llbracket M \rrbracket) \stackrel{\mathsf{def}}{=} \forall t \in \llbracket M \rrbracket, v \in \mathscr{R} \colon t_{0}(x_{0,i}) \neq v \Rightarrow \exists t' \in \llbracket M \rrbracket : \\ (\forall 0 \leq j \leq |L_{0}| : j \neq i \Rightarrow t_{0}(x_{0,j}) = t'_{0}(x_{0,j})) \\ \wedge t'_{0}(x_{0,i}) = v \\ \wedge \max_{j} t_{\omega}(x_{N,j}) = \max_{j} t'_{\omega}(x_{N,j}) \end{aligned}$$

Intuitively: any possible classification outcome is possible from any value of the sensitive input node $x_{0,i}$



Dependency Fairness







Dependency Fairness

 $\mathcal{F}_i \stackrel{\mathsf{def}}{=} \{\llbracket M \rrbracket \in \mathscr{P}(\Sigma^*) \mid \mathsf{UNUSED}_i(\llbracket M \rrbracket)\}$

 \mathcal{F}_i is the set of all neural networks M (or, rather, their semantics [[M]]) that **do not use** the value of the sensitive input node $x_{0,i}$ for classification

$$\begin{aligned} \mathsf{UNUSED}_i(\llbracket M \rrbracket) \stackrel{\mathsf{def}}{=} \forall t \in \llbracket M \rrbracket, v \in \mathscr{R} \colon t_0(x_{0,i}) \neq v \Rightarrow \exists t' \in \llbracket M \rrbracket : \\ (\forall 0 \leq j \leq |L_0| \colon j \neq i \Rightarrow t_0(x_{0,j}) = t'_0(x_{0,j})) \\ \wedge t'_0(x_{0,i}) = v \\ \wedge \max_j t_\omega(x_{N,j}) = \max_j t'_\omega(x_{N,j}) \end{aligned}$$

Intuitively: any possible classification outcome is possible from any value of the sensitive input node $x_{0,i}$

Theorem

 $M \models \mathscr{F}_i \Leftrightarrow \{\llbracket M \rrbracket\} \subseteq \mathscr{F}_i$

Hierarchy of Semantics

parallel semantics





Dependency Semantics

partitioning with respect to the outcome classification **induces a partition of the** space of **values** of the input nodes **used for classification**

\$

\$

\$\$

Lemma

F

\$\$

\$\$

 $M \models \mathcal{F}_i \Leftrightarrow \forall A, B \in \llbracket M \rrbracket_{\prec} \colon (A_{\omega} \neq B_{\omega} \Rightarrow A_0 |_{\neq i} \cap B_0 |_{\neq i} = \emptyset)$

\$

\$

(\$) (\$)

\$\$ \$\$

Naïve Abstraction

Naïve Backward Analysis

(2) forget the values of the sensitive input nodes





Naïve Backward Analysis



Back to the Semantics...

Hierarchy of Semantics

parallel semantics



Parallel Semantics



partitioning a set of traces that satisfies dependency fairness with respect to the non-sensitive inputs yields sets of traces that also satisfy dependency fairness



Parallel Semantics



partitioning a set of traces that satisfies dependency fairness with respect to the non-sensitive inputs yields sets of traces that also satisfy dependency fairness

Parallel Semantics



 $\alpha_{\mathbb{I}}(S) \stackrel{\text{def}}{=} \{ \{ \langle t_0, t_\omega \rangle \in R \mid t_0 \in I \} \mid R \in S \land I \in \mathbb{I} \}$

parallel abstraction

$\{ [M] \}_{\sim}^{\mathbb{I}} \stackrel{\text{def}}{=} \alpha_{\mathbb{I}}(\llbracket M \rrbracket_{\sim})$ = $\{ \{ \langle t_0, t_{\omega} \rangle \in \Sigma \times \Sigma \mid t \in \llbracket M \rrbracket \land t_0 \in I \land t_{\omega} \in O \} \mid I \in \mathbb{I} \land O \in \mathbb{O} \}$

Theorem

$$M \models \mathscr{F}_i \Leftrightarrow \gamma_{\prec}(\{[M]\}_{\prec}^{\mathbb{I}}) \subseteq \mathscr{F}_i$$

Lemma

 $M \models \mathscr{F}_i \Leftrightarrow \forall I \in \mathbb{I} \colon \forall A, B \in \{[M]\}_{\sim}^{\mathbb{I}} \colon (A_{\omega}^I \neq B_{\omega}^I \Rightarrow A_0^I|_{\neq i} \cap B_0^I|_{\neq i} = \emptyset)$

Better Abstraction

Forward and Backward Analysis

1 partition the space of values of the **non-sensitive input** nodes







Lesson 15











Lesson 15
Libra

📮 caterinaurban / Libra

P master → P 2	branches 🕟 0 tags	Go to file Code -	About
caterinaurban README 9f830db on Aug 8 🕚 53 commits			No description or website provided.
src	RQ5 and RQ6 reproducibility	4 months ago	#abstract-interpretation
.gitignore	RQ1 reproducibility	4 months ago	# static-analysis # machine-learning
LICENSE	Initial prototype	2 years ago	#neural-networks #fairnes
README.md	RQ5 and RQ6 reproducibility	4 months ago	🛱 Readme
README.pdf	README	4 months ago	제작 MPL-2.0 License
icon.png	icon	4 months ago	
🗋 libra.png	icon	4 months ago	Releases
requirements.txt	some documentation	4 months ago	No releases published
🗅 setup.py	some documentation	4 months ago	
README.md			Packages No packages published
Libra			Languages
			Python 98.7%Shell 1.3%

Lesson 15

Formal Verification of Machine Learning

Formal Methods for Model Training

Robust Training

Minimizing the Worst-Case Loss for Each Input

Adversarial Training

Minimizing a Lower Bound on the Worst-Case Loss for Each Input

Certified Training

Minimizing an Upper Bound on the Worst-Case Loss for Each Input







generate adversarial inputs and use them as training data



use upper bound as regularizer to encourage robustness

Bibliography

[Kurd03] **Zeshan Kurd, Tim Kelly**. Establishing Safety Criteria for Artificial Neural Networks. In KES, pages 63-169, 2003.

[Li19] Jianlin Li, Jiangchao Liu, Pengfei Yang, Liqian Chen, Xiaowei Huang, and Lijun Zhang. Analyzing Deep Neural Networks with Symbolic Propagation: Towards Higher Precision and Faster Verification. In SAS, page 296–319, 2019.

[Singh19] Gagandeep Singh, Timon Gehr, Markus Püschel, and Martin T. Vechev. An Abstract Domain for Certifying Neural Networks. In POPL, pages 41:1 - 41:30, 2019.

[Mazzucato21] **Denis Mazzucato and Caterina Urban**. Reduced Products of Abstract Domains for Fairness Certification of Neural Networks. In SAS, 2021.

Bibliography

[Julian16] Kyle D. Julian, Jessica Lopez, Jeffrey S. Brush, Michael P. Owen, Mykel J. Kochenderfer. Policy Compression for Aircraft Collision Avoidance Systems. In DASC, pages 1–10, 2016.

[Katz17] Guy Katz, Clark W. Barrett, David L. Dill, Kyle Julian, Mykel J. Kochenderfer. Reluplex: An Efficient SMT Solver for Verifying Deep Neural Networks. In CAV, pages 97–117, 2017.

[Galhotra17] Sainyam Galhotra, Yuriy Brun, and Alexandra Meliou. Fairness Testing: Testing Software for Discrimination. In FSE, pages 498–510, 2017.

[Urban20] Caterina Urban, Maria Christakis, Valentin Wüstholz, and Fuyuan Zhang. Perfectly Parallel Fairness Certification of Neural Networks. In OOPSLA, pages 185:1–185:30, 2020.

[Urban21] Caterina Urban and Antoine Miné. A Review of Formal Methods applied to Machine Learning. <u>https://arxiv.org/abs/2104.02466</u>, 2021.