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Multi-Dimensional Domain Splitting for Neural Network Verification

Msc Project Presentation

James Dorricott

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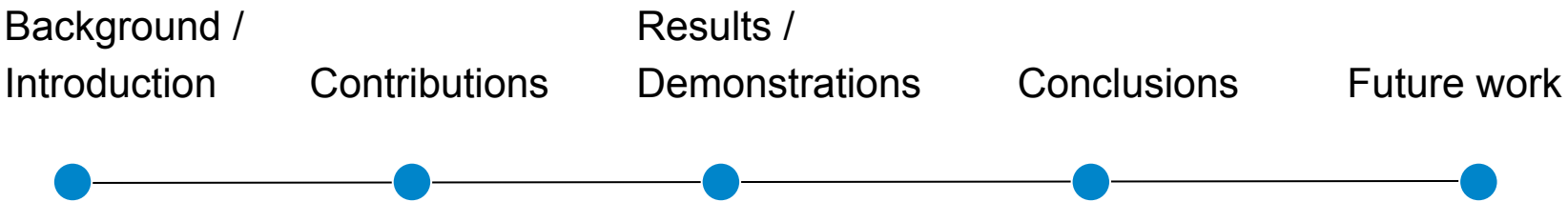
What I will cover



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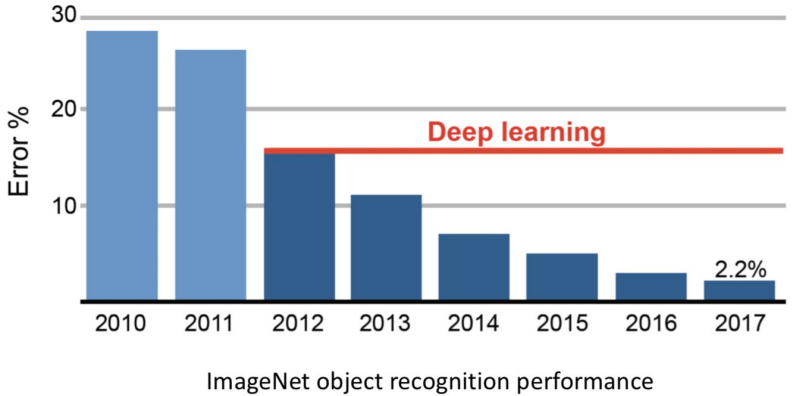
Explosion in deep learning...



ImageNet object recognition performance

Figures: M. Bronstein

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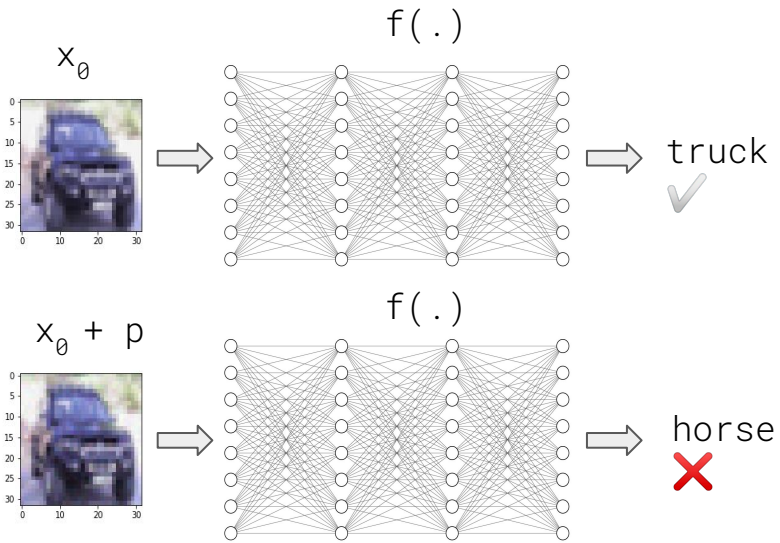
Neural network errors

- It's well-known that neural networks are vulnerable to *adversarial* images
- These are images that look the same to a human but lead to an incorrect classification
- These need to be identified before networks are deployed in safety-paramount applications



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Neural network verification

- The field of neural network verification deals with this *mathematically*
- To make it meaningful requires pre- and post-conditions on the network
- Showing that these hold is the “open-loop verification problem”
- Solving this problem on high-dimensional inputs is the core focus of this project

‘Preconditions’	=	*Input assumptions*
‘Postconditions’	=	*Output properties*
Neural Network	=	*Trained weights/biases*

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Terminology: the verification problem

- We can define this more formally...
- We use the infinity-norm the capture all possible input perturbations up to some ε-bound
- This problem allows for an exact representation as a **MILP program**[1]

Definition 1 *Verification problem. Let* $\mathcal{X}_0 \subseteq \mathbb{R}^m$ *and* $\mathcal{Y} \subseteq \mathbb{R}^n$ *be input and output constraints, respectively, imposed on a neural network network* $f : \mathbb{R}^m \to \mathbb{R}^n$. *Then, the verification problem is to establish whether for all* $\mathbf{x} \in \mathcal{X}_0$, $\mathbf{y} \in \mathcal{Y}$.

Definition 2 *Local robustness. Local robustness is a pair* $(\mathcal{X}_0, K)$, *where* $\mathcal{X}_0 \subseteq \mathbb{R}^m$ *defines a bounded input region and* $1 \leq K \leq n$ *represents the index of the desired class for all inputs in* $\mathcal{X}_0$. *A neural network is said to be locally robust if for all* $\mathbf{x} \in \mathcal{X}_0$, *we have that* $(f(\mathbf{x}))_K > (f(\mathbf{x}))_j$ *for all* $j \neq K$.

1: A. Lomuscio and L. Maganti, “An approach to reachability analysis for feed-forward relu neural networks,” 2017

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Terminology: MILP encodings

- To do so requires a way to linearly encode the non-linearity of the network
- The use of a Big-M encoding[1] can precisely capture the possible phases of the ReLU when the pre-activation pattern is unknown
- The encoding we use leverages the pre-activation **bounds** and modifies slightly the original formulation of Lomuscio & Maganti (2017)

$$
\begin{aligned}
z_{i,j} &\geq \hat{z}_{i,j} \\
z_{i,j} &\geq 0 \\
z_{i,j} &\leq \hat{u}_{i,j}\delta_{i,j} \\
z_{i,j} &\leq \hat{z}_{i,j} - \hat{l}_{i,j}(1-\delta_{i,j})
\end{aligned}
$$

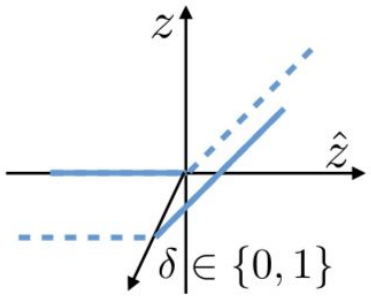

Figure: C. Liu

2: V. Tjeng, K. Xiao, and R. Tedrake, “Evaluating robustness of neural networks with mixed integer programming,” 2017

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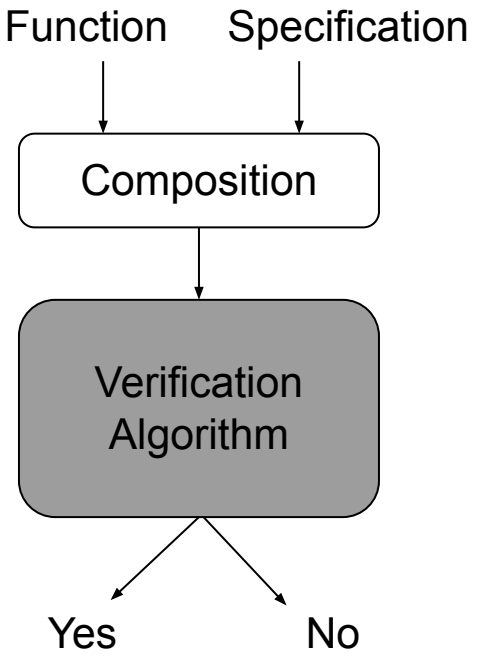
Verification pipeline: template

1. Define the input constraints
2. Define the output constraints
3. Starting from the input, propagate the bounds[3] throughout the network
4. Encode unstable nodes as MILP constraints
5. Dispatch all constraints to a MILP solver
6. If the **answer** to the satisfiability problem is NO, the network is proven to be robust within the given input region



3: We use the symbolic method for computing the bounds of Wang et al (2018)

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Domain splitting: bisection

- Tighter bounds still can be found by *bisecting* the input domain
- Bisection proceeds by dividing the input in half **one dimension** at a time
- Bisection has been shown to be effective for low-dimensional inputs[4,5]
- Different methods exist for how to optimise to dimension to split at each step

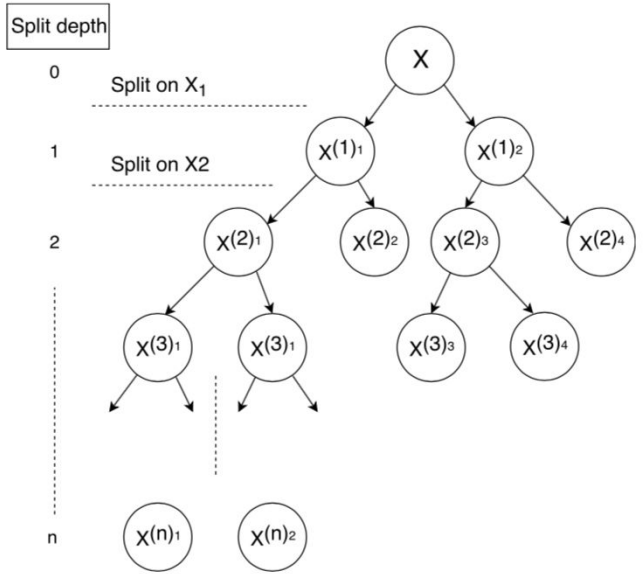

Figure: S. Wang

4: S. Wang, K. Pei, J. Whitehouse, J. Yang, and S. Jana, “Formal security analysis of neural networks using symbolic intervals,” 2018
5: R. Bunel, I. Turkaslan, P. H. Torr, P. Kohli, and M. P. Kumar, “A unified view of piecewise linear neural network verification,” 2018

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Multi-dimensional splitting: motivation

- The success of efficiently reaching an answer[6] to the verification problem when formulated with MILP constraints is related to:
  - The number of binary variables ≡ the number of unstable ReLUs
  - The strength of the relaxations ≡ the tightness of the pre-activation bounds
- This means that networks with high-dimensional inputs (often with many hidden nodes as well) can be very challenging to verify
- And bisection is not well-suited to high-dimensional inputs:
  - One split will be unlikely to reduce the overall problem complexity
  - Exponential blow-up of subregions if the splitting depth is not limited
  - Forced to randomly select which dimension to split

6: Modern commercial solvers apply the *branch and bound* algorithm for solving MILP problems

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Summary of contributions

- *In this project, we…*
- Present a new algorithm[7] for splitting the input domain along **multiple dimensions** which fixes a given ReLU node into the inactive or active state
- Perform extensive investigations to identify the best splitting strategies
- Engineer a distributed verification system for sharing jobs over a network
- Investigate the use of hybrid MILP formulations for checking a combination of the original verification problem and our new splitting procedure

7: Proposed by E. Botoeva (2020)

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The splitting algorithm

- Assume the input region is the multi-dimensional interval [**l**, **u**] and that the equation e(**x**) = **wx** + b estimates the upper bound of a given node y with input **x** ∈ R^m
- Finding split locations $s_{i1},...,s_{ik}$ in dimensions i,...,k that fix y into the inactive state can be solved by means of a MILP

Definition 3 *Splitting algorithm encoded as a MILP.*

- *Take m binary variables $\delta_i, \ldots, \delta_m$, with the meaning that $\delta_i = 1$ iff we split dimension i.*
- *Take m real variables $s_i, \ldots, s_m$, such that when $\delta_i = 1$, the value of $s_i \in [l_i, u_i]$ is the location of the split of input dimension i.*
- *Take m real variables $u_i^*, \ldots, u_m^*$, such that when $\delta_i = 1$, $u_i^* = s_i$, and when $\delta_i = 0$, u_i^* is equal to u_i or l_i depending on $sgn(w_i)$.*

The following constraints are added to the program:

- $e(\boldsymbol{u}^*) = 0$, *where* $\boldsymbol{u}^* = [u_1^*, \ldots, u_m^*]^T$.
- $\delta_i + \cdots + \delta_m \geq 1$.

We also add the following objective function:

- *Minimise the sum* $\delta_i + \cdots + \delta_m$.

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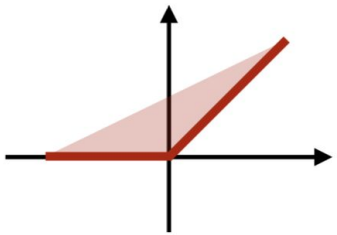
Splitting heuristics

- To decide which node to fix in the network, we make use of the triangle relaxation[8] as a measure of a node's *instability*:
  - The smaller the value of the area induced by the relaxation, the closer the node is to being stable



$\text{Area}_{\text{relax}} := \frac{1}{2}(-l)(u)$

Example: Picking the node with the *2*nd smallest over-approximation area

Node	$\text{Area}_{\text{relax}}$
(1,2)	0.8
(2,3)	1.6
(2,1)	3.4
⋮	⋮

8: R. Ehlers, "Formal verification of piece-wise linear feed-forward neural networks," 2017

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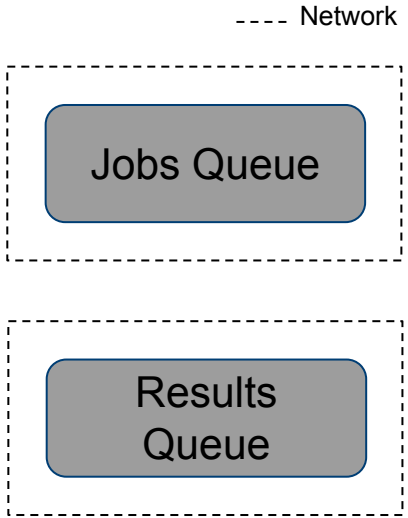
Distributed verification

- Because a splitting step creates a number of independent problems on each of the resulting subregions, we can check these in *parallel*
- A core contribution of this project: building on the existing parallelization scheme[9] by allowing verification jobs to be shared over a network of machines
- To achieve this, we:
  - Leveraged the server/client manager framework available in the Python std. library and the concept of *proxy* objects
  - Designed the system to allow for fully automatic connections



9: Included as part of the inherited verification toolkit for this project

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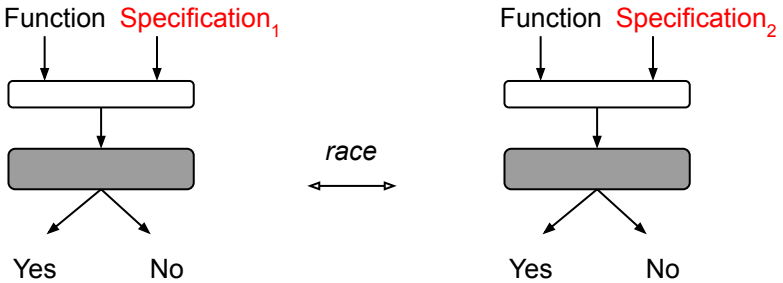
Hybrid MILP formulations

- *Infeasible* instances (solver returns NO) can often be verified more quickly using the standard MILP encoding
  - ...whereas (see next slide) our splitting procedure is good at speeding up the detection of counter-examples (solver returns YES)
- We have therefore investigated the use of hybrid/combined formulations that enter into a parallel race against each other to produce the answer



Example: checking the original problem (‘*spec 1*’) in parallel to our splitting procedure (‘*spec 2*’)

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Headline result

- We performed extensive experiments[10] on a five-layer CIFAR10 classifier with 3,072 inputs / 2,048 ReLUs
- Key finding: *our splitting procedure is able to speed up (x2) counter-example detection on networks with high-dimensional inputs*

Splitter	Queries solved	Total time (s)	Avg time (solved) (s)
None	84	44,309.51	184.62
Bisection	90	32,695.49	163.28
Multi-dim	93	23,733.63	119.71

Table 1: The best verification result of our multi-dimensional splitter applied to 100 mixed-difficulty, non-robust CIFAR instances at ε = 0.03. The timeout was set to 1,800 seconds. We compare it against the original problem (no domain splitting) and a bisection splitter.

10: We also observed good results (x3 speedup) on a smaller-sized MNIST network (784 inputs, 1,024 hidden nodes). We also extended our toolkit to work with the ACAS Xu safety networks, but initial experiments were inconclusive

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Additional insights

- Fixing unstable nodes via domain splitting serves to (a) reduce to search space for the MILP solver and (b) improve the strength of the LP relaxations
- Rather than waiting until a pre-specified stability ratio, e.g., 70%, has been reached (which may require many splitting steps), we found our most effective splitting strategy was to:
  - Perform one splitting step that can immediately produce subproblems for verification
  - Fix the *n*th almost-stable node as a *heuristic* for fixing all nodes with smaller $\text{Area}_{\text{relax}}$
  - Ensure the method for choosing *n* is such that *n* remains **small**
  - ...which suggests that it is only necessary to fix a few unstable nodes to significantly improve upon the original formulation (“dependency effect”)

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Demo: distributed system

Example: the server/client connections and readout from the remote workers are shown in real-time

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Hybrid investigation: results

- In the report, we demonstrate the correctness of our distributed system
- We also used it to investigate our hypothesis that if robustness is not known *a priori*, it's logical to check the original problem and our splitting procedure

Approach	Queries solved	Total time (s)
Baseline	83	54,249.04
Combination	88	37,766.93

Table 2: The result of our combined approach applied to 100 mixed-difficulty, robust AND non-robust CIFAR instances at ε = 0.03. The timeout was set to 1,800 seconds. The combined approach was performed on our distributed system with 2 client verifiers. We compare it against the original problem (no domain splitting).

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Conclusions

- We have introduced a new, multi-dimensional splitting algorithm that is able to more quickly detect counter-examples and brings some key advantages:
  - Based on exploiting information readily available, namely, ReLU stability
  - Aimed directly at reducing the number of binary variables to consider
  - Unlike bisection (which can't be optimised when the dimensionality is high), minimal overhead means it should be able to scale up to larger networks than tested in this project
- We have built a first prototype of a distributed verification system that is able to share jobs over a network, with positive initial demonstrations
- We have investigated the use of combined MILP formulations as an interesting solution to verification *in the wild*

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Future work

- Scaling verification algorithms, particularly complete methods, to real-world networks remains a key challenge. Does our approach hold promise here?
  - ...or do more hidden nodes simply imply more nodes need to be fixed in a splitting step, thus increasing the overhead from our splitting procedure?
  - This is a key trade-off to be considered
- How can we build a more scalable distributed system with less memory cost?
  - May require workarounds, or more production-grade tools than the Python std. library
- Are they other ways of approaching combined formulations?
  - A different approach[11] is to first check the original problem and then only split the input domain when a pre-specified timeout has been reached

11: H. Wu, A. Ozdemir, A. Zeljic, A. Irfan, K. Julian, D. Gopinath, S. Fouladi, G. Katz, C. Pasareanu, and C. Barrett, “Parallelization techniques for verifying neural networks,” 2020

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Thank you!