Automated Repair of Neural Networks

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Introduction

- Artificial Neural Networks (NNs) have been widely used recently
- NNs excel at solving image and natural language processing tasks
- However, they were also found to be susceptible to **Adversarial Attacks**
- This drawback limits the usage of NNs in **safety-critical** systems

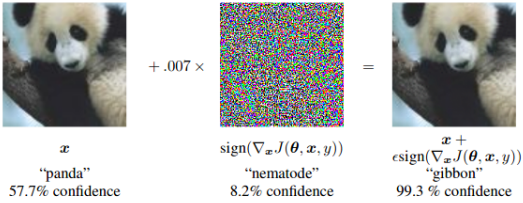

Figure: Depicts the effect of adding noise to an input example - this slight modification shifted the network prediction. Image is borrowed from [goodfellow2015explaining]

Verification of Neural Networks

- As a result, tools for verifying the safety of NNs were developed (e.g., [katz2017reluplex])
- Such tools provide a **safety certificate** given NN and desired properties
- Or, a counter-example in case the NN does not satisfy the specification

Verification of Neural Networks

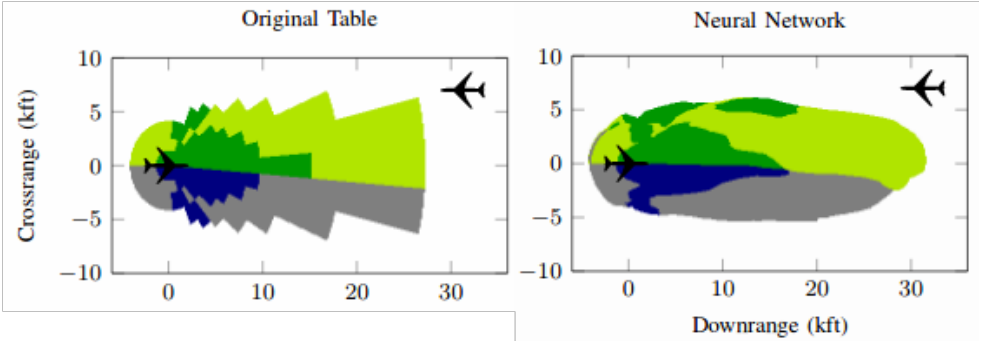

Figure: Taken from [julian2016policy] - depicted at left are the decision boundaries derived from the original *ACAS Xu* hash table. At the right figure, we can observe the trained NN boundaries. Each color depicts a different action that the aircraft should carry, with respect to the intruder position. It can be seen how the NN imposes unsafe regions, in contrast to the original table.

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Repair of Neural Networks

Problem definition: Consider a NN model denoted by $f_{w_A}(x)$ (model A). Assume that $f_{w_A}(x)$ is not safe w.r.t. a required specification φ. In the task of provably repairing a NN, we search for a new model $f_{w_B}(x)$ (model B) which satisfies φ and its decision boundaries are similar as possible to model A.

- Can be achieved naively via verification and re-training, until convergence
- In this work, we attempt to mitigate the repair process by utilizing tools from the field of *formal verification*

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Preliminaries - Linear classification for visual recognition

- Class score as a weighted sum of all of its pixel values
- E.g., we'd expect a ship classifier to have positive values in its blue channel weights

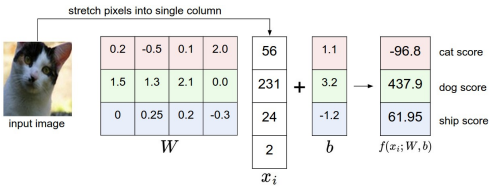


Figure: Taken from CS231N - Stanford's course for Visual Recognition with NNs - This is an example of mapping an image to class scores by using a linear classifier.

Preliminaries - Neural Network (NN) definition

- A mapping: $f_w : X \rightarrow Y$
  - $X \in \mathbb{R}^n$, $Y \in \mathbb{R}^m$, $n, m \in \mathbb{N}$ and w denotes the set of function **parameters**.
- Usually a composition of k functions: $f_w(x) = f^k(...(f^2(f^1(x))))$,
  - where k is referred to as the **number of layers**
- Typically, each layer performs a linear transformation followed by non-linear: $f^i(x) \equiv g_i(W_i x + b_i)$,
  - g_i denotes the non-linear operation (ReLU is a common one: $g(x) = max(0, x)$)
  - The shapes of W_i, b_i indicate the number of neurons for specific layer i

Preliminaries - Neural Network (NN) example

- For example, a two-layer NN with d ReLU neurons, an input $x \in \mathbb{R}^n$ and output $y \in \mathbb{R}^m$ will have the following form:

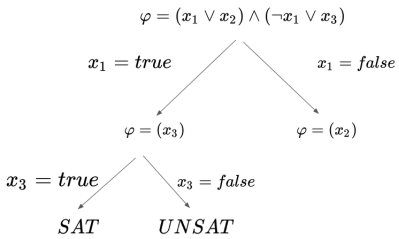
$$f_w(x) = W_2 * max(0, W_1 x + b_1) + b_2 \tag{1}$$

- where $W_1 \in \mathbb{R}^{d \times n}$, $b_1 \in \mathbb{R}^d$, $W_2 \in \mathbb{R}^{m \times d}$, $b_2 \in \mathbb{R}^m$

SAT Problem

- A Boolean formula φ is said to be in *CNF* if it's a **logical conjunction** of a set of clauses $C_1, ..., C_n$, where each clause C is a **logical disjunction** of a set of literals
- SAT: deciding if there exists an **assignment** that satisfies φ

- Example: $\varphi = (x_1 \vee x_2) \wedge (\neg x_1 \vee x_3)$
- Satisfying assignment: $\{x_1 = 1, x_2 = 1, x_3 = 1\}$, $\rightarrow \varphi$ is SATISFIABLE
- Solved by DPLL in practice (a backtracking based search algorithm)



Satisfiability modulo theories (SMT)

- Extends the SAT problem by supporting more theories (e.g., linear real arithmetic)
- Fundamentally solved with DPLL (similar to SAT) and a corresponding theory solver

- For instance, consider the real variables x, y in this formula: $\varphi = (y > 3x) \wedge (x >= 3)$
- Can re-write as: $\varphi = A \wedge B$
- At first, let's try to assign $B = \mathit{True}$
- A theory solver is invoked and assigns $x = 3$, which satisfies $B = \mathit{True}$
- After simplification, we get $y > 9$
- Finally, a possible solution is: $x = 3, y = 10$

(NN) Verification

- Verification methods allow to prove whether functions fulfill a certain **specification**
- Let f_w be such a function, with a given parameter set w
- A general specification can be formulated in first-order logic as follows:

$$\forall x \;\; C_{in}(x) \implies C_{out}(f_w, x) \tag{2}$$

where C_{in} and C_{out} denote input and output constraints functions respectively.

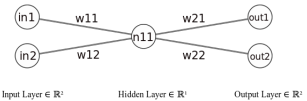
NN Repair

- Consider the case where f_w has an **unsafe** property
- We can slightly modify Eq. 2 to search for a new model $f_{\hat{w}}$
- The new model shall satisfy the specification, assuming such model exists
- That is by adding an existential quantifier:

$$\exists \hat{w} \;\; \forall x \;\; C_{in}(x) \implies C_{out}(f_{\hat{w}}, x) \tag{3}$$

Example - SMT formula to repair an NN

Consider the following NN, it has two inputs ($in1, in2$), a hidden layer with one **ReLU** neuron ($n11$), two outputs ($out1, out2$) and 6 weights ($w11, w12, w21, w22, bias11, bias21, bias22$):



Assume that this NN violates a required **specification**: $\forall in_1 \in [0, 0.5] \ .out_1 > out_2$. We then search for a repaired NN, by choosing to free two weights (while the rest remain constant):

$$
\begin{aligned}
&\exists w_{21}, bias_{21} \ (\\
&\quad \forall in_1, in_2 \ (\\
&\quad n_{11} = \text{if-then-else}(in_1 * w_{11} + in_2 * w_{12} + bias_{11} > 0, in_1 * w_{11} + in_2 * w_{12} + bias_{11}, 0) \wedge \\
&\quad out_1 = w_{21} * n_{11} + bias_{21} \wedge \\
&\quad out_2 = w_{22} * n_{11} + bias_{22} \wedge \\
&\quad (in_1 >= 0) \wedge (in_1 <= 0.5) \implies (out_1 > out_2) \\
&) \ )
\end{aligned}
$$

Adversarial Robustness property

Adversarial robustness defines **invariance to noise** in a δ neighborhood of x_0 as follows:

$$\forall x.\ \|x - x_0\| \leq \delta \implies D(f_w(x)) = D(f_w(x_0)), \tag{4}$$

where D denotes the decision function, usually $D(f(x)) = \underset{j}{\text{argmax}}(f(x))$ where j denotes the model predicted category.

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Repair w.r.t. Adversarial Robustness property

To generate a repaired network f_{w_B} which satisfies the safety properties, we search for a **subset** of weights $w_{B_{free}} \subseteq w_B$, and corresponding values, such that

$$\forall x. \quad \|x - x_0\| \leq \delta \implies D(f_{w_B}(x)) = D(x_0), \tag{5}$$

holds, where f_{w_B} is a NN in which the weights in $w_{B_{free}}$ are set to those values, and the rest are set to the values of the corresponding weights in the original NN.

Notice: we have many options for choosing $w_{B_{free}}$

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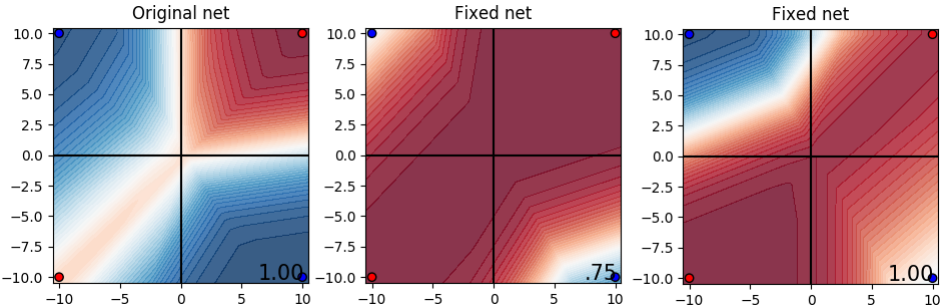
Initial Experiments

At first, we attempt to repair the following network (depicted on leftmost figure) to satisfy the **Adversarial Robustness** property w.r.t. point (-10, -10):



This experiment demonstrates that we should also preserve similarity

Experimental Setup

For the main part, we experiment with the following **neural networks** and their corresponding **data sets**:

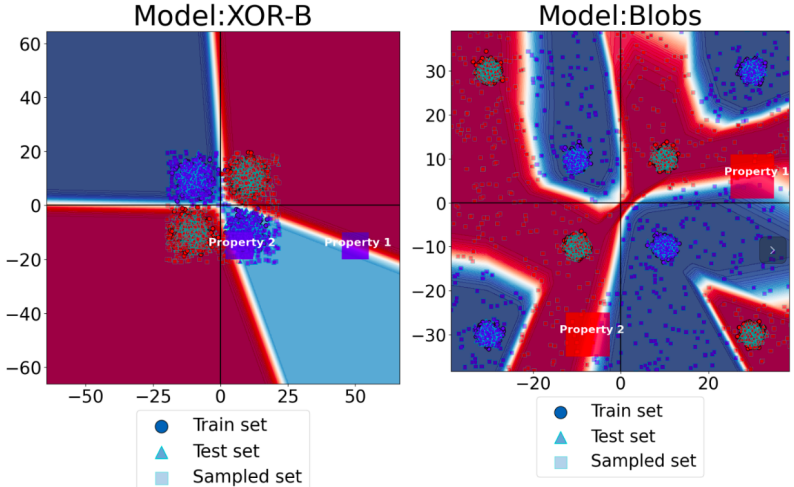
Model Name	Hidden Layers Sizes	Parameters	Train Set Size	Train Set Accuracy	Test Set Size	Test Set Accuracy	Sampled Set Size	Sampled Set Accuracy
XOR-B	[4]	22	1562	0.99743	1600	0.99125	500	1.0
Blobs	[10, 10]	162	6000	1.00000	4000	1.00000	1000	1.0

Further, we require these **properties** to hold:

Model Name	Property	Coordinate	Delta	Class	Norm	Violated
XOR-B	Property 1	[50, -15]	5	Blue (1)	L1	Yes
XOR-B	Property 2	[7, -15]	5	Blue (1)	L1	Yes
Blobs	Property 1	[30, 6]	5	Red (0)	L1	Yes
Blobs	Property 2	[-7.5, -30]	5	Red (0)	L1	Yes

Experimental Setup

Depicted below are the **decision boundaries** and **data sets** for each model, along with the required **specification**:



Experimental Setup - Technical Details

- **Z3** SMT solver and its **Python** wrapper to search for new weights assignments
- **PyTorch** with *Adam* optimizer to train the networks
- Experiments were performed on a computer with Intel(R) Core(TM) i5-8250U CPU @ 1.60GHz, using 8Gb of RAM, running Linux Ubuntu version 16.04.1
- Each repair trial was given a timeout of 600 seconds

Experiments - Similarity Heuristics

- As our initial experiments demonstrate, we shall employ **similarity-preserving** heuristics to keep the repaired NN decision boundaries as close as possible to the originals
- For this purpose we use three different heuristics which are illustrated below

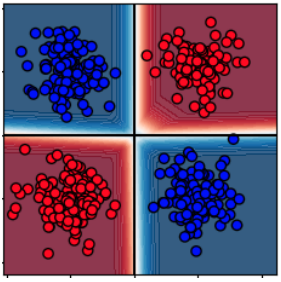


Figure: **Samples** - Enforce the model prediction on certain input coordinates.

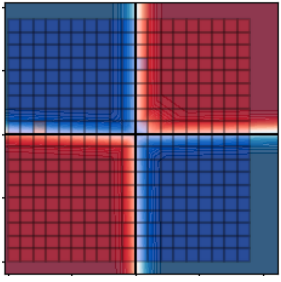


Figure: **Grid** - Divide the decision boundary into cells and enforce the same prediction for each cell.

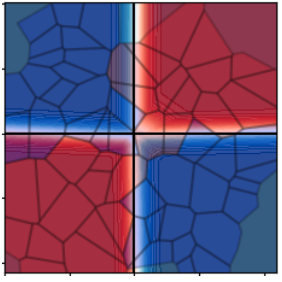
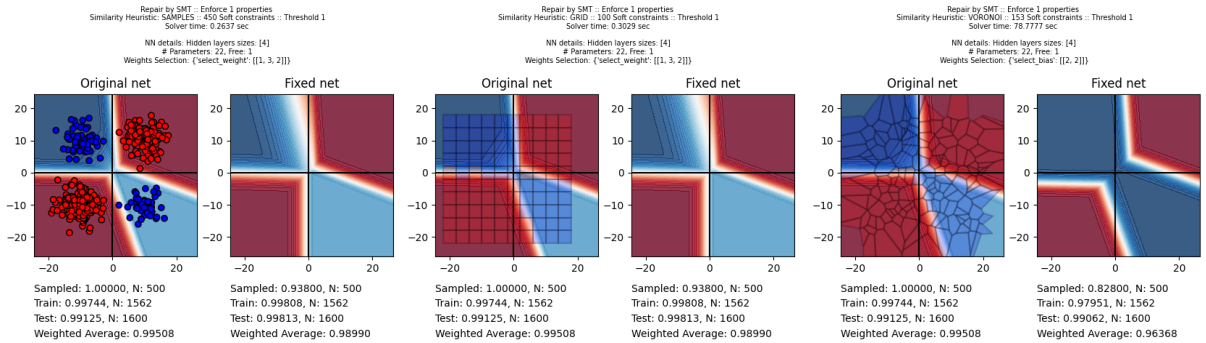


Figure: **Voronoi** - Build the cells according to Voronoi decomposition.

Experiments - Similarity Heuristics

- We perform extensive experiments to compare our proposed **similarity heuristics**.
- Following are visualizations for the repair of model *XOR-B*'s 1st property via each heuristic



Each similarity-preserving heuristic yields n additional constraints, in our experiments we require that **at least** $m \leq n$ constraints hold (we later use **threshold** to denote m).

Experiments - Similarity Heuristics

Attempts to repair each of ***XOR-B*** properties via each of our proposed heuristics:

Heuristic	Soft Constraints	Thresholds	Accuracy Before Repair	Max. Accuracy	Min. Accuracy	Average Accuracy	Trials	SAT	UNSAT	Timeout	Total Solver Time (sec.)
Weight selection tactic: **Individual weights**											
1st Property											
GRID	[100]	[1, 2]	99.5085%	85.9640%	37.5205%	60.1614%	44	9	26	9	6397
SAMPLES	[450]	[1, 250, 400]	99.5085%	86.9470%	37.5205%	71.8988%	66	15	51	0	32
VORONOI	[153]	[1, 2]	99.5085%	85.9640%	37.5205%	55.9803%	44	9	13	22	13994
2nd Property											
GRID	[100]	[1, 2]	99.5085%	**98.9896%**	37.5205%	65.5980%	44	10	24	10	6234
SAMPLES	[450]	[1, 250, 400]	99.5085%	**98.9896%**	37.5205%	83.6997%	66	24	42	0	32
VORONOI	[153]	[1, 2]	99.5085%	96.3681%	37.5205%	60.6827%	44	10	12	22	13843
Weight selection tactic: **Arbitrary combinations of weights, neurons or layers**											
1st Property											
GRID	[100, 400]	[1, 2, 10]	99.5085%	85.9640%	37.5205%	60.9448%	38	15	0	23	13812
SAMPLES	[450]	[1, 250, 400]	99.5085%	**98.6073%**	37.5205%	84.4578%	36	32	4	0	171
VORONOI	[268, 250, 153]	[1, 2, 10]	99.5085%	86.2370%	37.5205%	60.9030%	39	15	0	24	14424

The ***Samples*** similarity heuristic proves to be the most effective and efficient, as noticed by average accuracy and total solving time.

Experiments - Repair with *Samples* Similarity Heuristic

Aggregated search results for the repair of ***XOR-B*** network, with ***Samples*** similarity heuristics, results are grouped by soft constraints threshold value:

Threshold / Soft Constraints	Accuracy Before Repair	Max. Accuracy	Min. Accuracy	Average Accuracy	Trials	SAT	UNSAT	Timeout	Skipped	Total Solver Time (sec.)
1st Property										
Weight selection: **Combinations of two weights**										
1/1562	99.50847%	99.20808%	33.72474%	65.91046%	231	156	61	14	0	9127
325/1562	99.50847%	99.12616%	37.73894%	68.05714%	231	103	0	53	75	42027
750/1562	99.50847%	**99.26270%**	48.90770%	71.35950%	231	92	0	11	128	18004
1000/1562	99.50847%	98.60732%	61.22338%	80.55633%	230	74	11	6	139	13321
1500/1562	99.50847%	**99.26270%**	93.11851%	96.96887%	230	18	51	5	156	9529
2nd Property										
Weight selection: **Individual weights**										
1/1562	99.50847%	98.98962%	38.09394%	74.23539%	22	10	12	0	0	141
325/1562	99.50847%	97.95194%	37.52048%	74.13435%	22	10	12	0	0	75
750/1562	99.50847%	97.95194%	49.80885%	77.06475%	22	9	13	0	0	63
1000/1562	99.50847%	97.95194%	64.09066%	89.54806%	22	8	14	0	0	68
1500/1562	99.50847%	**99.31731%**	96.36810%	97.50137%	22	4	18	0	0	64
1561/1562	99.50847%	NA	NA	NA	22	0	22	0	0	27
1st And 2nd Property										
Weight selection: **Combinations of two weights**										
1/1562	99.50847%	97.21464%	20.04369%	57.71723%	231	119	95	14	0	8933
325/1562	99.50847%	90.44238%	36.15511%	63.79459%	231	76	0	43	112	34731
750/1562	99.50847%	**97.35117%**	48.90770%	68.24854%	231	65	0	11	155	11555
1000/1562	99.50847%	90.44238%	63.62643%	80.96122%	231	40	16	9	166	11202
1500/1562	99.50847%	97.05079%	96.28618%	96.66849%	231	2	37	1	191	3676

Produce safe networks by freeing up to two weights, with only a mild loss of accuracy

Experiments - Repair with *Samples* Similarity Heuristic

Aggregated search results for the repair of the ***Blobs*** network, with the ***Samples*** similarity heuristic, results are grouped by soft constraints threshold value:

Threshold / Soft Constraints	Accuracy Before Repair	Max. Accuracy	Min. Accuracy	Average Accuracy	Trials	SAT	UNSAT	Timeout	Skipped	Total Solver Time (sec.)
1st Property (individual weights)										
1/6000	100.00000%	99.43636%	64.10000%	89.52500%	107	48	44	15	0	18968
500/6000	100.00000%	99.41818%	86.50909%	95.03438%	107	32	0	16	59	11723
1000/6000	100.00000%	**99.50000%**	86.50909%	94.11420%	107	32	0	0	75	2046
2000/6000	100.00000%	99.43636%	86.47273%	94.44403%	107	32	0	0	75	2330
5500/6000	100.00000%	99.34545%	90.49091%	95.55016%	107	29	3	0	75	3518
2nd Property (individual weights)										
1/6000	100.00000%	99.72727%	51.12727%	86.66129%	143	31	95	17	0	23884
500/6000	100.00000%	99.72727%	86.15455%	92.72323%	143	18	0	13	112	9573
1000/6000	100.00000%	99.72727%	86.30909%	93.59798%	143	18	0	0	125	1406
2000/6000	100.00000%	**99.75455%**	64.67273%	90.52121%	143	18	0	0	125	1789
5500/6000	100.00000%	99.63636%	90.47273%	94.50160%	143	17	1	0	125	2580
1st And 2nd Property										
Combinations of size 2, assembled from top-5 repair setups of individual weights										
1/6000	100.00000%	99.49091%	62.45455%	89.15565%	45	33	12	0	0	5137
500/6000	100.00000%	99.10909%	74.16364%	93.26263%	45	9	0	24	12	15823
1000/6000	100.00000%	**99.56364%**	86.30909%	93.08636%	45	4	0	5	36	3477
2000/6000	100.00000%	86.89091%	86.30909%	86.55455%	45	3	0	1	41	747
5500/6000	100.00000%	98.81818%	97.35455%	98.23636%	45	3	0	0	42	638

Information from repairing single properties might be useful to further attempts of repairing multiple properties simultaneously. ***Blobs*** network has 162 parameters, and 13041 options to choose 2 parameters.

Experiments - Comparison to baseline

- We compare the results of repairing ***XOR-B*** and ***Blobs*** to a naive baseline
- Baseline: a repair loop which alternates between verification and re-training

Depicted are the accuracy measures for each of the networks and their repaired properties:

Model	XOR-B			Blobs		
Property	1st	2nd	Both	1st	2nd	Both
Our method	**99.2627%**	**99.3173%**	**97.3511%**	**99.5000%**	**99.7545%**	**99.5636%**
Naive method	97.2678%	96.4469%	94.5724%	97.3533%	97.8333%	96.0733%

Our method outperforms the naive method in terms of accuracy across all configurations

Automated Repair of Neural Networks

- Challenge in enumerating all possible weight combinations (n choose k)
- We suggest to perform the search in a greedy manner
- Provide a heuristic which attempts to minimize the UNSAT formulas we tackle

Thesis includes an algorithm to automatically repair NNs, a brief description:

Greedy repair (sketch)

1. Traverse a **search tree** where its nodes are combinations of free weights, and the tree level indicates the number of free weights.
2. Each **node** traversed corresponds to a **trial** which attempts to repair the network by freeing the given subset of weights.
3. Stop traversing according to timeout, return the most similar network as measured by accuracy.

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Contributions

- Demonstrate how off-the-shelf SMT solvers can be utilized to repair NNs
- Propose and experiment with similarity-preserving heuristics
- Perform additional experiments with the winning heuristic (Samples), and compare it to a naive baseline
- Suggest a greedy search algorithm to automatically repair NNs, and further strategies to improve its efficiency

Future work

- Perform additional experiments with larger benchmarks such as *Acas XU* networks, compare the results to related techniques
- Suggest further improvements to the algorithm
- Experiment with additional SMT solvers, attempt to fine-tune solvers to this specific task

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The End