ECE/CS 584: Verification of Embedded and Cyber-physical Systems

Lecture 9: Integer and Linear Programming Formulations for Neural Network Verification

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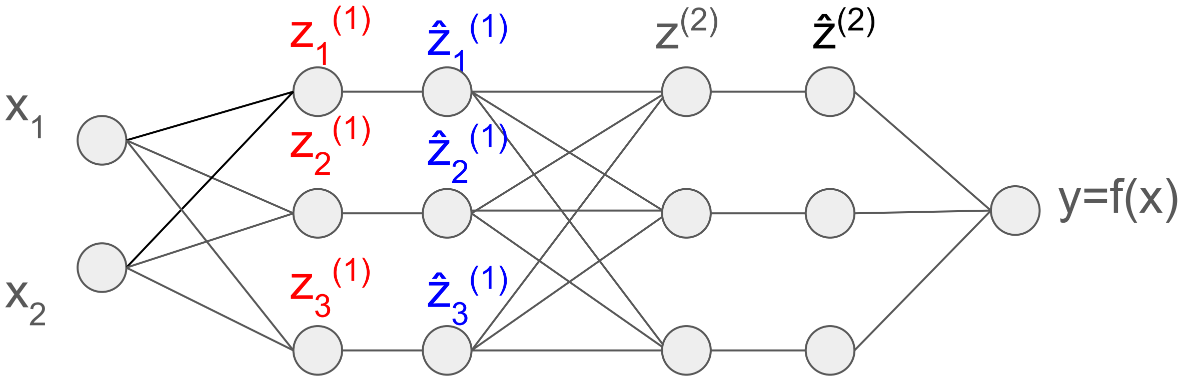
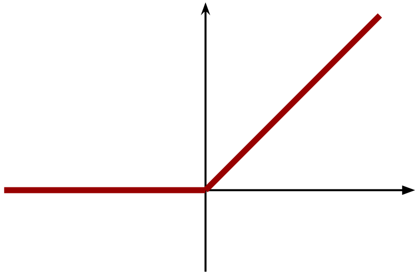
Review: neural networks

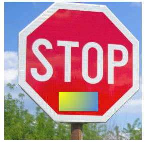


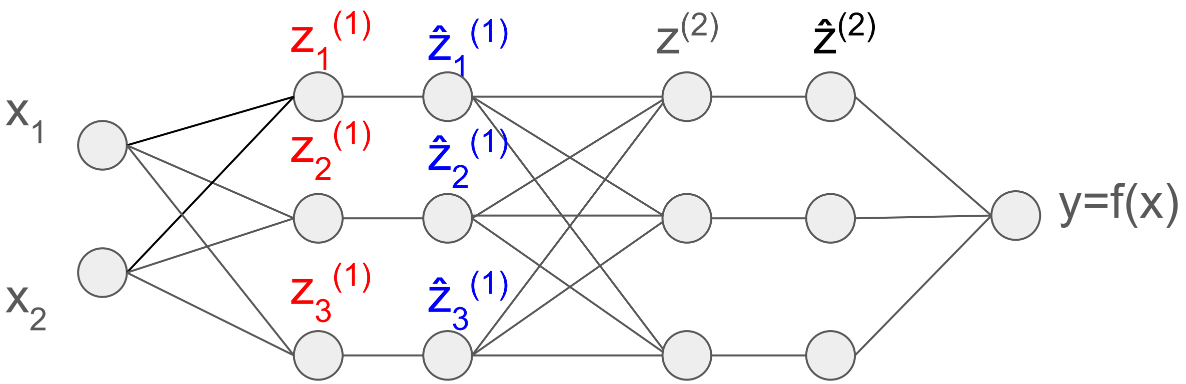


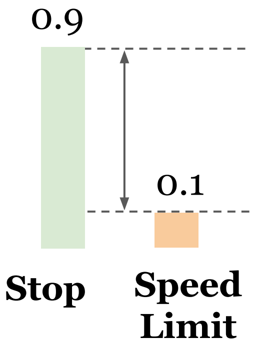
Linear layers: $z^{(1)} = W^{(1)} x$ $\quad z^{(2)} = W^{(2)} \hat{z}^{(1)}$ $\quad y = w^{(3)T} \hat{z}^{(2)}$

Nonlinear layers: $\hat{z}_j^{(i)}=\sigma(z_j^{(i)})$ (assume σ is ReLU for now)

Review: neural network verification as a satisfiability problem







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

Input domain under consideration

Negation of the desired property

Defines the neural network

Review: neural network verification as a satisfiability problem

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

$x_i \leq u_i \ \wedge\ x_i \geq l_i$ (assuming box constraints)

$((z_j^{(i)} \geq 0 \ \wedge\ \hat{z}_j^{(i)} = z_j^{(i)}) \vee (z_j^{(i)} < 0 \ \wedge\ \hat{z}_j^{(i)} = 0))$ for each ReLU neuron

$z_1 = W^{(1)} x \quad \wedge \quad z^{(2)} = W^{(2)} \hat{z}^{(1)} \quad \wedge \quad y = w^{(3)T} \hat{z}^{(2)} \quad \wedge \quad y \leq 0$

Add all clauses to the formula and solve using DPLL(T) with **Linear Real Arithmetic**.

In general this is very slow! Faster methods in the next a few lectures.

How does a SMT solver solve this problem?

First step: obtain the abstract version of the problem

$x_i \leq u_i \;\wedge\; x_i \geq l_i$ (assuming box constraints)

$((z_j^{(i)} \geq 0 \;\wedge\; \hat{z}_j^{(i)} = z_j^{(i)}) \;\vee\; (z_j^{(i)} < 0 \;\wedge\; \hat{z}_j^{(i)} = 0))$ for each ReLU neuron

$z_1 = W^{(1)} x \quad \wedge \quad z^{(2)} = W^{(2)} \hat{z}^{(1)} \quad \wedge \quad y = w^{(3)T} \hat{z}^{(2)} \quad \wedge \quad y \leq 0$

How does a SMT solver solve this problem?

Obtain the abstract version of the problem

$x_i \leq u_i \ \wedge \ x_i \geq l_i$ (assuming box constraints)

$((z_j^{(i)} \geq 0 \ \wedge \ \hat{z}_j^{(i)} = z_j^{(i)}) \ \vee \ (z_j^{(i)} < 0 \ \wedge \ \hat{z}_j^{(i)} = 0))$ for each ReLU neuron

$z_1 = W^{(1)} x \quad \wedge \quad z^{(2)} = W^{(2)} \hat{z}^{(1)} \quad \wedge \quad y = w^{(3)T} \hat{z}^{(2)} \quad \wedge \quad y \leq 0$

For each ReLU neuron: $((p_j^{(i)} \wedge q_j^{(i)}) \vee (\neg p_j^{(i)} \wedge r_j^{(i)}))$

All other clauses contain only a single literal, and must be set to True

How does a SMT solver solves this problem?

Now convert to CNF form

For each ReLU neuron: $((p_j^{(i)} \wedge q_j^{(i)}) \vee (\neg p_j^{(i)} \wedge r_j^{(i)}))$

Distribution: $((p_j^{(i)} \vee \neg p_j^{(i)}) \wedge (p_j^{(i)} \vee r_j^{(i)}) \wedge (q_j^{(i)} \vee \neg p_j^{(i)}) \wedge (q_j^{(i)} \vee r_j^{(i)}))$

Rewrite: $(p_j^{(i)} \vee r_j^{(i)}) \wedge (\neg p_j^{(i)} \vee q_j^{(i)}) \wedge (q_j^{(i)} \vee r_j^{(i)}))$

Observe that when $p_j^{(i)}$=True, $q_j^{(i)}$ must be true; $p_j^{(i)}$=False, $r_j^{(i)}$ must be true;

So the clause $q_j^{(i)} \vee r_j^{(i)}$ is redundant

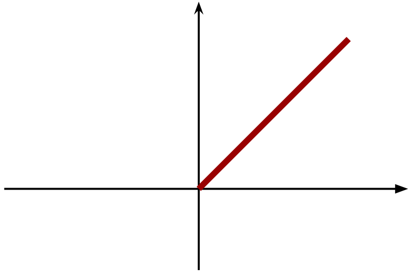
How does a SMT solver solves this problem?

$(p_j^{(i)} \vee r_j^{(i)}) \wedge (\neg p_j^{(i)} \vee q_j^{(i)})$

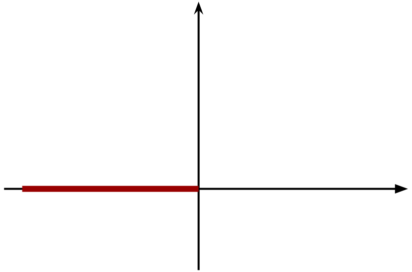
When $p_j^{(i)}$=True, $q_j^{(i)}$ must be true; $p_j^{(i)}$=False, $r_j^{(i)}$ must be true;

SAT solver must try both cases of $p_j^{(i)}$

$p_j^{(i)}$=True ($z_j^{(i)} \geq 0$)



$p_j^{(i)}$=False ($z_j^{(i)} < 0$)



Why using a SMT solver is very slow?

$(p_j^{(i)} \vee r_j^{(i)}) \wedge (\neg p_j^{(i)} \vee q_j^{(i)})$

When $p_j^{(i)}$=True, $q_j^{(i)}$ must be true; $p_j^{(i)}$=False, $r_j^{(i)}$ must be true;

SAT solver must try both cases of $p_j^{(i)}$. In a satisfiable solution from DPLL, each $p_j^{(i)}$ is set to True or False, then a theory solver (Simplex) invoked.

There are exponential number of cases here… and modern neural networks can have millions of neurons!

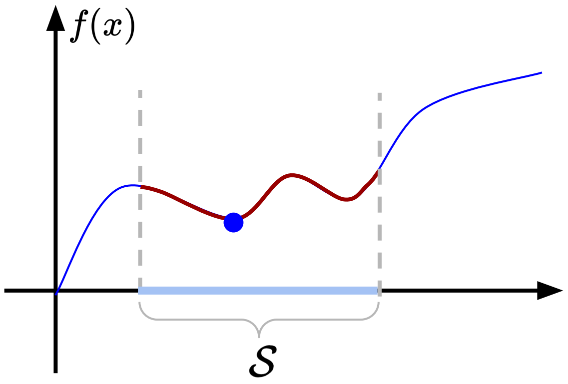
Can we solve the problem without setting every $p_j^{(i)}$?

We will tack this problem from an **optimization** point of view today

Mathematical optimization problems

Given a **objective function** f: S → R

Seek an **optimal solution** x^* such that $f(x^*) \leq f(x)$ for all $x \in S$



Some optimization problems are hard, some are easy

Given a **objective function** $f: S \rightarrow R$

Hardness depends on the properties of f and S. For tractable solving they cannot be arbitrary!

- Easy ones: convex optimization, linear programming, semidefinite programming
  - E.g., in linear programming, objective function and constraints must be linear functions

- Hard ones: integer programming, general quadratic programming, general nonlinear programming, …

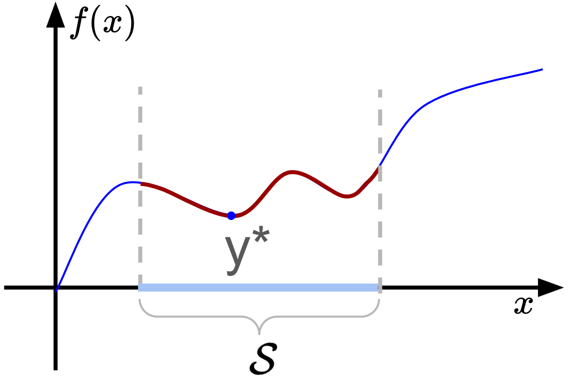
Verification Problem as an optimization problem

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

Can be solved with the following **minimization problem:**

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

If the optimal objective y*≤0, then the original Problem is satisfiable



Verification Problem as an optimization problem

Now we rewrite the neural network verification problem as a **constrained optimization problem** (still using the simple network example):

$$
\begin{aligned}
&\min\; y \\
\text{s.t.}\quad & y = w^{(3)T}\,\hat{z}^{(2)} && \text{(linear layers)} \\
& \hat{z}^{(2)} = \max(z^{(2)}, 0) && \text{(ReLU activation)} \\
& z^{(2)} = W^{(2)}\,\hat{z}^{(1)} \\
& \hat{z}^{(1)} = \max(z^{(1)}, 0) \\
& z^{(1)} = W^{(1)}\,x \\
& x_i \le u_i && \text{(element-wise input bounds)} \\
& x_i \ge l_i
\end{aligned}
$$

Verification Problem as an optimization problem

Now we rewrite the neural network verification problem as a **constrained optimization problem** (still using the simple network example):

$$\min y$$

$$\text{s.t.} \quad y = w^{(3)T} \hat{z}^{(2)} \qquad \text{(linear constraints)}$$

$$\hat{z}^{(2)} = \max(z^{(2)}, 0) \qquad \text{(nonlinear constraints)}$$

$$z^{(2)} = W^{(2)} \hat{z}^{(1)}$$

$$\hat{z}^{(1)} = \max(z^{(1)}, 0)$$

$$z^{(1)} = W^{(1)} x$$

$$x_i \leq u_i$$

$$x_i \geq l_i$$

(inputs bounds are also linear constraints)

Optimization formulation for ReLU neurons

Let's look at this constraint more carefully: $\hat{z}_j^{(i)} = \max(z_j^{(i)}, 0)$ (for all i, j)

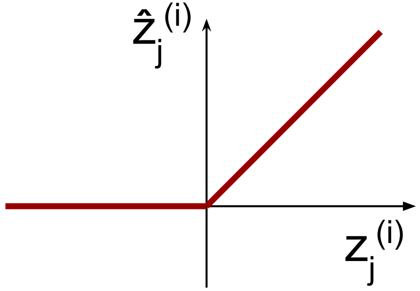
One way to handle it is through the **mixed integer linear programming (MILP)** formulation. Create an **integer variable** $p_j^{(i)} \in \{0,1\}$, the constraint $\hat{z}_j^{(i)} = \max(z_j^{(i)}, 0)$ can be equivalently written as (here M is a "big" number):

$$\hat{z}_j^{(i)} \le z_j^{(i)} - M_1(1 - p_j^{(i)})$$

$$\hat{z}_j^{(i)} \le M_2 p_j^{(i)}$$

$$\hat{z}_j^{(i)} \ge z_j^{(i)}$$

$$\hat{z}_j^{(i)} \ge 0$$



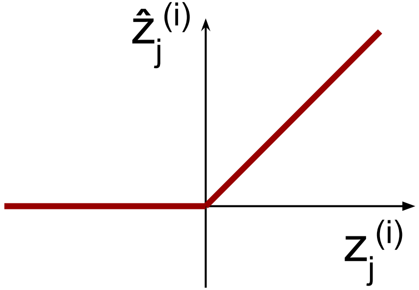
Optimization formulation for ReLU neurons

$$\hat{z}_j^{(i)} \leq z_j^{(i)} - M_1(1 - p_j^{(i)})$$

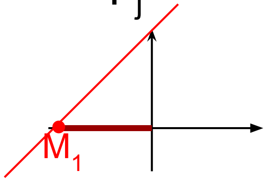
$$\hat{z}_j^{(i)} \leq M_2 p_j^{(i)}$$

$$\hat{z}_j^{(i)} \geq z_j^{(i)}$$

$$\hat{z}_j^{(i)} \geq 0$$



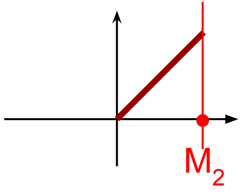
When $p_j^{(i)} = 0$:



$$\boxed{\hat{z}_j^{(i)} \leq z_j^{(i)} - M_1} \qquad \hat{z}_j^{(i)} \leq 0$$

$$\hat{z}_j^{(i)} \geq z_j^{(i)} \qquad \hat{z}_j^{(i)} \geq 0$$

When $p_j^{(i)} = 1$:



$$\hat{z}_j^{(i)} \leq z_j^{(i)} \qquad \boxed{\hat{z}_j^{(i)} \leq M_2}$$

$$\hat{z}_j^{(i)} \geq z_j^{(i)} \qquad \hat{z}_j^{(i)} \geq 0$$

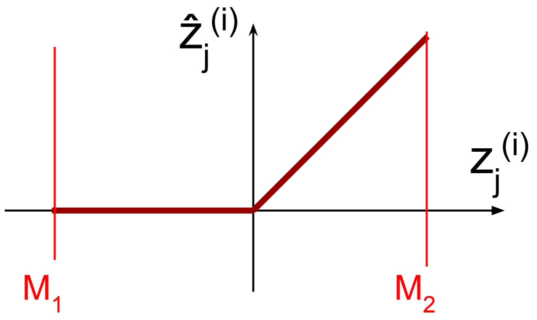
M_1 needs to be **small** (negative) **enough**

M_2 needs to be **large enough**

Pre-activation bounds

For this formulation to work, M_1 and M_2 must be properly selected.

If set too conservatively, like $M_1 = 100000$ and $M_2 = -100000$, solver can be very slow



How to find the tightest M_1 and M_2?

Pre-activation bounds

For this formulation to work, M_1 and M_2 must be properly selected.

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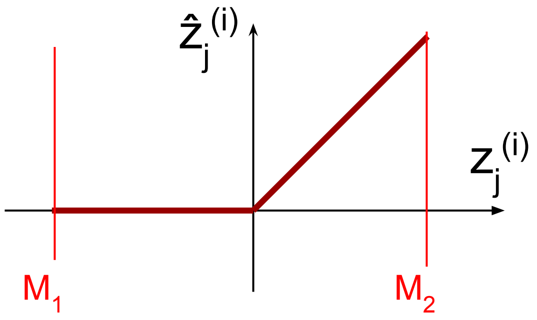
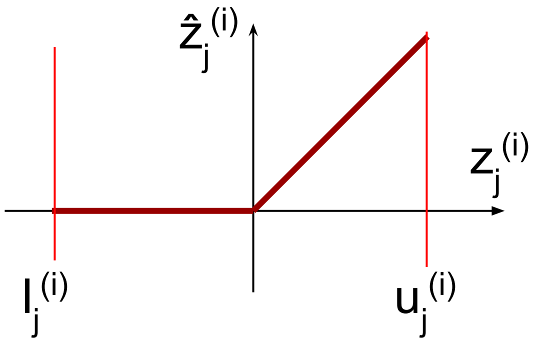


How to find the tightest M_1 and M_2?

Pre-activation bounds

For this formulation to work, M_1 and M_2 must be properly selected (usually denoted as l and u)



$$l_j^{(i)} := \min z_j^{(i)}$$

$$u_j^{(i)} := \max z_j^{(i)}$$

We can use optimization to find these pre-activation bounds - the same formulation as our verification problem before, just changing the optimization variables.

MILP, LP, or more efficient methods (next lecture) can be used to find these.

Pre-activation bounds

$$\cancel{\min y}$$
$$\text{s.t.} \quad y = w^{(3)T}\,\hat{z}^{(2)}$$
$$\hat{z}^{(2)} = \max(z^{(2)}, 0)$$
$$z^{(2)} = W^{(2)}\,\hat{z}^{(1)}$$
$$\hat{z}^{(1)} = \max(z^{(1)}, 0)$$
$$z^{(1)} = W^{(1)}\,x$$
$$x_i \leq u_i^{(0)}$$
$$x_i \geq l_i^{(0)}$$

$$l_j^{(i)} := \min z_j^{(i)} \quad \text{or} \quad u_j^{(i)} := \max z_j^{(i)}$$

We can use optimization to find these pre-activation bounds - the same formulation as our verification problem before, just changing the optimization variables.

Mixed Integer Linear Programming formulation

We rewrite the neural network verification problem as a **constrained optimization problem** (still using the simple network example):

$$
\begin{aligned}
\mathbf{y^*_{MILP}} &:= \min y \\
\text{s.t.} \quad y &= w^{(3)T} \hat{z}^{(2)} \\
&\cancel{\hat{z}^{(2)} = \max(z^{(2)}, 0)} \\
z^{(2)} &= W^{(2)} \hat{z}^{(1)} \\
&\cancel{\hat{z}^{(1)} = \max(z^{(1)}, 0)} \\
z^{(1)} &= W^{(1)} x \\
x_i &\le u_i^{(0)} \\
x_i &\ge l_i^{(0)}
\end{aligned}
$$

Each ReLU is represented by

$$
\hat{z}_j^{(i)} \le z_j^{(i)} - l_j^{(i)}(1 - p_j^{(i)})
$$

$$
\hat{z}_j^{(i)} \le u_j^{(i)} p_j^{(i)}
$$

$$
\hat{z}_j^{(i)} \ge z_j^{(i)}
$$

$$
\hat{z}_j^{(i)} \ge 0
$$

$$
p_j^{(i)} \in \{0, 1\}
$$

Mixed Integer Linear Programming formulation

However, the integer variables $p_j^{(i)}$ are still hard to handle! (NP-hard)

$$
\begin{aligned}
\color{red}{y^*_{MILP}} &:= \min y \\
\text{s.t.} \quad y &= w^{(3)T} \hat{z}^{(2)} \\
&\cancel{\hat{z}^{(2)} = \max(z^{(2)}, 0)} \\
z^{(2)} &= W^{(2)} \hat{z}^{(1)} \\
&\cancel{\hat{z}^{(1)} = \max(z^{(1)}, 0)} \\
z^{(1)} &= W^{(1)} x \\
x_i &\le u_i^{(0)} \\
x_i &\ge l_i^{(0)}
\end{aligned}
$$

Each ReLU is represented by

$$
\begin{aligned}
\hat{z}_j^{(i)} &\le z_j^{(i)} - l_j^{(i)}(1 - p_j^{(i)}) \\
\hat{z}_j^{(i)} &\le u_j^{(i)} p_j^{(i)} \\
\hat{z}_j^{(i)} &\ge z_j^{(i)} \\
\hat{z}_j^{(i)} &\ge 0 \\
p_j^{(i)} &\in \{0, 1\}
\end{aligned}
$$

Relaxation of integer variables: Linear programming

Now **relaxing** the integer constraints into continuous ones.

How does this affect the solution?

$$y^*_{LP} := \min y$$
$$\text{s.t.} \quad y = w^{(3)T} \hat{z}^{(2)}$$
$$\cancel{\hat{z}^{(2)} = \max(z^{(2)}, 0)}$$
$$z^{(2)} = W^{(2)} \hat{z}^{(1)}$$
$$\cancel{\hat{z}^{(1)} = \max(z^{(1)}, 0)}$$
$$z^{(1)} = W^{(1)} x$$
$$x_i \leq u_i^{(0)}$$
$$x_i \geq l_i^{(0)}$$

Each ReLU is represented by

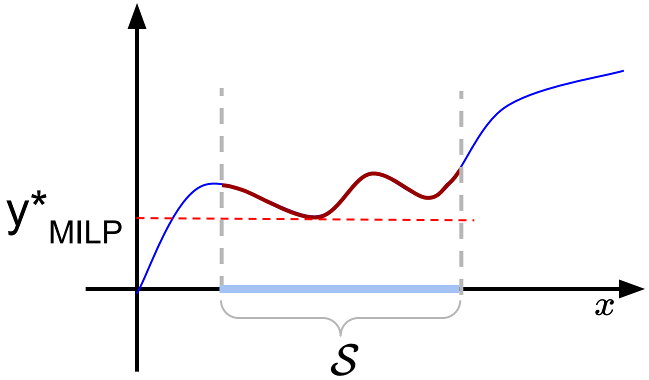
$$\hat{z}_j^{(i)} \leq z_j^{(i)} - l_j^{(i)}(1 - p_j^{(i)})$$
$$\hat{z}_j^{(i)} \leq u_j^{(i)} p_j^{(i)}$$
$$\hat{z}_j^{(i)} \geq z_j^{(i)}$$
$$\hat{z}_j^{(i)} \geq 0$$
$$\cancel{p_j^{(i)} \in \{0, 1\}} \quad 0 \leq p_j^{(i)} \leq 1$$

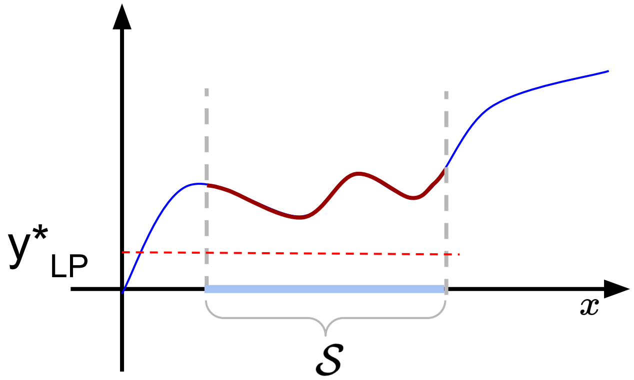
MILP vs LP

$$y^*_{LP} \leq y^*_{MILP}$$

It's not the original MILP solution, but it is a guaranteed lower bound

Solving LP is polynomial time. Practically a few orders of magnitude faster.



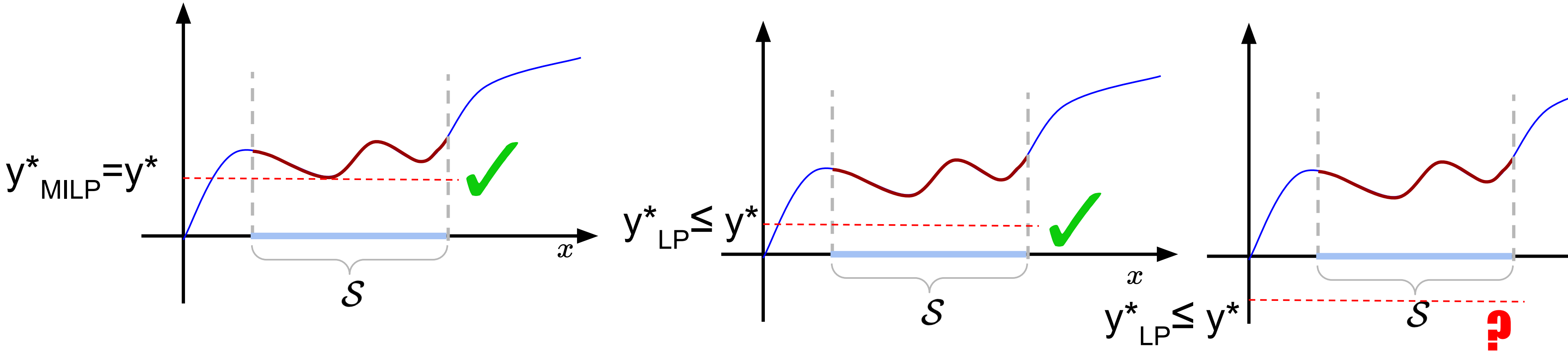


Sound but Incomplete Verification with a Lower Bound

Satisfiability problem: ∃ x ∈ S ∧ y ≤ 0 ∧ y = f(x)

If $y^*_{LP} \geq 0$ => $y^* \geq 0$ => requirement verified (unsatisfiable)

$y^*_{LP} \leq 0$ => return unknown (incomplete)



A closer look at the linear programming relaxation

Each ReLU is represented by

$$\hat{z}_j^{(i)} \leq z_j^{(i)} - l_j^{(i)}(1 - p_j^{(i)})$$

$$\hat{z}_j^{(i)} \leq u_j^{(i)} p_j^{(i)}$$

$$\hat{z}_j^{(i)} \geq z_j^{(i)}$$

$$\hat{z}_j^{(i)} \geq 0$$

$$0 \leq p_j^{(i)} \leq 1$$

$$\Rightarrow$$

$$p_j^{(i)} \leq \frac{\hat{z}_j^{(i)} - z_j^{(i)} + l_j^{(i)}}{l_j^{(i)}}$$

$$p_j^{(i)} \geq \frac{\hat{z}_j^{(i)}}{u_j^{(i)}}$$

$$\Rightarrow$$

Project out p

$$\hat{z}_j^{(i)} \leq \frac{u_j^{(i)}}{u_j^{(i)} - l_j^{(i)}} z_j^{(i)} - \frac{u_j^{(i)} l_j^{(i)}}{u_j^{(i)} - l_j^{(i)}}$$

(Please note that $l_j^{(i)}$ is negative during the above derivation)

A closer look at the linear programming relaxation

Each ReLU is represented by

$$\hat{z}_j^{(i)} \le z_j^{(i)} - l_j^{(i)}(1 - p_j^{(i)})$$

$$\hat{z}_j^{(i)} \le u_j^{(i)} p_j^{(i)}$$

$$\hat{z}_j^{(i)} \ge z_j^{(i)}$$

$$\hat{z}_j^{(i)} \ge 0$$

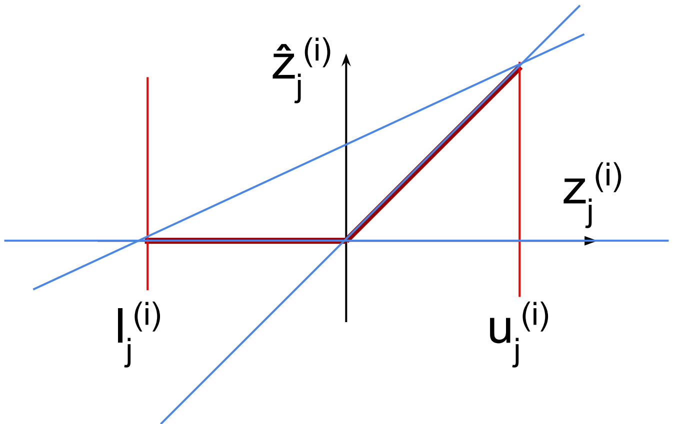
$$\Longrightarrow$$

$$\hat{z}_j^{(i)} \le \frac{u_j^{(i)}}{u_j^{(i)} - l_j^{(i)}} z_j^{(i)} - \frac{u_j^{(i)} l_j^{(i)}}{u_j^{(i)} - l_j^{(i)}}$$

$$\hat{z}_j^{(i)} \ge z_j^{(i)}$$

$$\hat{z}_j^{(i)} \ge 0$$

"Triangle" relaxation



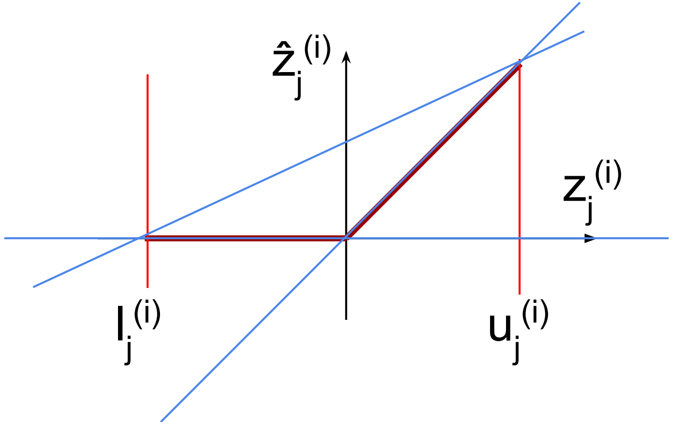
A closer look at the linear programming relaxation

MILP: solutions are constrained on ReLU function
Linear programming: solutions are constrained on the triangle

$$\hat{z}_j^{(i)} \leq \frac{u_j^{(i)}}{u_j^{(i)} - l_j^{(i)}} z_j^{(i)} - \frac{u_j^{(i)} l_j^{(i)}}{u_j^{(i)} - l_j^{(i)}}$$

$$\hat{z}_j^{(i)} \geq z_j^{(i)}$$

$$\hat{z}_j^{(i)} \geq 0$$



MILP vs LP vs DPLL(T)

MILP:

- Branch and bound is used to make decisions only on certain number of binary variables
- Specialized methods to accelerate solving (e.g., branching heuristics, cutting planes)
- Complete (solve y* exactly)
- Typically scales much better than DPLL(T)

Linear programming:

- No integer variables
- No variable decisions needed (no exponential time search)
- Simplex algorithm can solve it relatively fast, a few thousands neurons are ok
- Incomplete (has to return unknown in some cases)

Summary

- Neural network verification problem
- Solving the verification problem with SMT solvers
- Integer programming formulation
- Linear programming formulation and linear relaxation of ReLUs
- Next lecture: linear bound propagation method (CROWN) for efficient neural network verification
- **Reading for the next lecture**:
  - http://arxiv.org/pdf/1811.00866.pdf
  - https://arxiv.org/pdf/1902.08722.pdf
- Homework 1 due on Sunday (2/11) 11:59 pm