ECE598HZ: Advanced Topics in Machine Learning and Formal Methods

Lecture 9: Neural Network Verification with Bound Propagation Algorithms (Part II)

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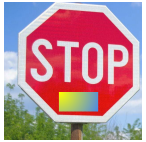
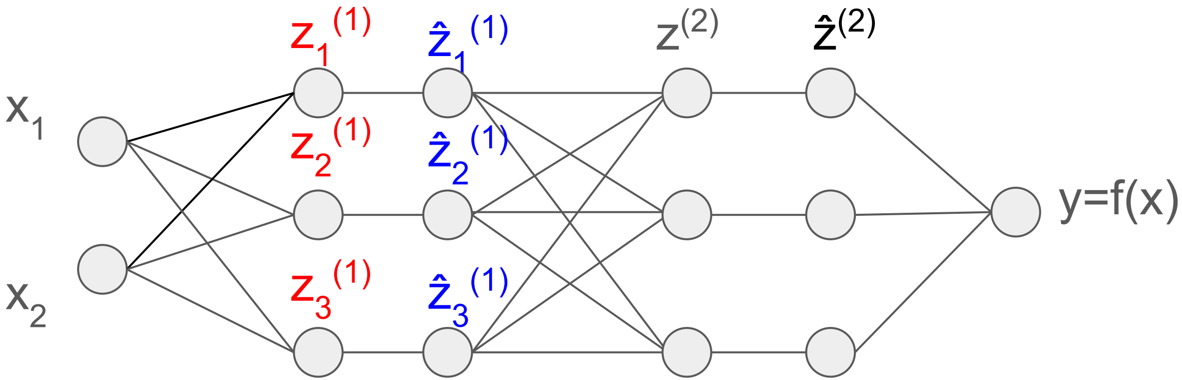
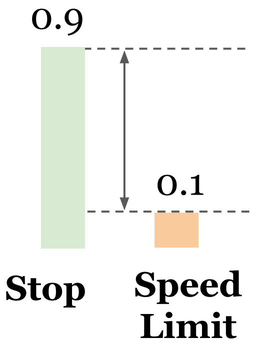
Review: NN verification as an **optimization** problem







$$\exists\ x \in S\ \wedge\ y \leq 0\ \wedge\ y = f(x)$$

Input domain under consideration

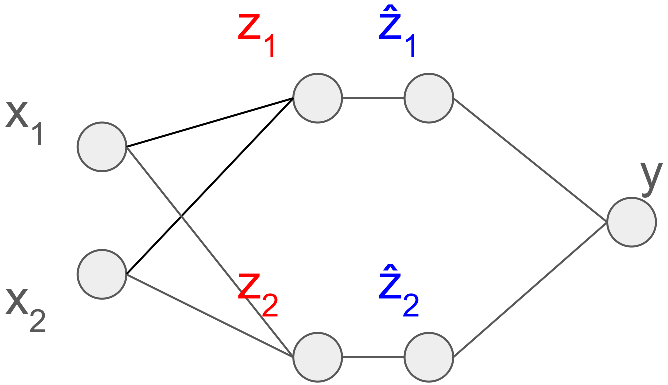
Negation of the desired property

$$y^* = \min_{x \in \mathcal{S}} f(x)$$

MILP and LP

Review: bound propagation with linear bounds (CROWN)

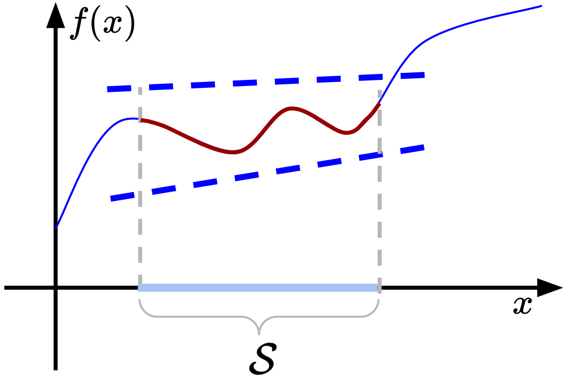
Simple example: linear -> ReLU -> linear



$$x_1 \in [-1, 2],\ x_2 \in [-2, 1]$$

$$z_1 = x_1 - x_2 \qquad z_2 = 2x_1 - x_2$$

$$y = \mathrm{ReLU}(z_1) - \mathrm{ReLU}(z_2)$$



Goal: bound y using symbolic linear functions of x
(linear inequalities)

Review: bound propagation with linear bounds (CROWN)

Prerequisite: all pre-activation bounds (can be computed using CROWN by treating z_1 and z_2 as the output neuron)

$$x_1 \in [-1, 2],\ x_2 \in [-2, 1] \qquad z_1 = x_1 - x_2 \qquad z_2 = 2x_1 - x_2$$

$$z_1 \in [-2, 4] \qquad z_2 \in [-3, 6]$$

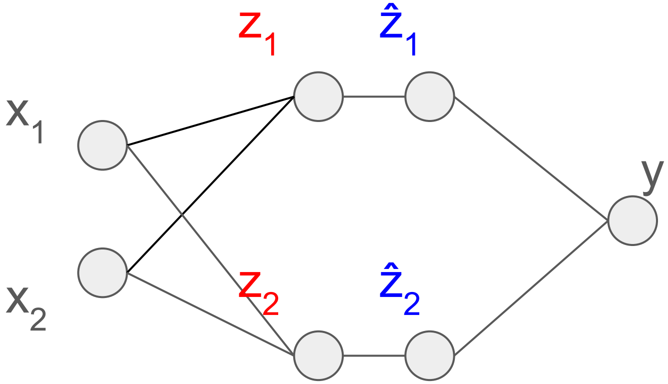
Pre-activation bounds needed for linear bounds of ReLU or other non-linear functions

Review: bound propagation with linear bounds (CROWN)

Propagation starts from the output y.

Step 1: bound **y** using linear functions of **y** (base case): y <= y, y >= y

Step 2: bound **y** using linear functions of $\hat{\mathbf{z}}$: simply plugin the definition of the second linear layer: $y = \hat{z}_1 - \hat{z}_2$



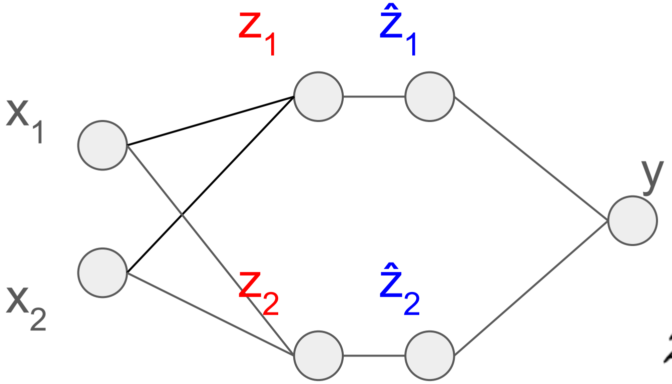
$y \le \hat{z}_1 - \hat{z}_2$, $y \ge \hat{z}_1 - \hat{z}_2$

Linear layer: simple substitution

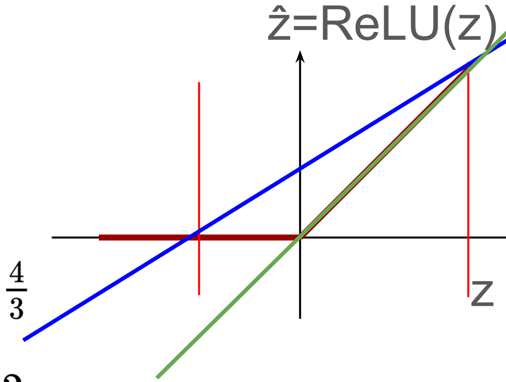
Review: bound propagation with linear bounds (CROWN)

Step 3: bound **y** using linear functions of **z**: need linear bounds for ReLU functions, which allows us to replace ẑ with z

ReLU layer: use linear bound
Check **sign** of coefficients and take the lower or upper bound



y <= **1**· $\hat{z}_1$ + (**-1**) · $\hat{z}_2$
y >= **1**· $\hat{z}_1$ + (**-1**) · $\hat{z}_2$



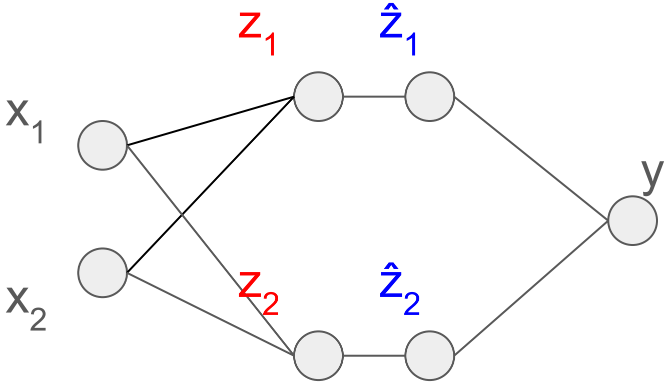
$$z_1 \leq \mathrm{ReLU}(z_1) \leq \frac{2}{3} z_1 + \frac{4}{3}$$

$$z_2 \leq \mathrm{ReLU}(z_2) \leq \frac{2}{3} z_2 + 2$$

$$z_1 - \left(\frac{2}{3} z_2 + 2\right) \leq y \leq \left(\frac{2}{3} z_1 + \frac{4}{3}\right) - z_2$$

Review: bound propagation with linear bounds (CROWN)

Step 4: bound **y** using linear functions of **x**



$$z_1 - \left(\frac{2}{3}z_2 + 2\right) \leq y \leq \left(\frac{2}{3}z_1 + \frac{4}{3}\right) - z_2$$

$$z_1 = x_1 - x_2$$

$$z_2 = 2x_1 - x_2$$

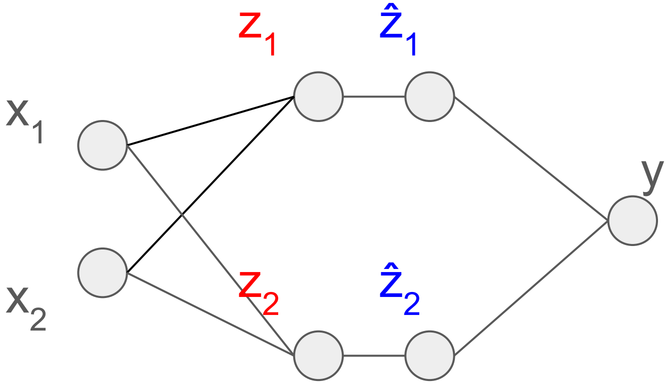
$$\Downarrow$$

$$-\frac{1}{3}x_1 - \frac{1}{3}x_2 - 2 \leq y \leq -\frac{4}{3}x_1 + \frac{1}{3}x_2 + \frac{4}{3}$$

Linear layer: simple substitution

Review: bound propagation with linear bounds (CROWN)

Step 5: concretize linear bounds



$$-\frac{1}{3}x_1 - \frac{1}{3}x_2 - 2 \le y \le -\frac{4}{3}x_1 + \frac{1}{3}x_2 + \frac{4}{3}$$

$$x_1 \in [-1, 2],\ x_2 \in [-2, 1]$$

$$y \in [-3, 3]$$

How to improve bound propagation

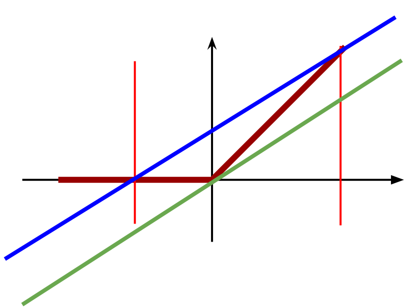
Bound propagation is fast, but what if the bounds are not tight enough?

Goal: use more time to “refine” the bounds. Two techniques:

- Bound optimization (previous lecture)
- **Branch and bound (this lecture)**

Bound optimization (α-CROWN)

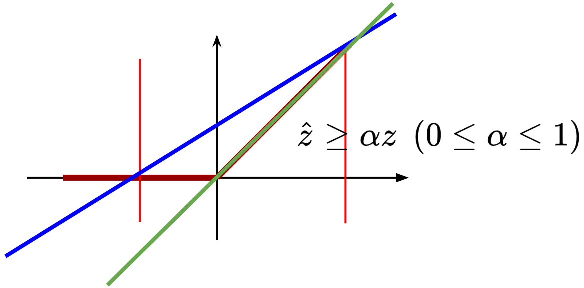
In the previous lecture, we discussed the possibility of making the lower bound of a ReLU function optimizable. α can be optimization used gradient descent.



$$\frac{2}{3}z_1 \leq \mathrm{ReLU}(z_1) \leq \frac{2}{3}z_1 + \frac{4}{3}$$

$$\frac{2}{3}z_2 \leq \mathrm{ReLU}(z_2) \leq \frac{2}{3}z_2 + 2$$

$$y \in [-\frac{10}{3}, 2]$$



$$z_1 \leq \mathrm{ReLU}(z_1) \leq \frac{2}{3}z_1 + \frac{4}{3}$$

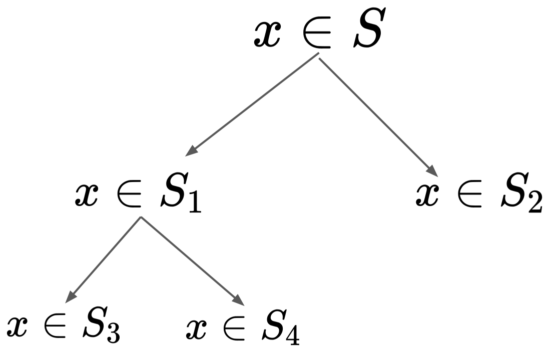
$$z_2 \leq \mathrm{ReLU}(z_2) \leq \frac{2}{3}z_2 + 2$$

$$y \in [-3, 3]$$

Branch and bound

General idea: split (branch) the original problem into easier subproblems; obtain bounds on each subproblem

Define **LB(*S*)** as the lower bound obtained using bound propagation for $\min_{x \in S} f(x)$



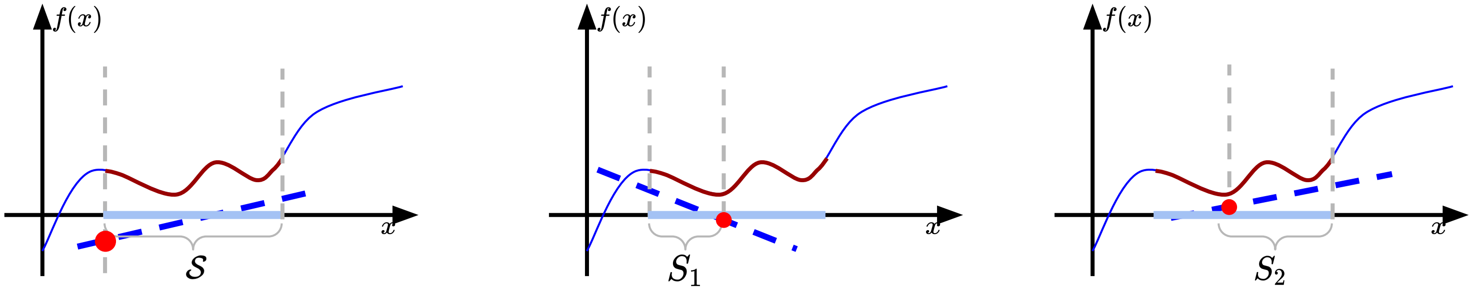
$LB(S)$

$S_1 \cup S_2 = S$ $\quad\quad$ $\min(LB(S_1), LB(S_2))$

$S_3 \cup S_4 \cup S_2 = S$ $\quad\quad$ $\min(LB(S_3), LB(S_4), LB(S_2))$

All leaf nodes

Branch and bound: why the lower bounds become tighter?



$x \in S$

$x \in S_1$ $\quad$ $x \in S_2$

$x \in S_3$ $\quad$ $x \in S_4$

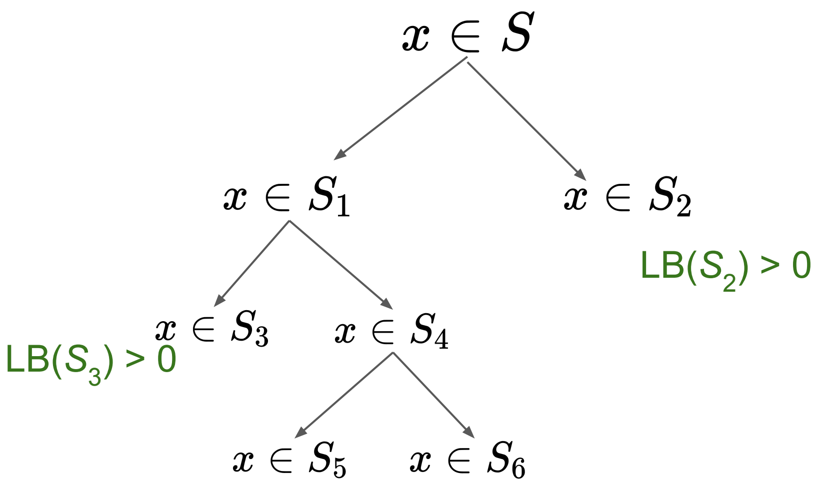
$LB(S)$

$S_1 \cup S_2 = S$ $\qquad$ $\min(LB(S_1), LB(S_2))$

$S_3 \cup S_4 \cup S_2 = S$ $\qquad$ $\min(LB(S_3), LB(S_4), LB(S_2))$

Branch and bound

If LB(S_i) > 0, it can be removed from our problem since the property is verified on this subdomain S_i; branch and bound is needed for unverified subdomains only.



List of unverified subproblems

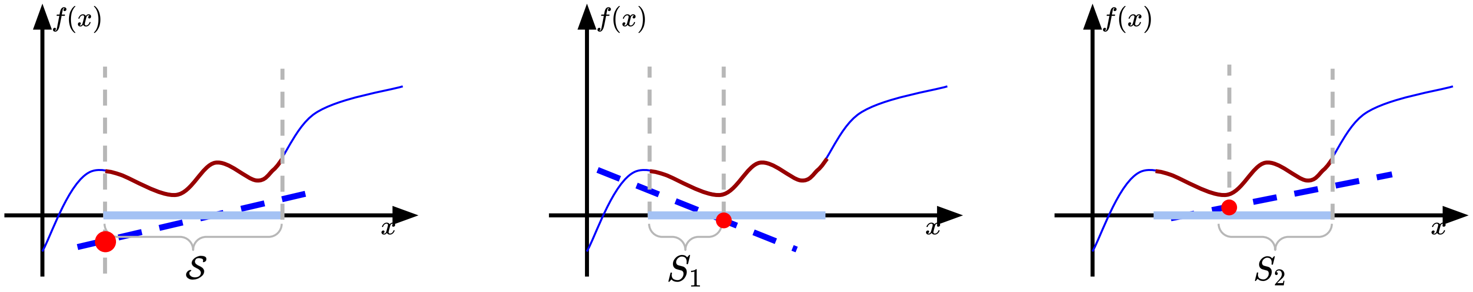
{S}

{S_1 , ~~S_2~~}

{~~S_3~~ , S_4}

{S_5 , S_6}

Branch and bound on input



Split each into domain S, typically by

$S = \{x_1 \in [-1, 1], x_2 \in [-1, 1]\}$ =>

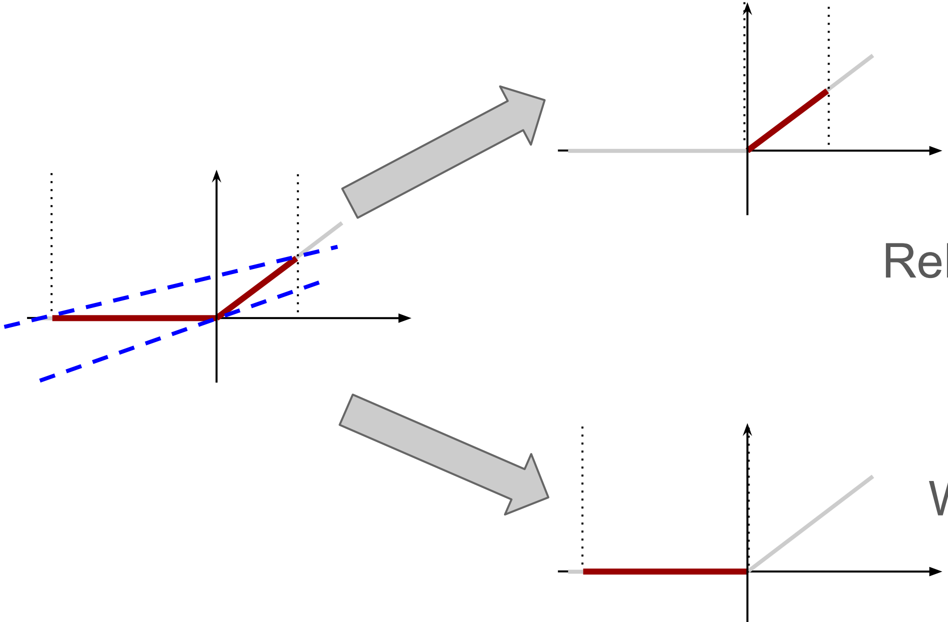
$S_1 = \{x_1 \in [-1, 0], x_2 \in [-1, 1]\}$, $S_2 = \{x_2 \in [0, 1], x_2 \in [-1, 1]\}$

Implementation is easy

Does not work well when input dimension is very high (e.g., image inputs)

Branch and bound on ReLU

Implicitly split input domain S by considering a ReLU neuron in two cases: active and inactive.



ReLU becomes **linear** in both subproblems

Works best when the number of unstable neurons is not very large

Branch and bound on ReLU

Implicitly split input domain S by considering a ReLU neuron in two cases: active and inactive.

$S = \{x_1 \in [-1, 1], x_2 \in [-1, 1]\}$ =>

$S_1 = \{x_1 \in [-1, 1], x_2 \in [-1, 1], z^{(i)}_j(x_1, x_2) \geq 0\}$,

$S_2 = \{x_2 \in [-1, 1], x_2 \in [-1, 1], z^{(i)}_j(x_1, x_2) \leq 0\}$

z is a function of input x

E.g., for our example $x_1 \in [-1, 2],\ x_2 \in [-2, 1]$ $z_1 = x_1 - x_2$

Splitting z_1 essentially consider two cases $x_1 - x_2 \geq 0$ and $x_1 - x_2 \leq 0$

Let's go over our example again with split

Prerequisite: all pre-activation bounds

$$x_1 \in [-1, 2],\ x_2 \in [-2, 1] \qquad z_1 = x_1 - x_2 \qquad z_2 = 2x_1 - x_2$$

Split constraint: $z_1 \leq 0$

$$z_1 \in [-2, 0] \qquad z_2 \in [-3, 6]$$

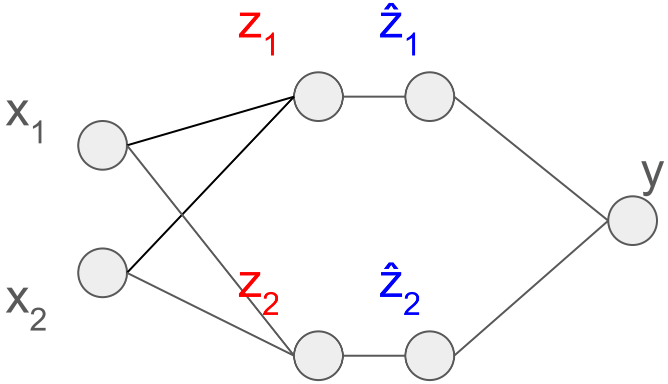
Pre-activation bounds for z_1 updated!

CROWN with neuron split

Let's look at the **lower bound** only (since only lower bound is needed)

Step 1: bound **y** using linear functions of **y** (base case): y <= y, y >= y

Step 2: bound **y** using linear functions of **ẑ**: simply plugin the definition of the second linear layer: $y = \hat{z}_1 - \hat{z}_2$



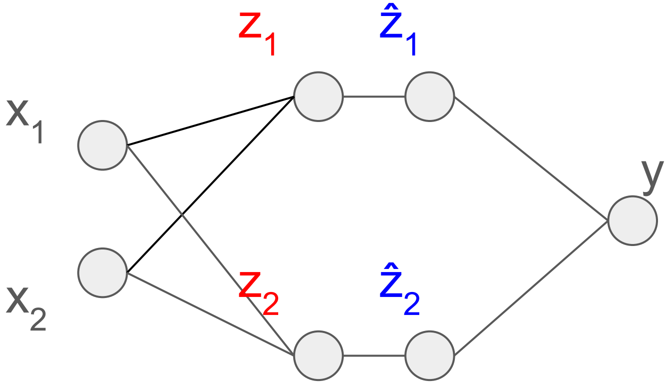
$y >= \hat{z}_1 - \hat{z}_2$

Linear layer: simple substitution

CROWN with neuron split (changed with the split)

Step 3: bound **y** using linear functions of **z**: need linear bounds for ReLU functions, which allows us to replace ẑ with z

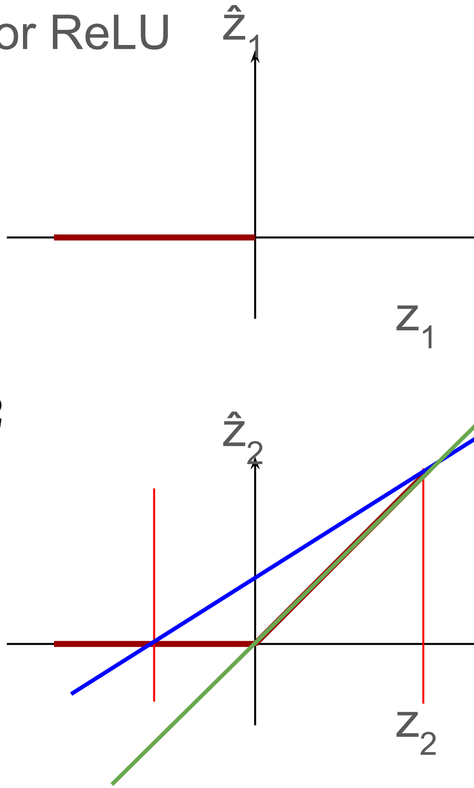
ReLU layer: use linear bound
Check **sign** of coefficients and take the lower or upper bound



y >= **1** · $\hat{z}_1$ + (**-1**) · $\hat{z}_2$

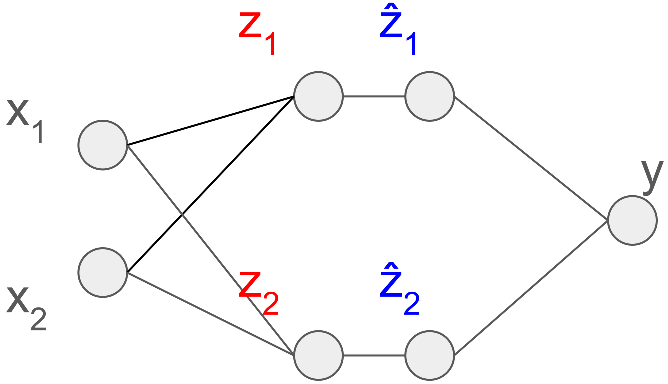
$$0 \le \mathrm{ReLU}(z_1) \le 0$$
$$z_2 \le \mathrm{ReLU}(z_2) \le \frac{2}{3} z_2 + 2$$

$$y \ge -\frac{2}{3} z_2 - 2$$



CROWN with neuron split (changed with the split)

Step 4: bound **y** using linear functions of **x**



$$y \geq -\frac{2}{3} z_2 - 2$$

$$z_1 = x_1 - x_2$$

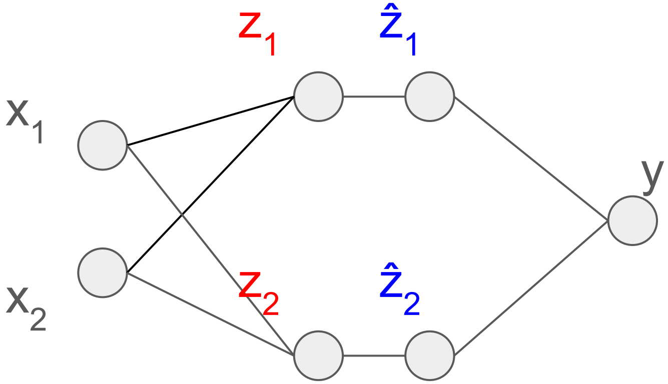
$$z_2 = 2x_1 - x_2$$

$$y \geq -\frac{4}{3} x_1 + \frac{2}{3} x_2 - 2$$

Linear layer: simple substitution

CROWN with neuron split (changed with the split)

Step 5: concretize linear bounds



$$y \geq -\frac{4}{3}x_1 + \frac{2}{3}x_2 - 2$$

$$x_1 \in [-1, 2],\ x_2 \in [-2, 1]$$

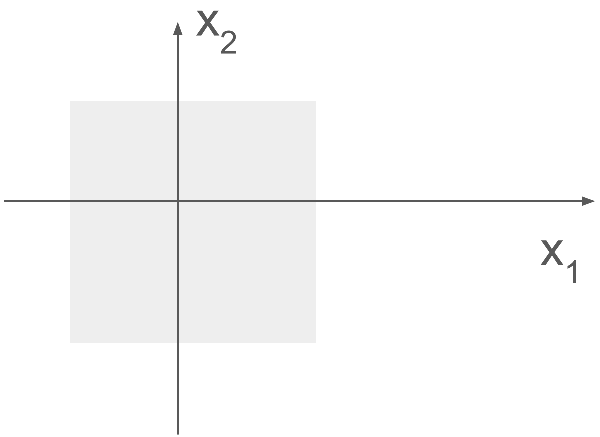
$$y \geq -6$$

Recall that without the split, we have y >= -3
With the split we expect the lower bound to improve??

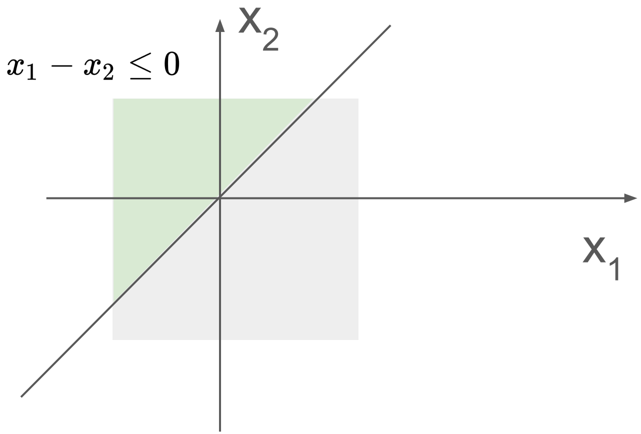
What is going wrong with CROWN?

The split constraint is not fully used during the process.

$$z_1 \leq 0 \implies x_1 - x_2 \leq 0$$



$x_1 \in [-1, 2],\ x_2 \in [-2, 1]$

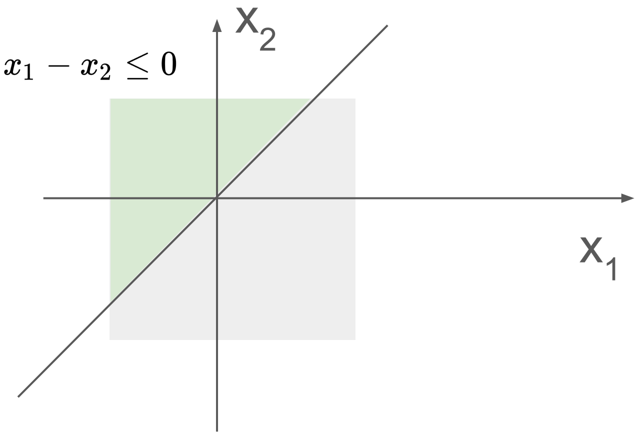


What is going wrong with CROWN?

In the concretization step, we still consider the worst case scenario in the larger box, rather than the green triangle.

$$y \geq -\frac{4}{3}x_1 + \frac{2}{3}x_2 - 2$$

$$x_1 \in [-1, 2],\ x_2 \in [-2, 1]$$



How to address the problem?

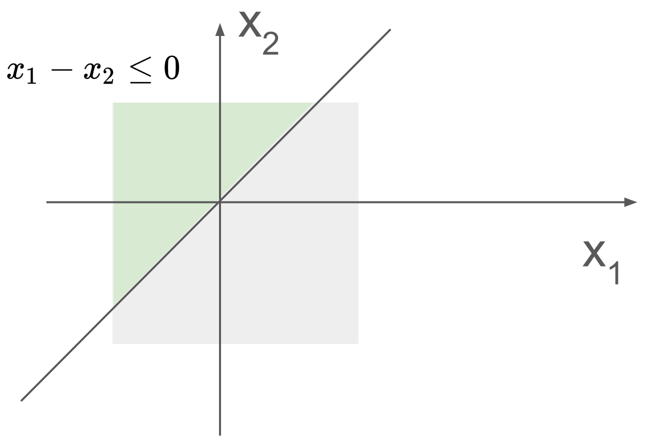
Instead we should solve this optimization problem during concretization:

$$\min_{x_1, x_2} -\frac{4}{3}x_1 + \frac{2}{3}x_2 - 2$$

$$\text{s.t. } z_1 \leq 0$$

$$x_1 \in [-1, 2],\ x_2 \in [-2, 1]$$

CROWN cannot handle this constraint!



β-CROWN: bound propagation with split constraint

We use *Lagrangian multipliers* to handle this constraint.

To solve a constrained optimization problem:

$$\begin{aligned} &\min f_0(x) \\ &\text{such that } f_i(x) \leq 0 \qquad\qquad \forall i \in 1, \ldots, m \end{aligned}$$

We can define Lagrangian with $\lambda_i \geq 0$:

$$L(x, \lambda) = f_0(x) + \sum_i \lambda_i f_i(x)$$

So the optimization problem can be written as

$$\min_x \max_\lambda L(x, \lambda)$$

β-CROWN: bound propagation with split constraint

$$\min_x \max_\lambda L(x, \lambda)$$

It is hard to solve directly. But we can then apply *weak duality*, which gives a lower bound

$$\max_\lambda \boxed{\min_x L(x, \lambda)} \leq \min_x \max_\lambda L(x, \lambda)$$

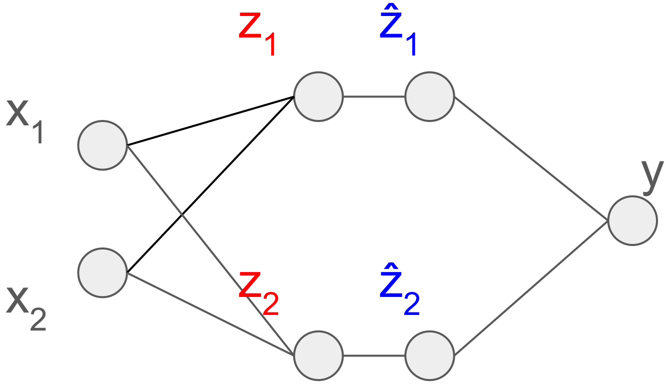
It has an intuitive game-theoretic explanation: whoever plays second may have an advantage, because they know the move of the first player.

Closed form solution exist for the inner minimization
(basically the concretization process without constraints)

β-CROWN with neuron split

Step 3: bound **y** using linear functions of **z**: need linear bounds for ReLU functions, which allows us to replace ẑ with z

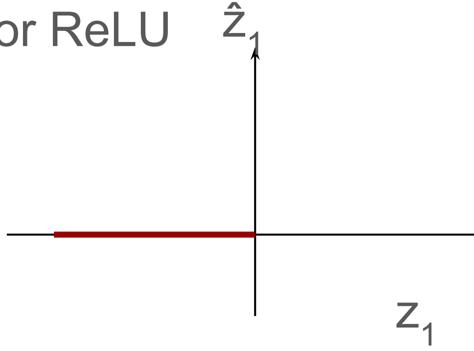
ReLU layer: use linear bound
Check **sign** of coefficients and take the lower or upper bound

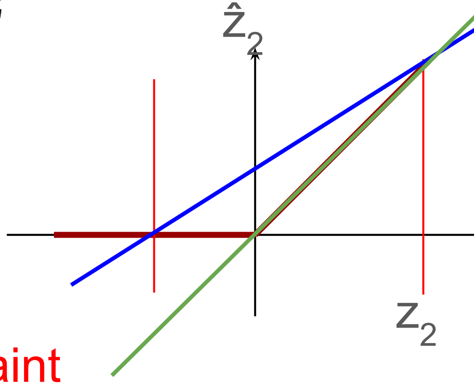


y >= **1**· $\hat{z}_1$ + (**-1**) · $\hat{z}_2$

$$0 \le \mathrm{ReLU}(z_1) \le 0$$
$$z_2 \le \mathrm{ReLU}(z_2) \le \frac{2}{3} z_2 + 2$$

$$y \ge -\frac{2}{3} z_2 - 2 + \beta z_1$$
$$\beta \ge 0$$





Change in bound propagation: add *β* for each split constraint

β-CROWN with neuron split

Step 4: bound **y** using linear functions of **x**, Now our bound has a parameter β

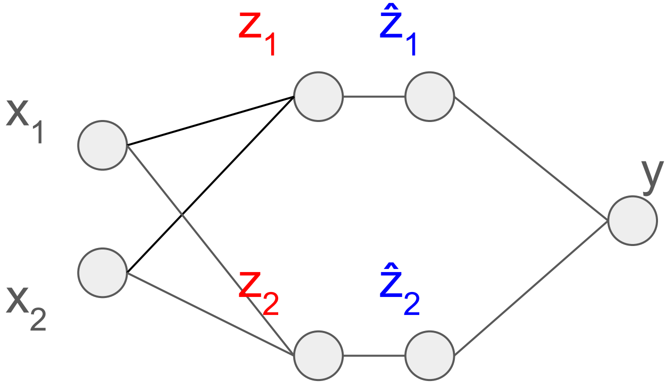
$$y \geq -\frac{2}{3} z_2 - 2 + \beta z_1$$

$$z_1 = x_1 - x_2$$

$$z_2 = 2x_1 - x_2$$

$$\Downarrow$$

$$y \geq (\beta - \frac{4}{3}) x_1 + (\frac{2}{3} - \beta) x_2 - 2$$



Linear layer: simple substitution

β-CROWN with neuron split

Step 5: concretize linear bounds

$$y \geq (\beta - \frac{4}{3})x_1 + (\frac{2}{3} - \beta)x_2 - 2$$

$$x_1 \in [-1, 2],\ x_2 \in [-2, 1]$$

Concretization depends on the sign of the coefficients, so we must discuss three cases:

$$0 \leq \beta \leq \frac{2}{3}$$

$$\frac{2}{3} \leq \beta \leq \frac{4}{3}$$

$$\beta \geq \frac{4}{3}$$

β-CROWN with neuron split

Step 5: concretize linear bounds

$$y \geq (\beta - \frac{4}{3})x_1 + (\frac{2}{3} - \beta)x_2 - 2$$

$$x_1 \in [-1, 2],\ x_2 \in [-2, 1]$$

$$0 \leq \beta \leq \frac{2}{3}$$

$$y \geq (\beta - \frac{4}{3}) \cdot 2 + (\frac{2}{3} - \beta) \cdot (-2) - 2$$

The optimal β to maximize y is 2/3, with objective = -10/3

$$\frac{2}{3} \leq \beta \leq \frac{4}{3}$$

$$y \geq (\beta - \frac{4}{3}) \cdot 2 + (\frac{2}{3} - \beta) \cdot 1 - 2$$

The optimal β is 4/3, with objective = **-8/3**

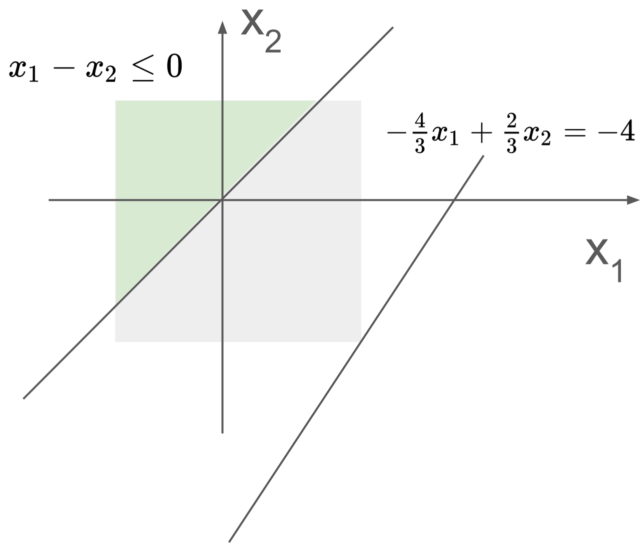
$$\beta \geq \frac{4}{3}$$

$$y \geq (\beta - \frac{4}{3}) \cdot (-1) + (\frac{2}{3} - \beta) \cdot 1 - 2$$

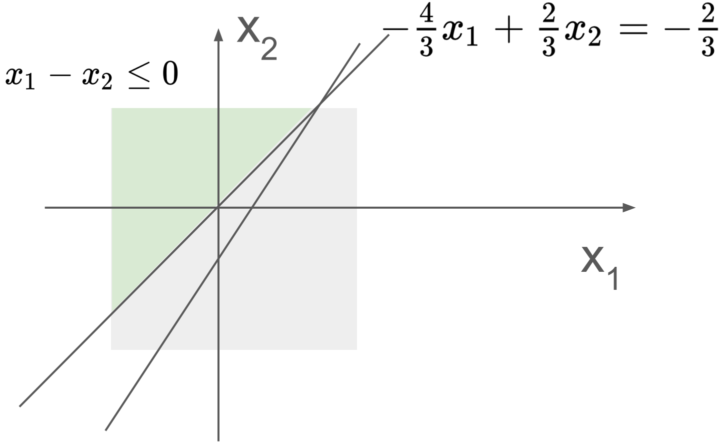
The optimal β is 4/3, with objective = **-8/3**

Geometric interpretation

$$\min_{x_1, x_2} -\frac{4}{3}x_1 + \frac{2}{3}x_2 - 2$$



No constraint, obj = -6



With constraint, obj = -8/3, improved!

Which dimension/which neuron to branch?

Similar to the backtracking process in DPLL, the selection of which dimension (for input split) or which neuron (ReLU split) is very important.

Strong branching: try every possible branch and choose the one with actual largest improvements in lower bound

Heuristic branching: estimate how good a branch is, and choose the neuron/dimension with highest score.

Example branching heuristic

$S = \{x_1 \in [-1, 1], x_2 \in [-1, 1]\}$ =>

$S_1 = \{x_1 \in [-1, 0], x_2 \in [-1, 1]\}$, $S_2 = \{x_2 \in [0, 1], x_2 \in [-1, 1]\}$

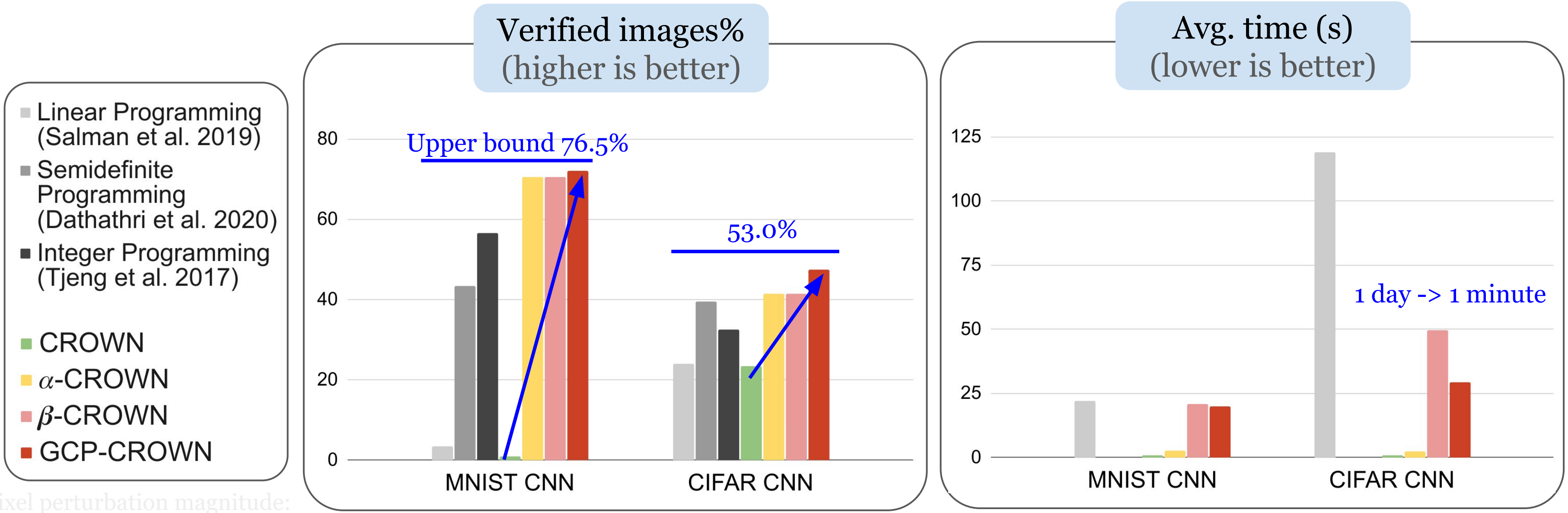
OR

$S_1 = \{x_1 \in [-1, 1]\ x_2 \in [-1, 0]\}$, $S_2 = \{x_2 \in [-1, 1], x_2 \in [0, 1]\}$

We can estimate the impact on lower bound given changes on x_1 and x_2

Given the CROWN linear bound $y >= a_1 x_1 + a_2 x_2 + c$, we branch on dimension i where $|a_i|$ is largest.

Benchmarks: CROWN-family bound propagation algorithms



Pixel perturbation magnitude:
0.3 for MNIST, 2/255 for CIFAR

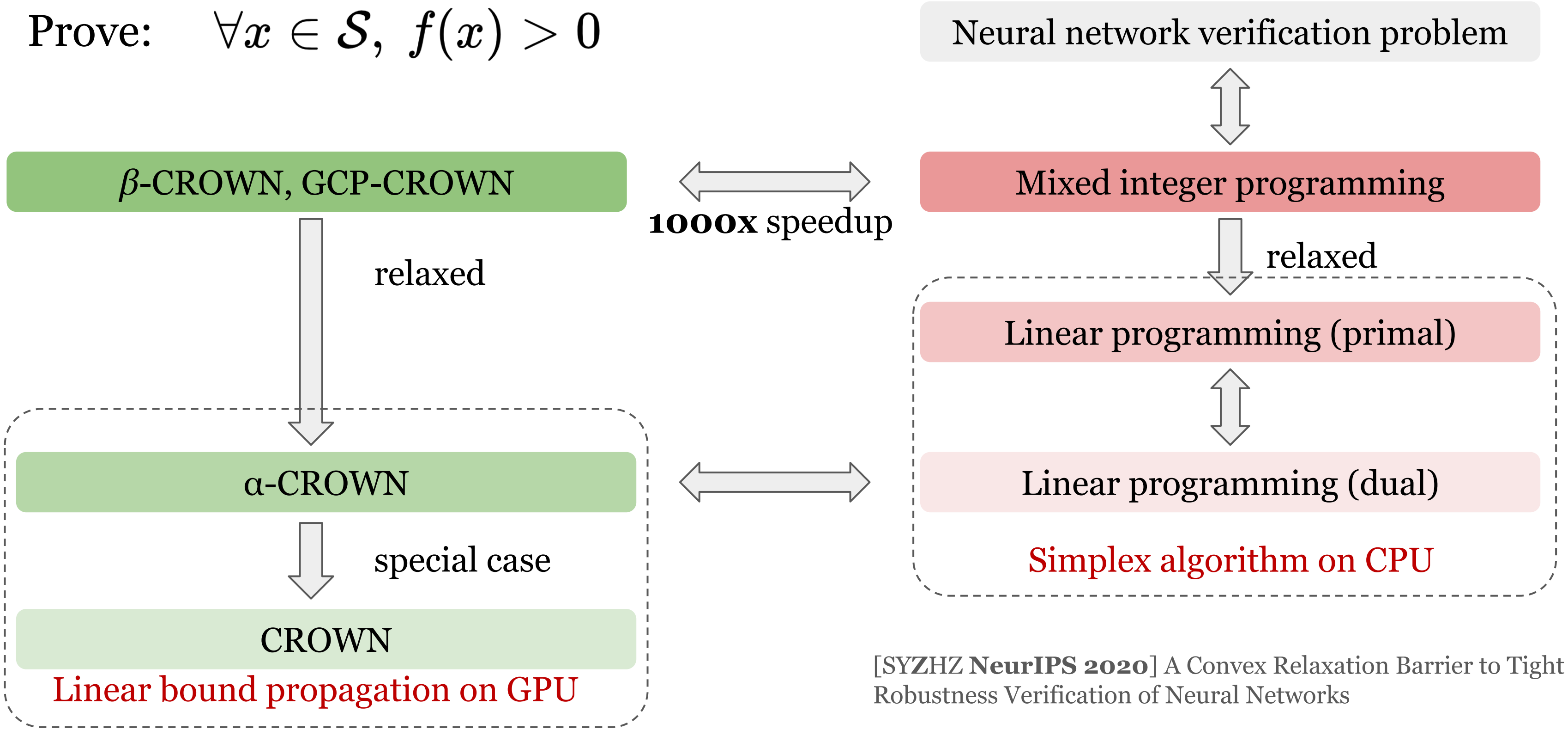
Model size: ~5k neurons

Integer programming and semidefinite programming **not plotted (~1 day)**

Key enablers: specialized bound propagation solver + GPU acceleration + BaB

Theoretical Connections: CROWN vs MIP/LP

Prove: $\forall x \in \mathcal{S},\ f(x) > 0$



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