Imperial College London

computational optimisation group

EPSRC
Engineering and Physical Sciences Research Council

Partition-based formulations for mixed-integer optimization of trained ReLU neural networks

Calvin Tsay, Jan Kronqvist, Alexander Thebelt, & Ruth Misener

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Papers Kronqvist, Misener, Tsay, *CPAIOR*, 2021; *arXiv:2101.12708*
Tsay, Kronqvist, Thebelt, Misener, *arXiv:2102.04373*, 2021

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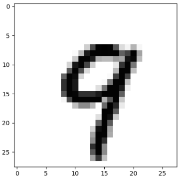
Optimization problems over trained neural networks



Given . . . .

Trained NN

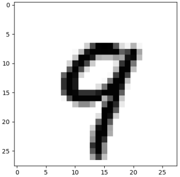
Image $\bar{\boldsymbol{x}}$

Label $j = 9$

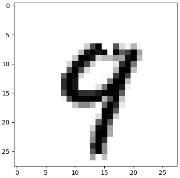
Adversary? $k = 4$

- **Verification** *[Feasibility]* Is there an adversary labeled k within a given perturbation ℓ_1 or ℓ_∞?
- **Optimal adversary** What image within perturbation ℓ_1 or ℓ_∞ maximizes the prediction difference?
- **Minimally distorted adversary** [Croce and Hein, 2020] Smallest perturbation ℓ_1 or ℓ_∞ over which the NN predicts label k?
- **Lossless compression** [Serra et al., 2020] Can I safely remove NN nodes or layers?

Optimization problems over trained neural networks



$\downarrow \ell_1$



$k = 4,$

$\|\boldsymbol{x} - \bar{\boldsymbol{x}}\|_1 = 4$

Given . . . .

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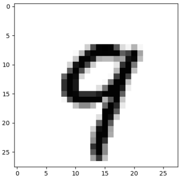

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Trained NN	
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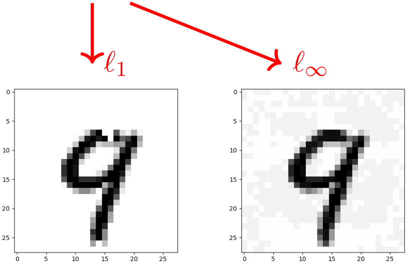

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$k = 4,$ $\|\boldsymbol{x} - \bar{\boldsymbol{x}}\|_\infty = 0.05$

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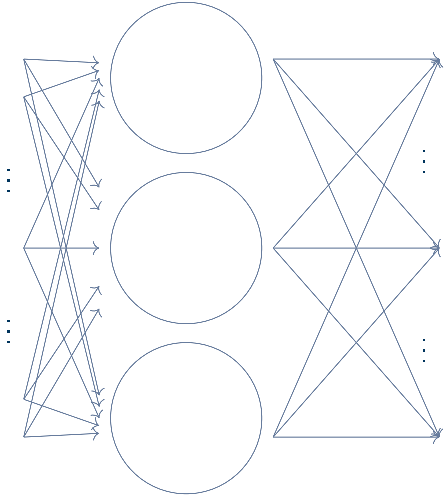
Big-M formulation of a learned ReLU neural network

Lomuscio and Maganti [2017], Fischetti and Jo [2018]



$$y \geq (\boldsymbol{w}^T \boldsymbol{x} + b)$$
$$y \leq (\boldsymbol{w}^T \boldsymbol{x} + b) - (1 - \sigma) LB^0$$
$$0 \leq y \leq \sigma UB^0$$
$$\sigma \in \{0, 1\}$$

Big-M coefficients $LB^0, UB^0 \in \mathbb{R}$

$(\boldsymbol{w}^T \boldsymbol{x} + b) \in [LB^0, UB^0]$

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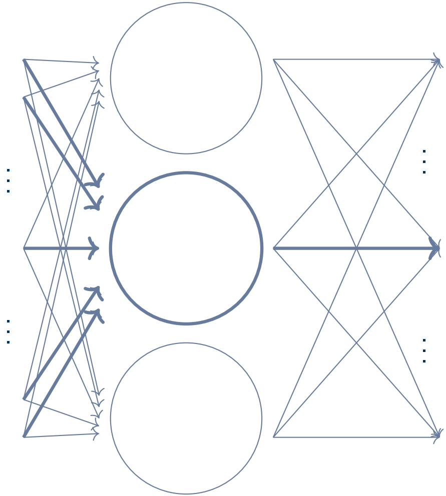

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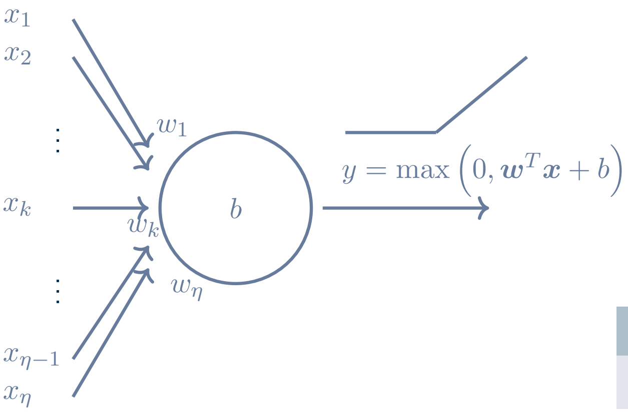

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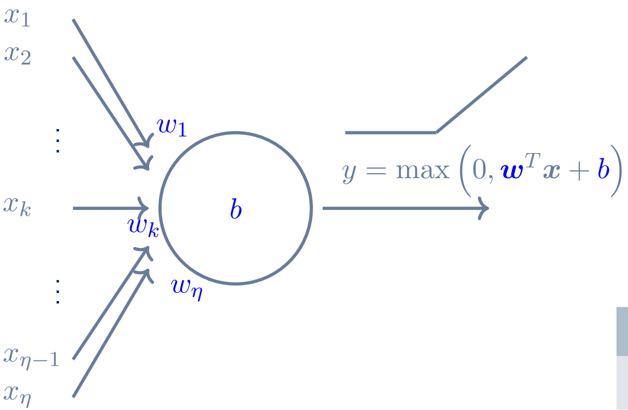

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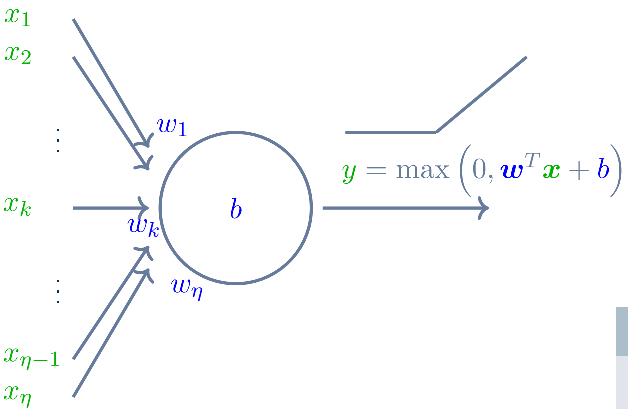

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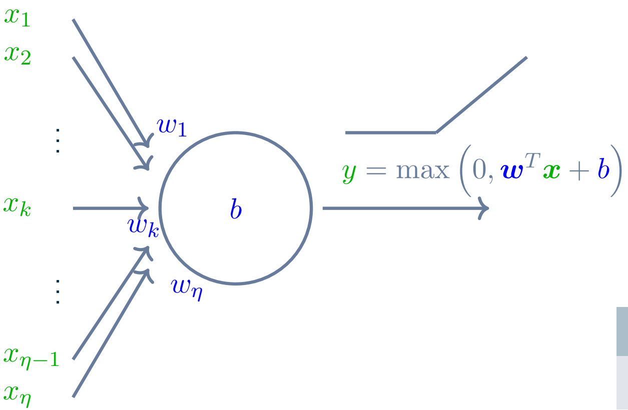

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Why do we want to improve big-M?

State-of-the-art verification tools rely on big-M

MIPVerify [Tjeng et al., 2017] • NSVerify [Akintunde et al., 2018]

Applications using big-M

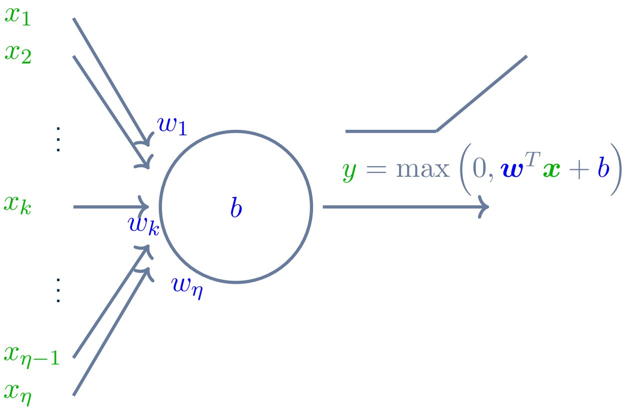
Optimize NN [Dutta et al., 2018, Lomuscio and Maganti, 2017, Wu et al., 2020, Grimstad and Andersson, 2019] • Get perturbation bounds [Cheng et al., 2017] • Compress NN [Serra et al., 2020] • Count regions [Serra et al., 2018] • Find adversarial examples [Fischetti and Jo, 2018]

Develop alternatives to dynamic cut generation

Anderson et al. [2020] develop exponentially many cuts from a node's convex hull. This method does not scale well to large NNs [De Palma et al., 2021]. Botoeva et al. [2020] find callback frequencies $<0.025\%$ balance computational burden and model tightening.

Idea: Partition-based formulation of a learned ReLU neural network

Use disjunctive programming [Balas, 2018] to develop intermediate relaxations [Kronqvist et al., 2021]



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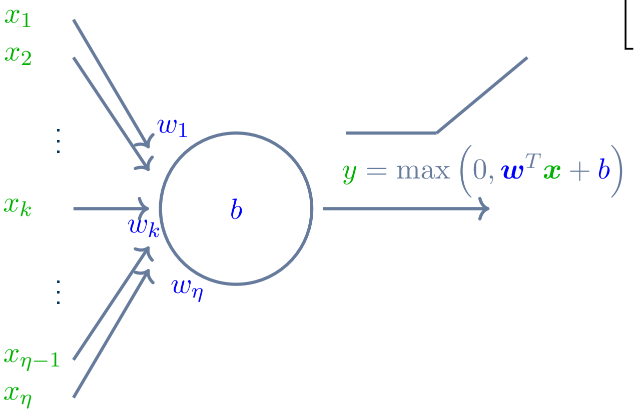

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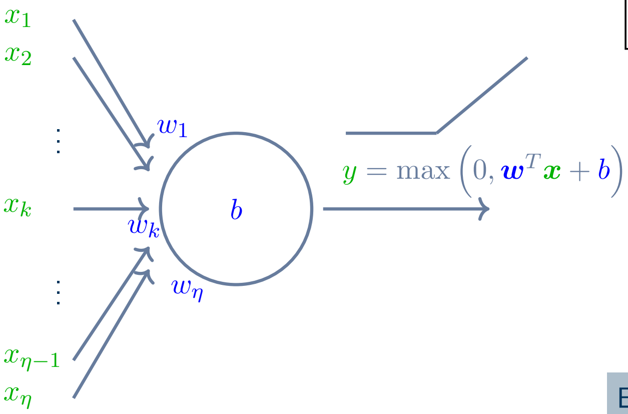

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$$\begin{aligned}
\boldsymbol{w}^T\boldsymbol{x} &= z^a + z^b \\
z^a + \sigma b &\leq 0 \\
z^b + (1-\sigma)b &\geq 0 \\
y &= z^b + (1-\sigma)b \\
\sigma LB^a \leq\ & z^a \leq \sigma UB^a \\
(1-\sigma)LB^b \leq\ & z^b \leq (1-\sigma)UB^b
\end{aligned}$$

Extra: 1 variable z^b, 4 constraints

Equivalent to the big-M formulation

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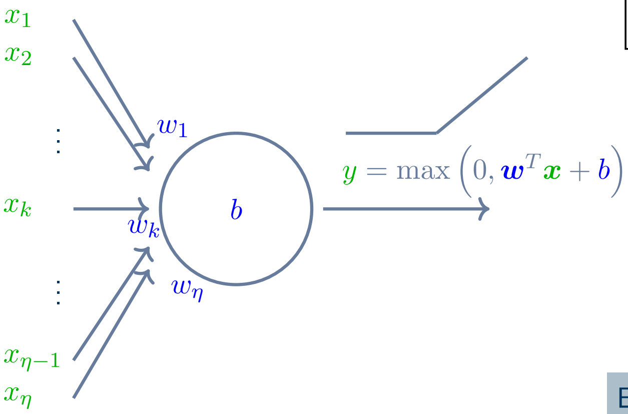

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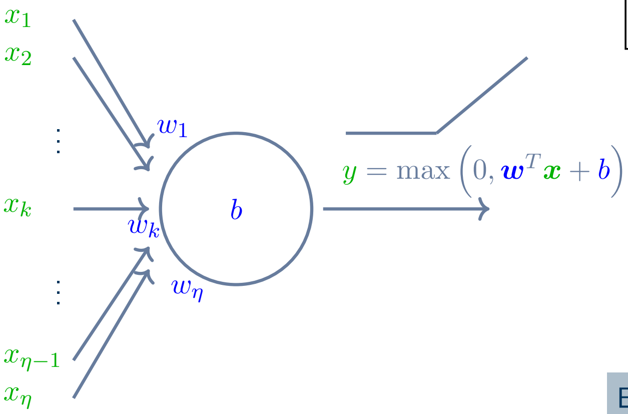

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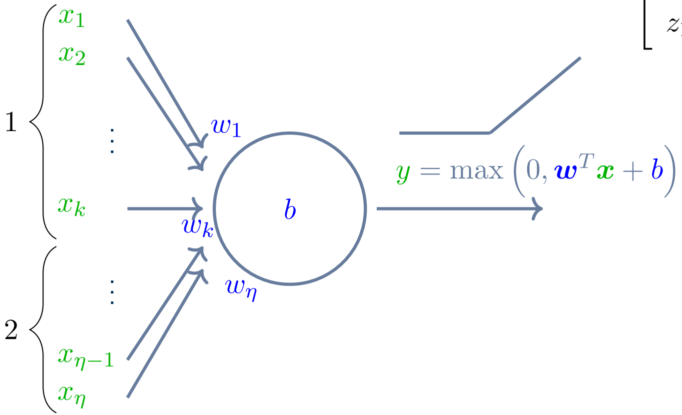

$$\begin{bmatrix} y = 0 \\ z_1 + z_2 + b \leq 0 \end{bmatrix} \vee \begin{bmatrix} y = z_1 + z_2 + b \\ z_1 + z_2 + b \geq 0 \end{bmatrix}$$

$$\sum_{i=1}^{k} w_i x_i = z_1^a + z_1^b$$

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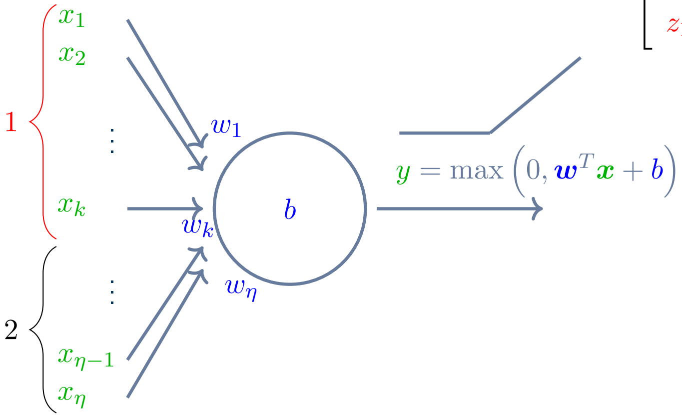

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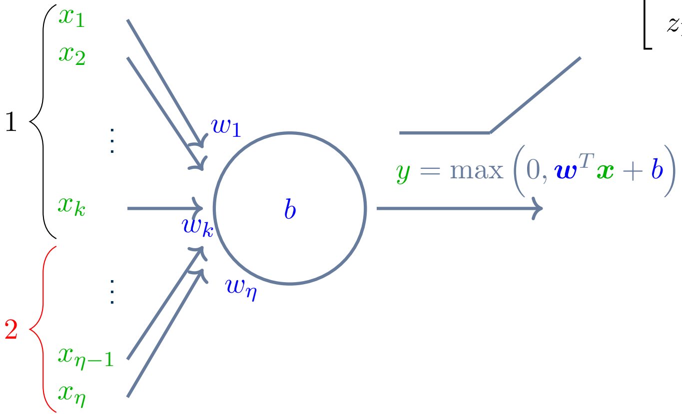

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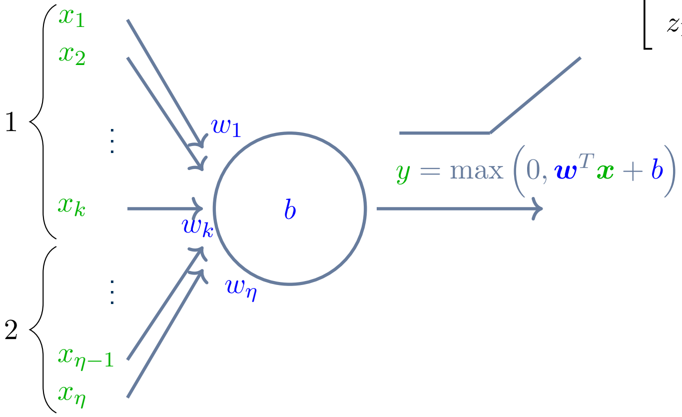

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$$z_1^a + z_2^a + \sigma b \leq 0$$

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$$y = z_1^b + z_2^b + (1-\sigma) b$$

$$\sigma LB_n^a \leq z_n^a \leq \sigma UB_n^a, \forall n = 1,2$$

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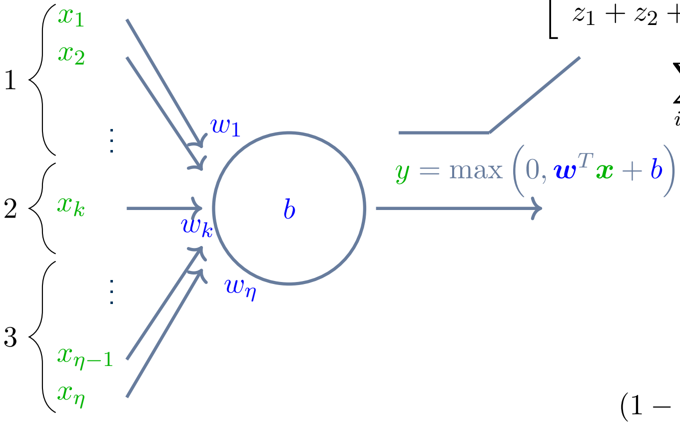

$$\sum_{i=1}^{k} w_i x_i = z_n^a + z_n^b, \quad \forall n = 1, 2, 3$$

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Proposed formulation & observations

Tsay et al. [2021]

$$\sum_n \left(\sum_{i \in \mathbb{S}_n} w_i x_i - z_n^b \right) + \sigma b \leq 0$$

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Differences from big-M

Partition parameter N • Choose subsets $\mathbb{S}_1 \cup \ldots \cup \mathbb{S}_N = \{1, \ldots, \eta\}$; $\mathbb{S}_n \cap \mathbb{S}_{n'} = \emptyset$ $\forall n \neq n'$ • N new auxiliary variables z_n^b after eliminating z_n^a • $4N$ new constraints

Observations

$N = 1$ eqv. to big-M • $N = \eta$ eqv. to convex hull • Eqv. non-lifted formulation has 2^N constraints • Can have hierarchy of relaxations with increasing tightness/size

Tighten bounds LB_n^a, UB_n^a, LB_n^b, UB_n^b

Interval arithmetic? Optimization-based bounds tightening (OBBT)? [Tjeng et al., 2017, Dvijotham et al., 2018]

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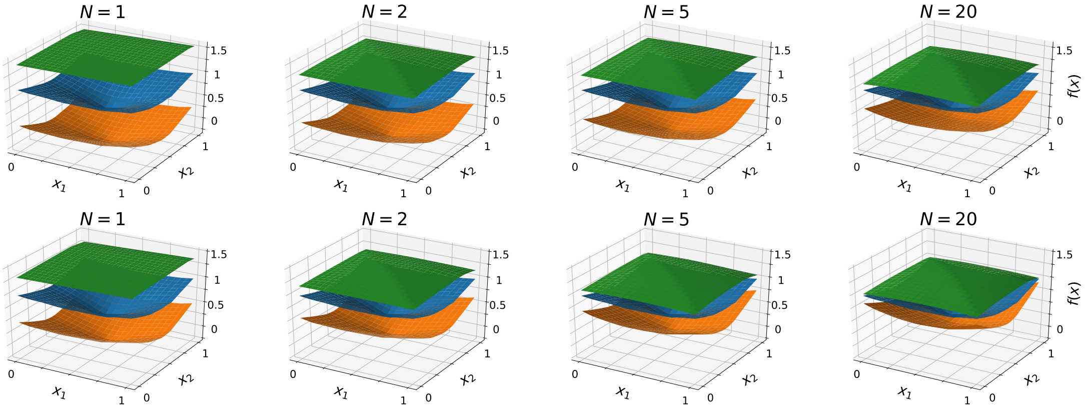
Increasing relaxation tightness with increasing N

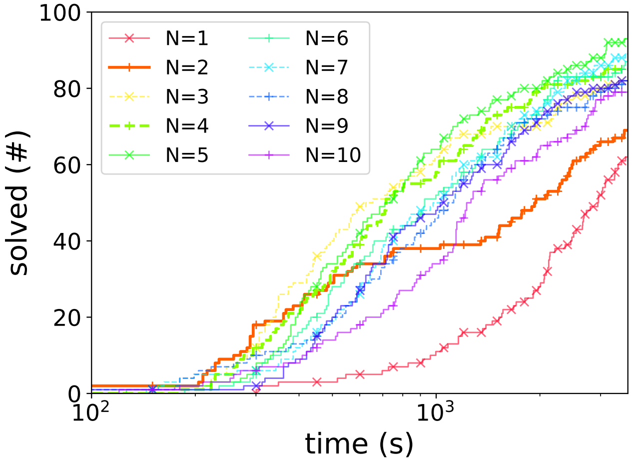


Example: two-input (x_1, x_2) NN trained on scaled Ackley function

$N = 1$ and $N = 20$ equiv. to big-M and convex hull, respectively. The z_n^b bounds were obtained using interval arithmetic (top row) and optimization-based bounds tightening (bottom row).

Importance of parameter N: Number solved vs. run time $\left(\|\boldsymbol{x} - \bar{\boldsymbol{x}}\|_1 = 5\right)$

Optimal adversary CIFAR-10; CNN with $n_{\text{Layers}} = 2$ & $n_{\text{Hidden}} = 100$; Each line averages 100 examples $\bar{\boldsymbol{x}}$



Observations

- $N = 1$ (equivalent to big-M) performs worst;
- $N = 2$ good for easy problems;
- Intermediate N balances model size vs. tightness;
- Performance declines $N \geq 7$

Effect of input partitioning choice

Consider $\boldsymbol{w} = [1, 1, 100, 100]$ and $x_i \in [0, 1], i = 1, ..., 4$

$$\begin{bmatrix} x_1 \leq \sigma 1 \\ x_2 + 100x_3 + 100x_4 \leq \sigma 201 \end{bmatrix} \text{or} \begin{bmatrix} x_1 + 100x_3 \leq \sigma 101 \\ x_2 + 100x_4 \leq \sigma 101 \end{bmatrix} \text{or} \begin{bmatrix} x_1 + x_2 \leq \sigma 2 \\ x_3 + x_4 \leq \sigma 2 \end{bmatrix}$$

Proposed partitioning: Want similar weights $\boldsymbol{w}$

- **Equal size** $|\mathbb{S}_1| = |\mathbb{S}_2| = ... = |\mathbb{S}_N|$ with weights in each partition as similar as possible
- **Equal range** $\underset{i \in \mathbb{S}_1}{\mathrm{range}}(w_i) = ... = \underset{i \in \mathbb{S}_N}{\mathrm{range}}(w_i)$, reduce outliers effect w/ 2 extra bins, $N \geq 3$

Weak partitioning: Dissimilar weights

- **Random partitions** Assign indices $\{1, ..., \eta\}$ randomly to partitions $\mathbb{S}_1, ..., \mathbb{S}_N$
- **Uneven magnitudes** Weights "dealt" in a snake-draft order by decreasing magnitude.

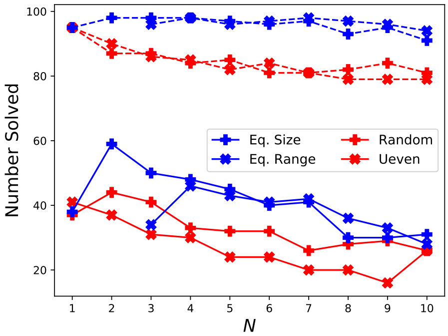
Experimental conditions [Tsay et al., 2021]

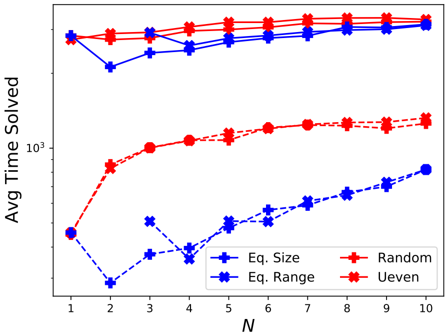
- 3.2 GHz Intel Core i7-8700 CPU (12 threads), 16 GB memory,
- Models implemented & solved: Gurobi v 9.1 [Gurobi Optimization, LLC, 2020],
- LP: Dual simplex, `cuts` 1, `TimeLimit` $3600s$, default termination criteria, `MIPFocus` 3,
- Trained NNs on MNIST [LeCun et al., 2010] & CIFAR-10 [Krizhevsky et al., 2009], Dense models: $n_{\text{Layers}} \times n_{\text{Hidden}}$ hidden & 10 output nodes. CNN2 from 'ConvSmall' [1]: {`Conv2D`(16, (4,4), (2,2)), `Conv2D`(32, (4,4), (2,2)), `Dense`(100), `Dense`(10)}. CNN1 halves channels in each layer: {`Conv2D`(8, (4,4), (2,2)), `Conv2D`(16, (4,4), (2,2)), `Dense`(100), `Dense`(10)}. CNN1/CNN2: 1,852/3,604 (MNIST) & 2,476/4,852 (CIFAR-10) nodes,
- NNs implemented in PyTorch [Paszke et al., 2019] using standard training (no regularization or methods to improve robustness).

[1] Based on ERAN dataset (`https://github.com/eth-sri/eran`)

Importance of partitioning strategy: Number Solved & Average Time Solved

Optimal adversary MNIST; CNN with $n_{\text{Layers}} = 2$ & $n_{\text{Hidden}} = 100$; Each line averages 100 runs; Max time 3600 s





Our partitioning strategies solve more problems faster than random & uneven partitions

Optimal adversary examples

Number solved (in 3600s) and average solve times for big-M vs equal-size partitions. Average times computed for problems solved by all 3 formulations

Dataset	Model	ϵ_1	Big-M		2 Partitions		4 Partitions	
			solved(#)	av.t (s)	solved(#)	av.t (s)	solved(#)	av.t (s)
MNIST	2×50	5	100	57.6	100	**42.7**	100	83.9
	2×50	10	97	431.8	98	**270.5**	98	398.4
	2×100	2.5	92	525.2	100	**285.1**	94	553.9
	2×100	5	32	1473.7	59	**494.6**	48	988.9
	CNN1*	0.25	68	1099.7	86	**618.8**	87	840.0
	CNN1*	0.5	2	2293.2	16	**1076.0**	11	2161.2
CIFAR-10	2×100	5	62	1982.3	69	1083.4	85	**752.8**
	2×100	10	23	2319.0	28	1320.2	34	**1318.1**

*OBBT performed on all NN nodes

Verification examples

Number solved (in 3600s) and average solve times for big-M vs equal-size partitions. Average times computed for problems solved by all 3 formulations. OBBT performed for all problems.

Dataset	Model	ϵ_∞	Big-M		2 Partitions		4 Partitions	
			solved(#)	av.t (s)	solved(#)	av.t (s)	solved(#)	av.t (s)
MNIST	CNN1	0.050	82	198.5	92	**27.3**	90	52.4
	CNN1	0.075	30	632.5	52	**139.6**	42	281.6
	CNN2	0.075	21	667.1	36	**160.7**	31	306.0
	CNN2	0.100	1	505.3	5	**134.7**	5	246.3
CIFAR-10	CNN1	0.007	99	100.6	100	**25.9**	99	45.4
	CNN1	0.010	98	85.1	100	**21.1**	100	37.5
	CNN2	0.010	40	2246.7	72	**859.9**	35	2449.4

ℓ_1-minimally distorted adversary examples

Number solved (in 3600s) and average solve times for big-M vs equal-size partitions. Average times and ϵ_1 are computed for problems solved by all 3 formulations. OBBT was performed for all problems.

Dataset	Model	$\mathrm{avg}(\epsilon_1)$	Big-M		2 Partitions		4 Partitions	
			solved(#)	av.t (s)	solved(#)	av.t (s)	solved(#)	av.t (s)
MNIST	2×50	6.51	52	675.0	93	**150.9**	89	166.6
	2×75	4.41	16	547.3	37	**310.5**	31	424.0
	2×100	2.73	7	710.8	13	**572.9**	10	777.9

Generalizing from NN: How to take steps *between* big-M & convex hull?

MI(NL)P with disjunctions

$$\bigvee_{l \in \mathcal{D}} \left[g_k(\boldsymbol{x}) \leq b_k \quad \forall k \in \mathcal{C}_l \right]$$

$$\boldsymbol{x} \in \mathcal{X} \subset \mathbb{R}^{\eta},$$

$\mathcal{D}$: disjunct indices, $\mathcal{C}_l$: constraint indices, $\mathcal{X}$: convex compact set

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$$\boldsymbol{x} \in \mathcal{X} \subset \mathbb{R}^\eta,$$

$\mathcal{D}$: disjunct indices, $\mathcal{C}_l$: constraint indices, $\mathcal{X}$: convex compact set

Assumptions

1. Functions $g_k : \mathbb{R}^\eta \to \mathbb{R}$ convex additively separable: $g_k(\boldsymbol{x}) = \sum_{i=1}^{\eta} h_{ik}(x_i)$ where $h_{ik} : \mathbb{R} \to \mathbb{R}$ are convex functions, and each disjunct is non-empty on $\mathcal{X}$.
2. Functions g_k are bounded over $\mathcal{X}$,
3. Far fewer constraints than # variables in each disjunction: $|\mathcal{C}_l| << \eta$.

Generalizing from NN: How to take steps *between* big-M & convex hull?

MI(NL)P with disjunctions

$$\bigvee_{l \in \mathcal{D}} \left[g_k(\boldsymbol{x}) \le b_k \quad \forall k \in \mathcal{C}_l \right]$$

$$\boldsymbol{x} \in \mathcal{X} \subset \mathbb{R}^\eta,$$

$\mathcal{D}$: disjunct indices, $\mathcal{C}_l$: constraint indices, $\mathcal{X}$: convex compact set

Applications?

Clustering [Papageorgiou and Trespalacios, 2018, Sağlam et al., 2006] • **Mixed-integer classification** [Liittschwager and Wang, 1978, Rubin, 1997] • **Coverage optimization** [Huang and Tseng, 2005] • **P_ball** [Kronqvist and Misener, 2020] • **ReLU NN**

Assumptions

1. Functions $g_k : \mathbb{R}^\eta \to \mathbb{R}$ convex additively separable: $g_k(\boldsymbol{x}) = \sum_{i=1}^{\eta} h_{ik}(x_i)$ where $h_{ik} : \mathbb{R} \to \mathbb{R}$ are convex functions, and each disjunct is non-empty on $\mathcal{X}$.
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N-split representation of original disjunction [Kronqvist et al., 2021]

Lift with $N \times |\mathcal{D}|$ new variables, Relax splitted constraints to global constraints, Feasible x space doesn't change

$$\bigvee_{l \in \mathcal{D}} \left[\sum_{i=1}^{\eta} h_{il}(x_i) \leq b_l \right]$$
$$\boldsymbol{x} \in \mathcal{X}$$

N-split representation of original disjunction [Kronqvist et al., 2021]

Lift with $N \times |\mathcal{D}|$ new variables, Relax splitted constraints to global constraints, Feasible x space doesn't change

$$\bigvee_{l \in \mathcal{D}} \left[\sum_{i=1}^{\eta} h_{il}(x_i) \le b_l \right] \qquad \longrightarrow \qquad \bigvee_{l \in \mathcal{D}} \begin{bmatrix} \sum_{i \in \mathcal{I}_1} h_{il}(x_i) \le \alpha_1^l \\ \vdots \\ \sum_{i \in \mathcal{I}_N} h_{il}(x_i) \le \alpha_N^l \\ \sum_{s=1}^{N} \alpha_s^l \le b_l \\ \underline{\alpha}_s^l \le \alpha_s^l \le \bar{\alpha}_s^l \\ \forall s \in \{1, \dots, N\} \end{bmatrix}$$

$$\boldsymbol{x} \in \mathcal{X}$$

$$\boldsymbol{x} \in \mathcal{X}, \boldsymbol{\alpha}^l \in \mathbb{R}^N \ \forall \ l \in \mathcal{D},$$

$$\underline{\alpha}_s^l := \min_{\boldsymbol{x} \in \mathcal{X}} \sum_{i \in \mathcal{I}_s} h_{il}(x_i),$$

$$\bar{\alpha}_s^l := \max_{\boldsymbol{x} \in \mathcal{X}} \sum_{i \in \mathcal{I}_s} h_{il}(x_i).$$

N-split representation of original disjunction [Kronqvist et al., 2021]

Lift with $N \times |\mathcal{D}|$ new variables, Relax splitted constraints to global constraints, Feasible $\boldsymbol{x}$ space doesn't change

$$\bigvee_{l \in \mathcal{D}} \left[\sum_{i=1}^{\eta} h_{il}(x_i) \le b_l \right] \quad \boldsymbol{x} \in \mathcal{X}$$

$$\longrightarrow$$

$$\bigvee_{l \in \mathcal{D}} \begin{bmatrix} \sum_{i \in \mathcal{I}_1} h_{il}(x_i) \le \alpha_1^l \\ \vdots \\ \sum_{i \in \mathcal{I}_N} h_{il}(x_i) \le \alpha_N^l \\ \sum_{s=1}^{N} \alpha_s^l \le b_l \\ \underline{\alpha}_s^l \le \alpha_s^l \le \bar{\alpha}_s^l \\ \qquad \forall s \in \{1, \ldots, N\} \end{bmatrix}$$

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$$\longrightarrow$$

$$\bigvee_{l \in \mathcal{D}} \begin{bmatrix} \sum_{s=1}^{N} \alpha_s^l \le b_l \\ \underline{\alpha}_s^l \le \alpha_s^l \le \bar{\alpha}_s^l \\ \qquad \forall s \in \{1, \ldots, N\} \end{bmatrix}$$

$$\sum_{i \in \mathcal{I}_s} h_{il}(x_i) \le \alpha_s^l$$

$$\forall s \in \{1, \ldots, N\},\ l \in \mathcal{D},$$

$$\boldsymbol{x} \in \mathcal{X}, \boldsymbol{\alpha}^l \in \mathbb{R}^N \ \forall\, l \in \mathcal{D},$$

$$\underline{\alpha}_s^l := \min_{\boldsymbol{x} \in \mathcal{X}} \sum_{i \in \mathcal{I}_s} h_{il}(x_i),$$

$$\bar{\alpha}_s^l := \max_{\boldsymbol{x} \in \mathcal{X}} \sum_{i \in \mathcal{I}_s} h_{il}(x_i).$$

N-split formulation

Represent the convex hull of the N-split disjunction using extended formulation [Balas, 1998]

$$\alpha_s^l = \sum_{d \in \mathcal{D}} \nu_d^{\alpha_s^l} \qquad \forall\ s \in \{1, \dots, N\},\ l \in \mathcal{D}$$

$$\sum_{s=1}^{N} \nu_l^{\alpha_s^l} \leq b_l \lambda_l \qquad \forall\ l \in \mathcal{D}$$

$$\underline{\alpha}_s^l \lambda_d \leq \nu_d^{\alpha_s^l} \leq \bar{\alpha}_s^l \lambda_d \qquad \forall\ s \in \{1, \dots, N\},\ l, d \in \mathcal{D}$$

$$\sum_{i \in \mathcal{I}_s} h_{il}(x_i) \leq \alpha_s^l \qquad \forall\ s \in \{1, \dots, N\}, l \in \mathcal{D}$$

$$\sum_{l \in \mathcal{D}} \lambda_l = 1, \quad \boldsymbol{\lambda} \in \{0, 1\}^{|\mathcal{D}|}$$

$$\boldsymbol{x} \in \mathcal{X}, \boldsymbol{\alpha}^l \in \mathbb{R}^N,\ \boldsymbol{\nu}^{\alpha_s^l} \in \mathbb{R}^N \qquad \forall\ s \in \{1, \dots, N\},\ l \in \mathcal{D}$$

Properties

- Feasible $\boldsymbol{x}$ space stays same,
- 1-split equiv. big-M,
- If h affine, η-split equiv. convex hull,
- If h affine, can get big-M to convex hull relaxation hierarchy.

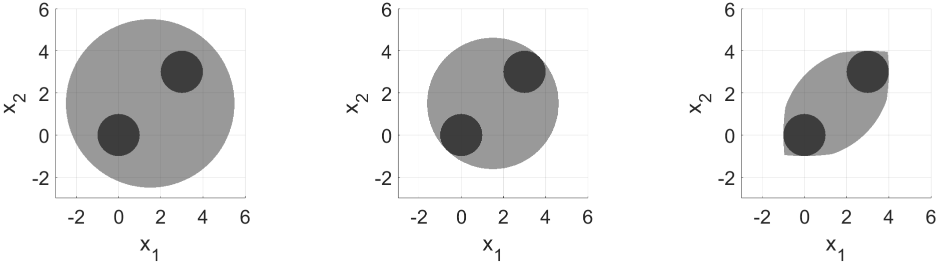
More in Kronqvist et al. [2021]

N-splits also may be useful with nonlinear functions

Illustrative example

$$\left[\sum_{i=1}^{4} x_i^2 \leq 1\right] \vee \left[\sum_{i=1}^{4} (3 - x_i)^2 \leq 1\right]$$

$$\boldsymbol{x} \in \mathbb{R}^4$$



1-split/big-M ($\{x_1, x_2, x_3, x_4\}$)

2-split ($\{x_1, x_2\}, \{x_3, x_4\}$)

4-split ($\{x_1\}, \{x_2\}, \{x_3\}, \{x_4\}$)

instance		big-M	2-split	4-split	8-split	16-split	32-split	convex hull
Cluster_g1	time	>1800	81.0	13.9	2.9	**1.7**	3.5	42.0
	nodes	>8998	2946	1096	256	98	91	**73**
Cluster_g2	time	>1800	106.3	7.7	4.3	**2.1**	4.5	40.6
	nodes	>10431	1736	481	217	104	86	**77**
Cluster_g3	time	>1800	>1800	870.6	**407.2**	597.5	NA	>1800
	nodes	>28906	>40820	19307	**14923**	16806		>7797
P_ball_1	time	403.0	235.4	285.1	**18.5**	NA	NA	42.2
	nodes	29493	7919	5518	2202			**1437**
P_ball_2	time	>1800	483.6	326.6	41.6	30.6	NA	**28.2**
	nodes	>19622	13602	5871	3921	1261		**531**
P_ball_3	time	>1800	>1800	>1800	149.3	91.1	**78.7**	114.0
	nodes	>7537	>6035	>6708	7042	3572	631	**554**
		big-M	14-split	28-split	56-split	196-split	392-split	convex hull
Cluster_m1	time	>1800	>1800	129.5	76.8	**32.0**	33.2	313.3
	nodes	>10680	>9651	2926	1462	524	**195**	228
Cluster_m2	time	>1800	1116.5	156.1	**27.1**	97.0	54.2	1260.1
	nodes	>4867	6220	1915	805	2752	1155	**131**
Cluster_m3	time	>1800	>1800	429.5	60.0	23.2	**19.8**	>1800
	nodes	>4419	>4197	3095	1502	741	**397**	>93

Between steps: Partition-based formulations

Summary

- New relaxations of disjunctions intermediate to big-M & convex hull, form a hierarchy under additional assumptions,
- Introduce parameter N (# splits) and aggregation choice (how to group variables), parameter choices robust across many instances,
- ReLU NN: Solve 25% more problems in 1 hr, average 2.2X speedup for solved problems,
- Promising computational results for other classes of problems.

Want to know more?

- **Papers** `https://arxiv.org/abs/2102.04373` • `https://arxiv.org/abs/2101.12708`
- **Twitter** @CogImperial • @CalvinTsay • @JanKronqvist • @AThebelt • @RuthMisener
- **YouTube** `https://www.youtube.com/channel/UCXRdjQRm9XfZj2c4XW1xpzg`

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