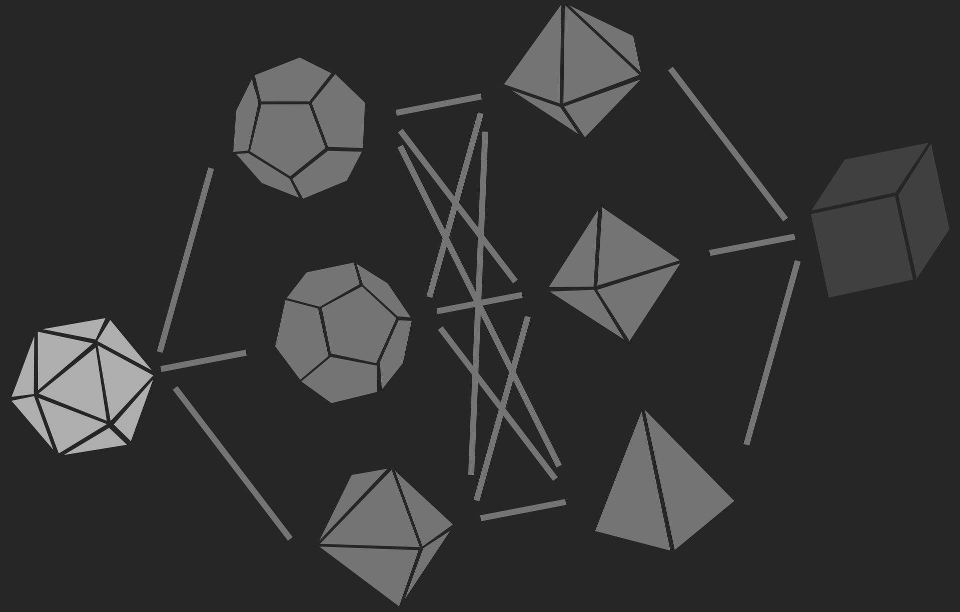
18th INFORMS Computing Society (ICS) Conference

L2O-MINLP

Learning to Optimize for Mixed-Integer Non-Linear Programming



Mechanical & Industrial Engineering
UNIVERSITY OF TORONTO

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Presented by Bo Tang
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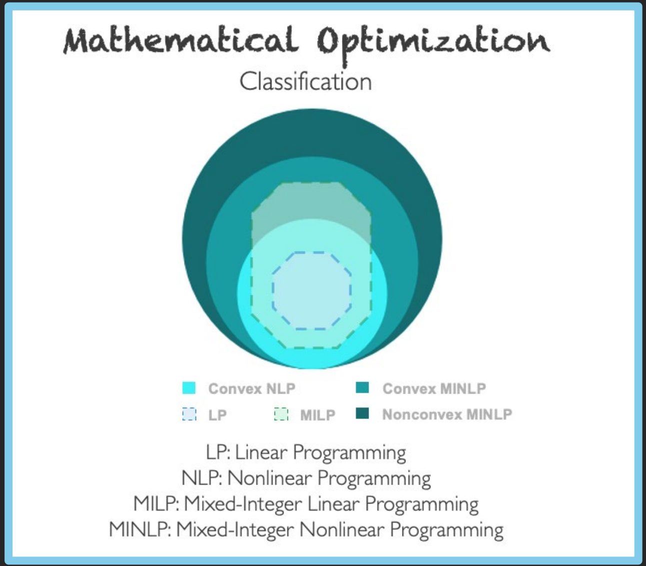
Motivation

Why does MINLP matter?

MINLP is general but very hard:

Combinatorial Complexity + Non-Convexity.



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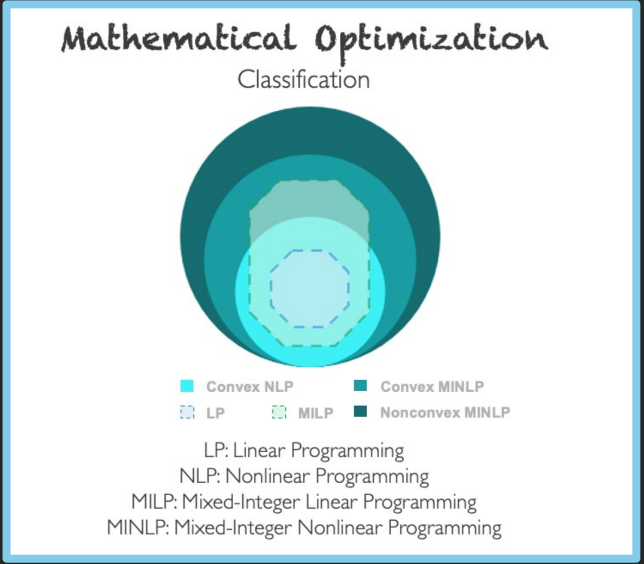

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Traditional solvers struggle with large-scale MINLP problems.

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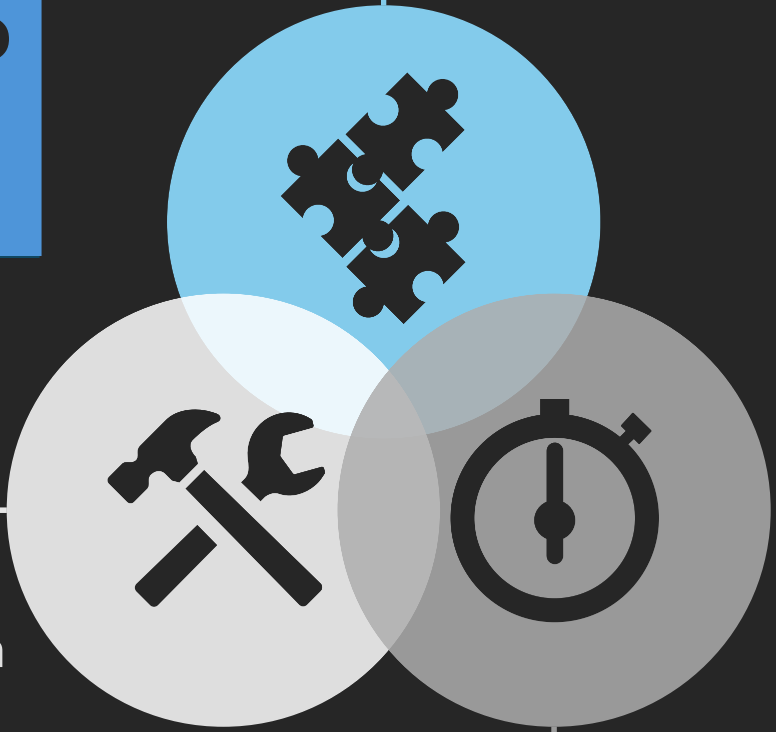

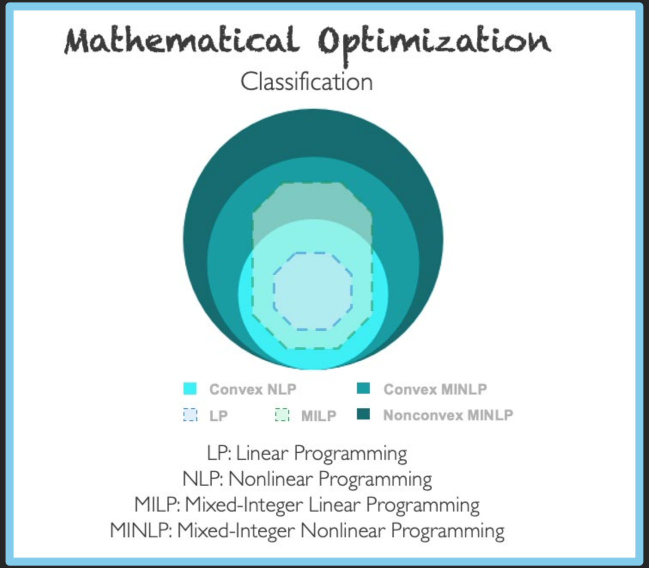

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Traditional solvers struggle with large-scale MINLP problems.

GUROBI OPTIMIZATION

Solution time is tight:

Real-world applications often require solutions within a short time window.

e.g., Optimal Control, Energy Management, etc.

Introduction to L2O

01 What is L2O?

L2O is a data-driven approach that leverages machine learning to improve optimization processes.

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03 How does L2O work?

L2O learns from optimal or near-optimal solutions to either generate solutions directly or guide solvers in narrowing the search space.

What we did here!

Traditional Methods vs. L2O Approaches

Traditional Methods

- **Require costly iterative procedures** (e.g., branch-and-bound, matrix inversion) that scale poorly with problem size.
- **Solve from scratch for every instance**, even if similar problems have been solved before.
- **Require manual tuning** of heuristics and parameters for good performance.
- **Optimality is theoretical guaranteed** through exact methods.

L2O Approaches

- **Bypass expensive iterations** by learning direct mappings or guiding solvers for faster convergence.
- **Leverage past patterns** to generalize and quickly generate solutions for new instances.
- **Automate tuning** by learning optimization strategies from data.
- **No guarantee** of optimality or even feasibility.

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Problem Formulation

MINLP Formulation:

$$\min_{\boldsymbol{x}} f(\boldsymbol{x})$$

$$\text{s.t.} \quad \boldsymbol{g}(\boldsymbol{x}) \le 0$$

$$\boldsymbol{x} \in \mathbb{R}^{n_r} \times \mathbb{Z}^{n_z}$$

Problem Formulation

Parametric MINLP Formulation:

$$\min_{\boldsymbol{x}} f(\boldsymbol{x}, \xi)$$

$$\text{s.t.} \quad \boldsymbol{g}(\boldsymbol{x}, \xi) \le 0$$

$$\boldsymbol{x} \in \mathbb{R}^{n_r} \times \mathbb{Z}^{n_z}$$

$$\xi \in \Xi$$

Parameters ξ influence the objective and constraints of optimization problems.

Multiple Instances $\left\{ \begin{array}{l} \xi_1 \to \boldsymbol{x}_1^* \\ \xi_2 \to \boldsymbol{x}_2^* \\ \vdots \\ \xi_m \to \boldsymbol{x}_m^* \end{array} \right.$

Problem Formulation

Prediction for Parametric MINLP Formulation:

$$\min_{\boldsymbol{\Theta}} \mathbb{E}_{\boldsymbol{\Xi}}[f(\hat{\boldsymbol{x}}, \boldsymbol{\xi})]$$

Expected objective function:

$$\mathbb{E}_{\boldsymbol{\Xi}}[f(\hat{\boldsymbol{x}}, \boldsymbol{\xi})] \approx \frac{1}{m} \sum_{i=1}^{m} f(\hat{\boldsymbol{x}}_i, \boldsymbol{\xi}_i)$$

$$\text{s.t.} \quad \boldsymbol{g}(\hat{\boldsymbol{x}}, \boldsymbol{\xi}) \leq 0$$

$$\hat{\boldsymbol{x}} \in \mathbb{R}^{n_r} \times \mathbb{Z}^{n_z}$$

$$\boldsymbol{\xi} \in \boldsymbol{\Xi}$$

Machine learning model $\psi_{\boldsymbol{\Theta}}$ with inputs $\boldsymbol{\xi}$ and weights $\boldsymbol{\Theta}$

Solution prediction

$$\hat{\boldsymbol{x}} = \psi_{\boldsymbol{\Theta}}(\boldsymbol{\xi})$$

Problem Formulation

Prediction for Parametric MINLP Formulation:

$$\min_{\Theta} \mathbb{E}_{\Xi}[f(\hat{x}, \xi)]$$

Minimize expected objective function:

$$\mathbb{E}[f(\hat{x}, \xi)] \approx \frac{1}{m}\sum_{i=1}^{m} f(\hat{x}_i, \xi_i)$$

IT SEEMS IDEAL:

What Prevents L2O from Extending to this MINLP?

$$\hat{x} \in \mathbb{R}^{n_r} \times \mathbb{Z}^{n_z}$$

$$\xi \in \Xi$$

Machine learning model ψ_{Θ} with input ξ and weights Θ

Solution prediction

$$\hat{x} = \psi_{\Theta}(\xi)$$

Limitations of Existing L2O

01 Collecting Solutions as Training Label is Very Expensive

02 Neural Networks Cannot Directly Output Integer Values

03 It is Difficult to Ensure Feasibility, Especially in Integers

Limitations of Existing L2O

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Our Solution: We propose a Self-Supervised Approach without requiring solutions for training.

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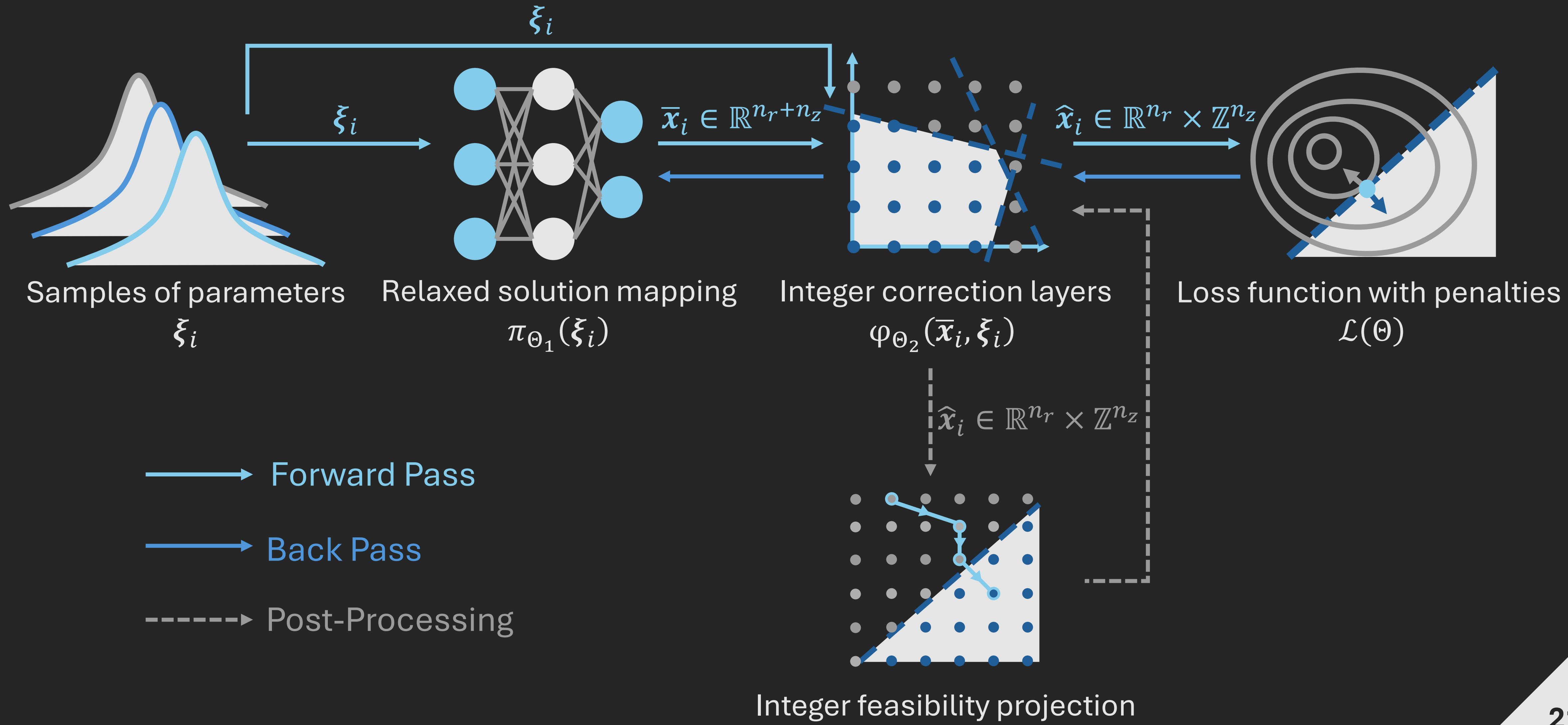
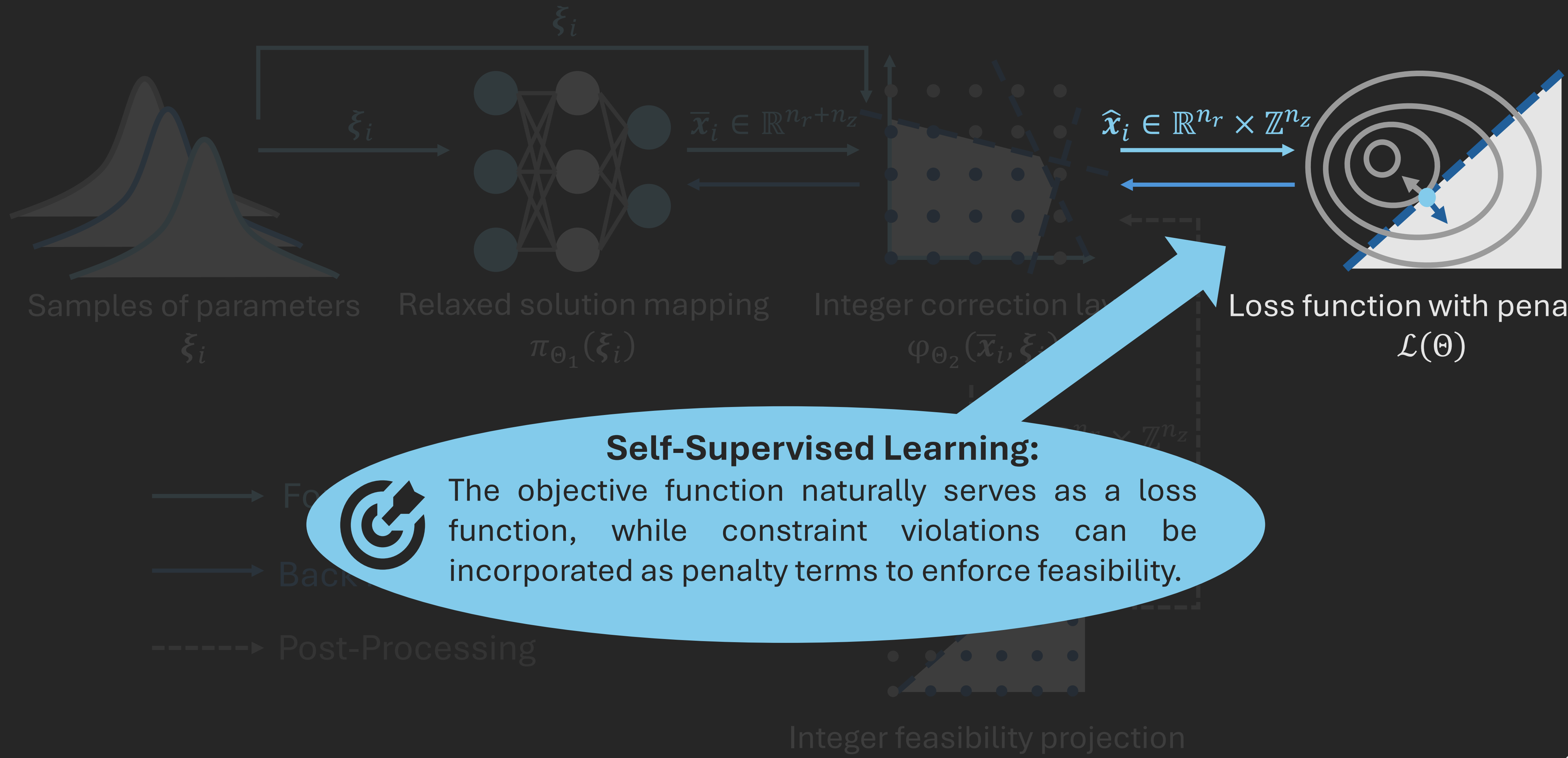
03 It is Difficult to Ensure Feasibility, Especially in Integers

Our Solution: We introduce a gradient-based Feasibility Projection to adjust integer solutions.

Methodology



Loss Function



Self-Supervised Learning:

The objective function naturally serves as a loss function, while constraint violations can be incorporated as penalty terms to enforce feasibility.

Loss Function

Loss Function with Penalty

$$\mathcal{L}(\Theta) = \sum_{i=1}^{m} \left[f(\hat{\boldsymbol{x}}_i, \xi_i) + \lambda \cdot \| \boldsymbol{g}(\hat{\boldsymbol{x}}_i, \xi_i)_+ \|_1 \right]$$

Loss Function

Loss Function with Penalty

$$\mathcal{L}(\Theta) = \sum_{i=1}^{m} [\underbrace{f(\hat{\boldsymbol{x}}_i, \xi_i)}_{\text{Objective Function}} + \lambda \cdot \|g(\hat{\boldsymbol{x}}_i, \xi_i)_+\|_1]$$

Loss Function

Loss Function with Penalty

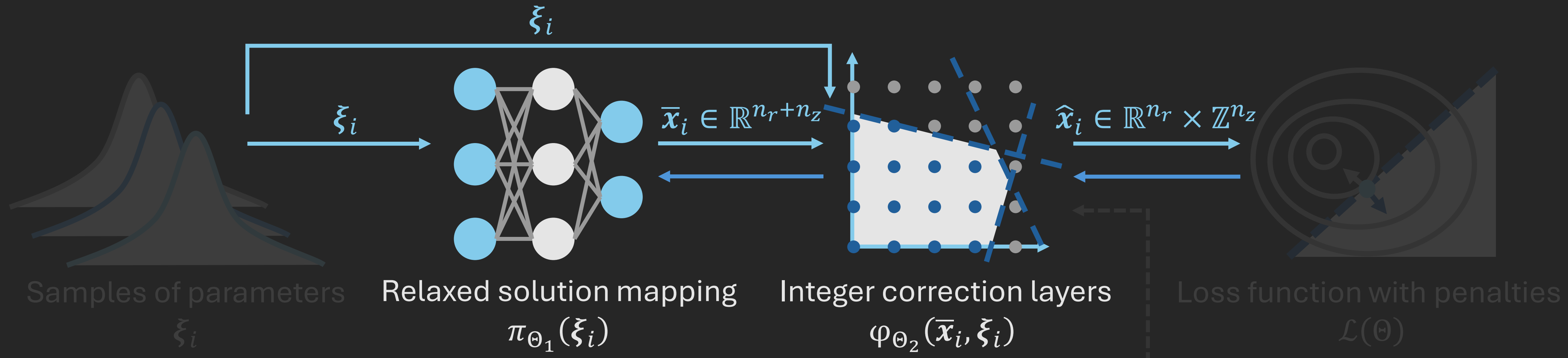
$$\mathcal{L}(\Theta) = \sum_{i=1}^{m} \Big[\underbrace{f(\hat{x}_i, \xi_i)}_{\text{Objective Function}} + \lambda \cdot \| \underbrace{g(\hat{x}_i, \xi_i)_+ \|}_{\text{Constraints Violation}}{}_1 \Big]$$

Loss Function

Loss Function with Penalty

$$\mathcal{L}(\Theta) = \sum_{i=1}^{m} [\underbrace{f(\hat{x}_i, \xi_i)}_{\text{Objective Function}} + \overbrace{\lambda}^{\text{Penalty Weight}} \cdot \underbrace{\|g(\hat{x}_i, \xi_i)_+\|_1}_{\text{Constraints Violation}}]$$

Integer Correction Layers



Bi-Level Neural Network Architecture

Relaxed Solution Mapping

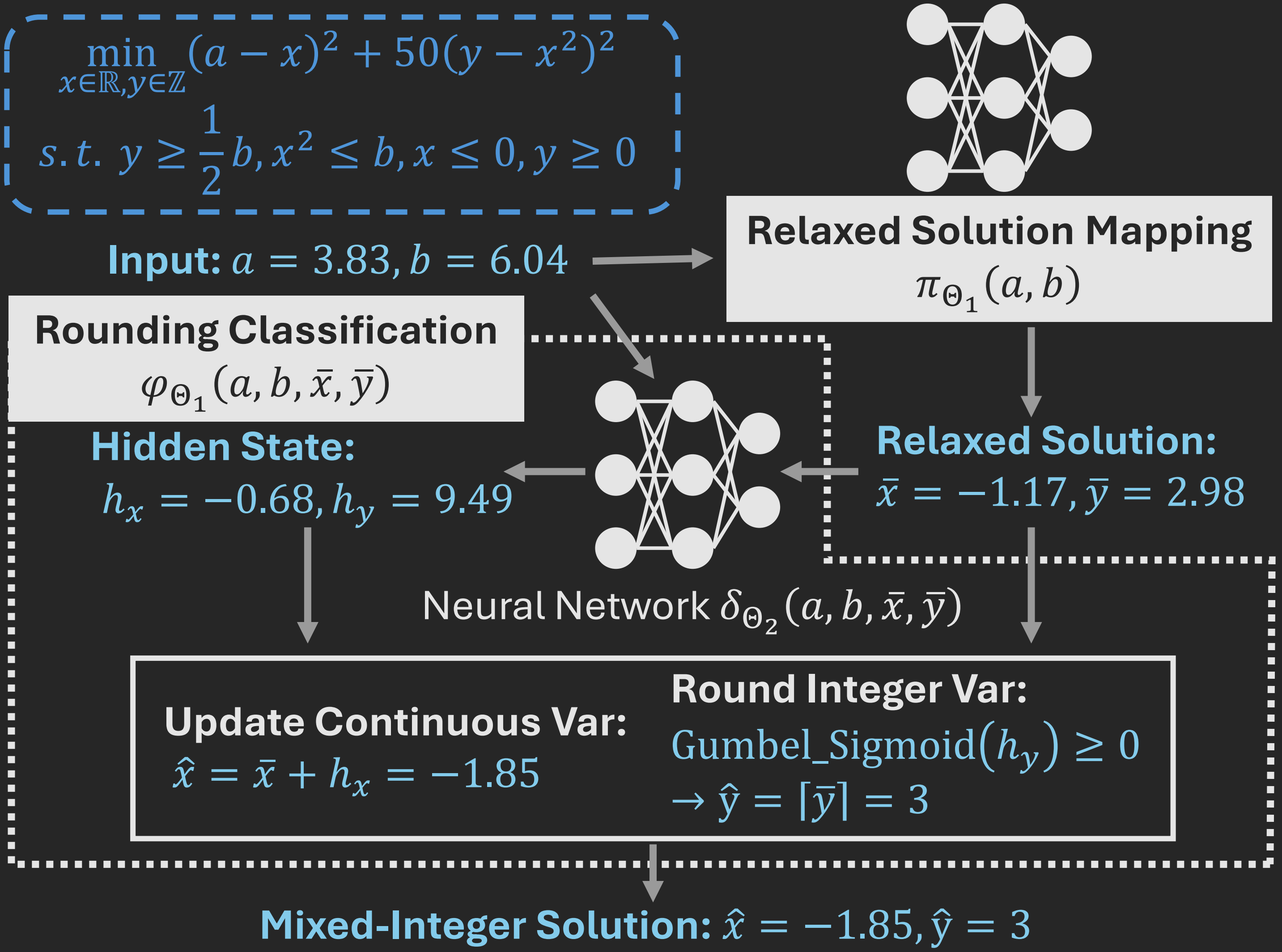
From
Parameters ξ
To
Relaxed Solution $\bar{x}$

Integer Correction

From
Relaxed Solution $\bar{x}$
To
Mixed-Integer Solution $\hat{x}$

Integer Correction Layers

Example

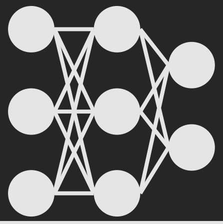


Integer Correction Layers

Example

$$\min_{x\in\mathbb{R},y\in\mathbb{Z}} (a-x)^2 + 50(y-x^2)^2$$
$$s.t.\ y \geq \frac{1}{2}b, x^2 \leq b, x \leq 0, y \geq 0$$

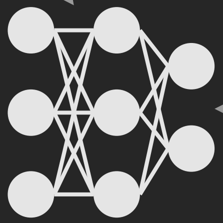
Input: $a = 3.83, b = 6.04$



Relaxed Solution Mapping
$\pi_{\Theta_1}(a, b)$

Relaxed Solution:
$\bar{x} = -1.17, \bar{y} = 2.98$

Rounding Classification
$\varphi_{\Theta_1}(a, b, \bar{x}, \bar{y})$



Neural Network $\delta_{\Theta_2}(a, b, \bar{x}, \bar{y})$

Hidden State:
$h_x = -0.68, h_y = 9.49$

Update Continuous Var:
$\hat{x} = \bar{x} + h_x = -1.85$

Round Integer Var:
$\text{Gumbel\_Sigmoid}(h_y) \geq 0$
$\rightarrow \hat{y} = \lceil \bar{y} \rceil = 3$

STE

Mixed-Integer Solution: $\hat{x} = -1.85, \hat{y} = 3$

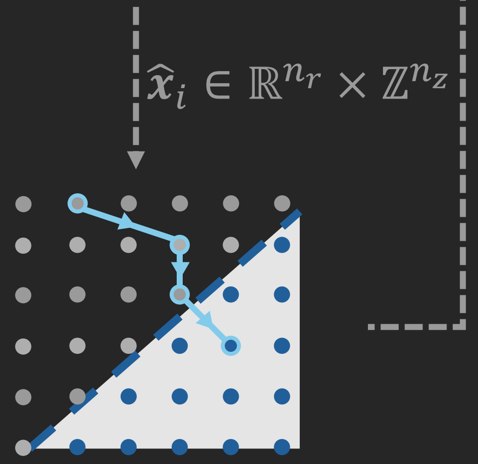
Integer Feasibility Projection

Feasibility projection is a computationally efficient post-processing heuristic that refines neural network outputs while preserving integer constraints.

- **Computational Efficiency:** Avoids the need for repeated projections and second-order gradient computation during training.
- **Stable Training:** Keeps projection separate from training, preventing interference with the output of model.

Integer correction layers
$\varphi_{\Theta_2}(\bar{x}_i, \xi_i)$

Loss function with penalties
$\mathcal{L}(\Theta)$

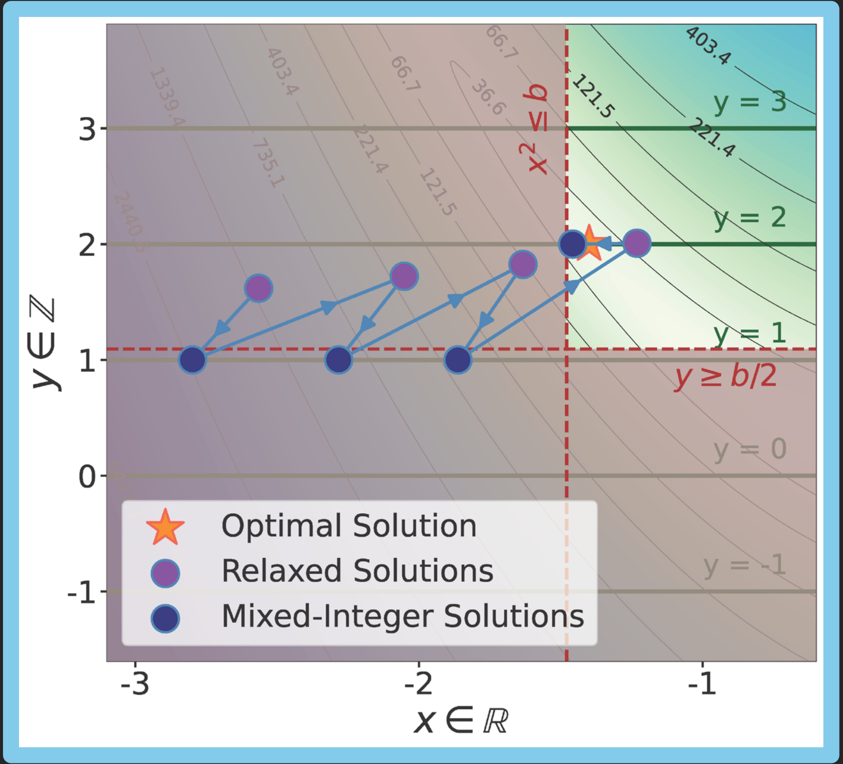


Integer feasibility projection

Integer Feasibility Projection

Algorithm 2 Integer Feasibility Projection: Inference

Input: parameters $\boldsymbol{\xi}^i$, layers $\pi_{\Theta_1}(\cdot)$ and $\varphi_{\Theta_2}(\cdot)$, step size η
Predict a continuously relaxed solution $\bar{\mathbf{x}}^i \leftarrow \pi_{\Theta_1}(\boldsymbol{\xi}^i)$
while True **do**
  Obtain a mixed-integer solution $\hat{\mathbf{x}}^i \leftarrow \varphi_{\Theta_2}(\bar{\mathbf{x}}^i, \boldsymbol{\xi}^i)$
  Compute feasibility violation $\mathcal{V}(\hat{\mathbf{x}}^i, \boldsymbol{\xi}^i) \leftarrow \|\mathbf{g}(\hat{\mathbf{x}}^i, \boldsymbol{\xi}^i)_+\|_1$
  if $\mathcal{V}(\hat{\mathbf{x}}^i, \boldsymbol{\xi}^i) = 0$ **then**
    Break
  else
    Update relaxed solution $\bar{\mathbf{x}}^i \leftarrow \bar{\mathbf{x}}^i - \eta \nabla_{\bar{\mathbf{x}}} \mathcal{V}(\hat{\mathbf{x}}^i, \boldsymbol{\xi}^i)$
  end if
end while
Output: a mixed-integer solution $\hat{\mathbf{x}}^i$



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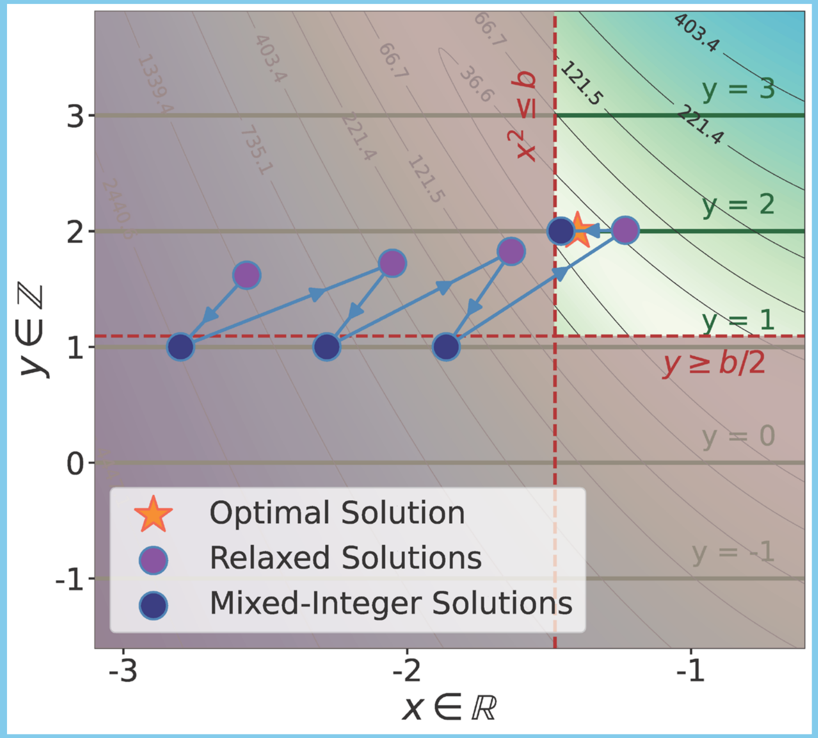
    Update relaxed solution $\bar{\mathbf{x}}^i \leftarrow \bar{\mathbf{x}}^i - \eta \nabla_{\bar{\mathbf{x}}} \mathcal{V}(\hat{\mathbf{x}}^i, \boldsymbol{\xi}^i)$
  end if   (1) Update relaxed solution to reduce violation
end while
Output: a mixed-integer solution $\hat{\mathbf{x}}^i$



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Predict a continuously relaxed solution $\bar{\mathbf{x}}^i \leftarrow \pi_{\Theta_1}(\boldsymbol{\xi}^i)$
while True **do** (2) Differentiable integer correction
  Obtain a mixed-integer solution $\hat{\mathbf{x}}^i \leftarrow \varphi_{\Theta_2}(\bar{\mathbf{x}}^i, \boldsymbol{\xi}^i)$
  Compute feasibility violation $\mathcal{V}(\hat{\mathbf{x}}^i, \boldsymbol{\xi}^i) \leftarrow \|\mathbf{g}(\hat{\mathbf{x}}^i, \boldsymbol{\xi}^i)_+\|_1$
  if $\mathcal{V}(\hat{\mathbf{x}}^i, \boldsymbol{\xi}^i) = 0$ **then**
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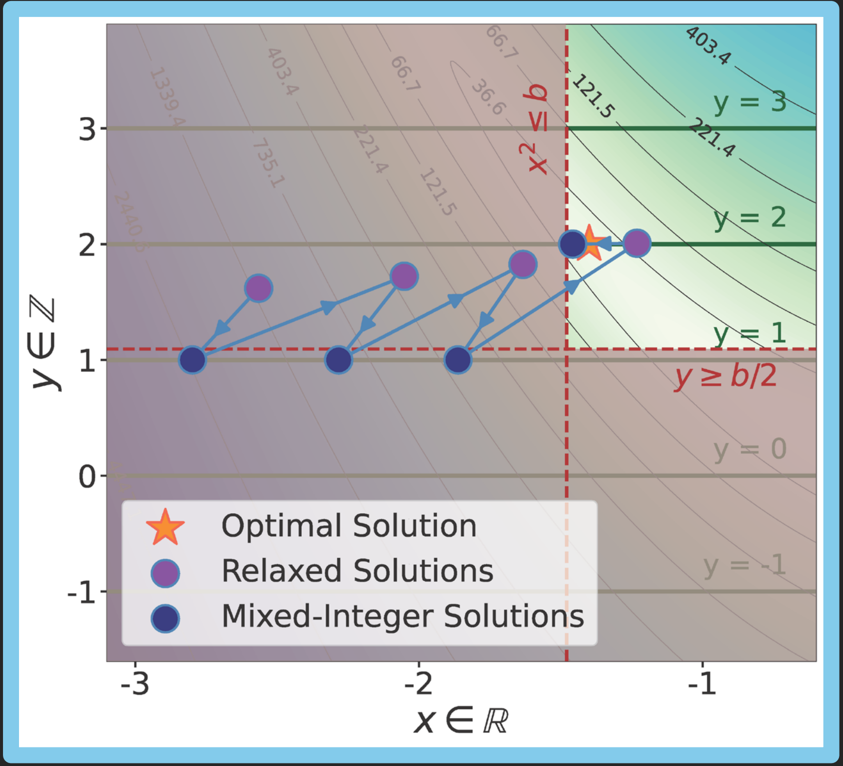
end while
Output: a mixed-integer solution $\hat{\mathbf{x}}^i$



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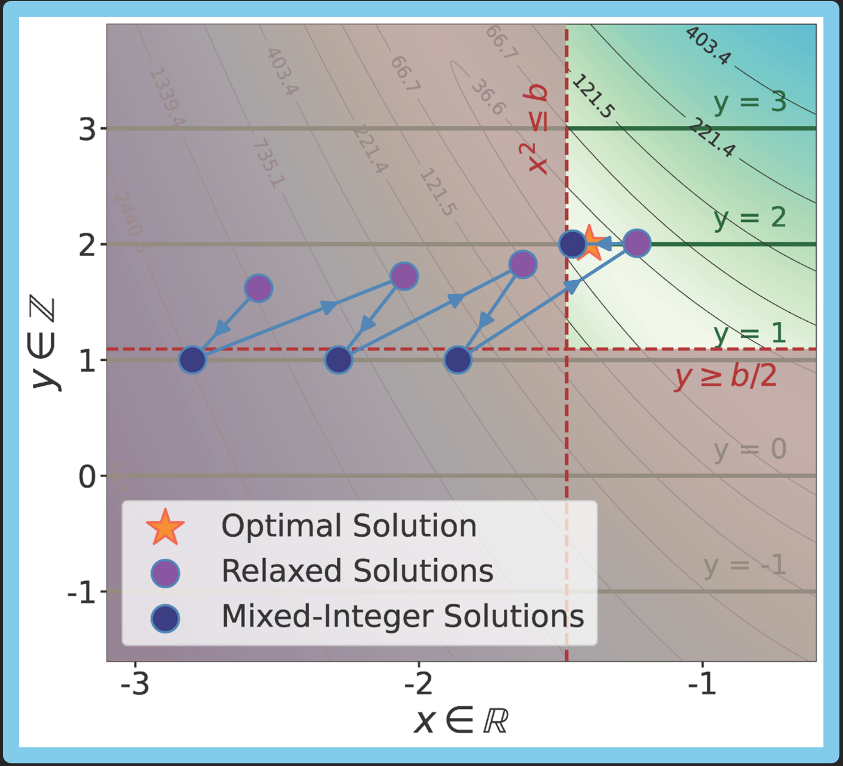
    end if
end while
Output: a mixed-integer solution $\hat{\mathbf{x}}^i$

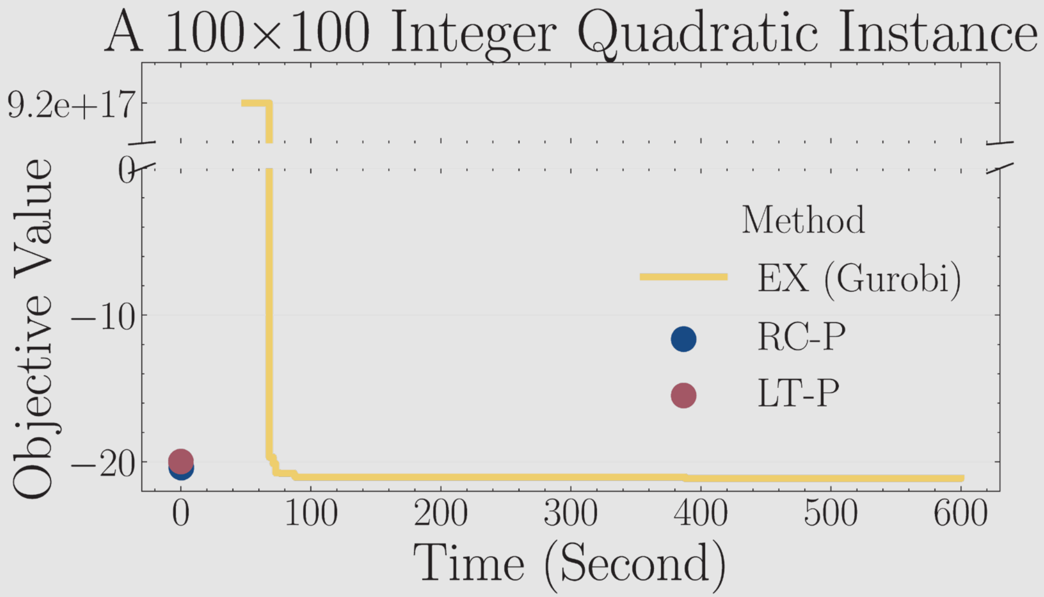
(3) Compute constraint violation based on mixed-integer solution

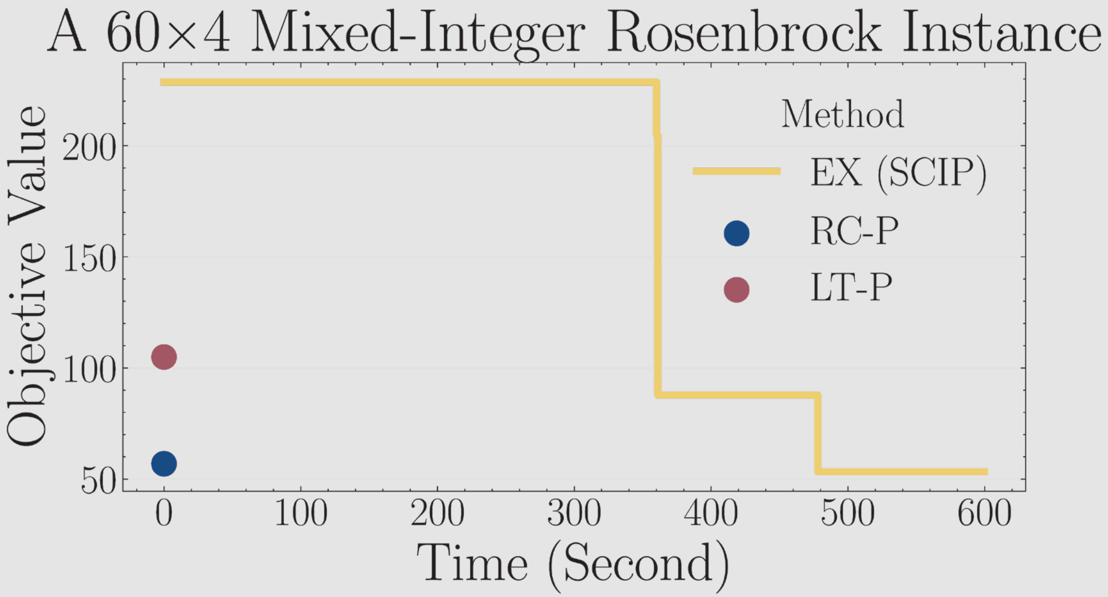


Key Methods in Comparison

Method	Description
EX (Exact Solver)	Solves problems exactly using traditional solver with 1000-sec time-limit as a benchmark.
N1 (Root Node Solution)	Finds the first feasible solution from the root node of the solver, combining various heuristics.
RC (Rounding Classification)	A neural network-based correction layer that learns a classification to determine how to round each integer variable.
LT (Learnable Thresholding)	A neural network-based correction layer that learns a threshold value to decide to round up or down for each integer variable.
RC-P (RC + Feasibility Projection)	RC combined with feasibility projection, which corrects infeasibilities while preserving integer constraints.
LT-P (LT + Feasibility Projection)	LT combined with feasibility projection, which corrects infeasibilities while preserving integer constraints.

Subsecond Solution





Exact solvers such as Gurobi and SCIP find better solutions over time but can be somewhat slow. In contrast, our methods (RC-P & LT-P) achieve high-quality feasible solutions within milliseconds.

More Experiments

Result for IQPs. Each problem size is evaluated on a test set of 100 instance

Method	RC				RC-P				LT			
Metric	Obj Mean	Obj Median	% Feasible	Time (Sec)	Obj Mean	Obj Median	% Feasible	Time (Sec)	Obj Mean	Obj Median	% Feasible	Time (Sec)
100×100	-13.54	-13.6	96%	0.0022	-13.54	-13.57	100%	0.005	-13.65	-13.77	93%	0.0023
200×200	-31.62	-31.71	97%	0.0021	-31.62	-31.71	100%	0.005	-31.34	-31.61	95%	0.0022
500×500	-73.31	-73.38	86%	0.0025	-73.31	-73.38	100%	0.0065	-72.36	-72.48	94%	0.0026
1000×1000	-142.7	-142.7	82%	0.0042	-142.7	-142.7	100%	0.009	-142.6	-142.6	100%	0.0047

Method	LT-P				EX				N1			
Metric	Obj Mean	Obj Median	% Feasible	Time (Sec)	Obj Mean	Obj Median	% Feasible	Time (Sec)	Obj Mean	Obj Median	% Feasible	Time (Sec)
100×100	-13.65	-13.77	100%	0.01	-20.79	-20.78	100%	1237	1.5E+18	1.4E+18	100%	104.2
200×200	-31.34	-31.61	100%	0.0064	-	-	-	-	-	-	-	-
500×500	-72.36	-72.48	100%	0.0063	-	-	-	-	-	-	-	-
1000×1000	-142.6	-142.6	100%	0.0086	-	-	-	-	-	-	-	-

More Experiments

Result for INPs. Each problem size is evaluated on a test set of 100 instance

Method	RC				RC-P				LT			
Metric	Obj Mean	Obj Median	% Feasible	Time (Sec)	Obj Mean	Obj Median	% Feasible	Time (Sec)	Obj Mean	Obj Median	% Feasible	Time (Sec)
100×100	1.664	1.594	100%	0.0022	1.664	1.594	100%	0.0060	0.669	0.649	96%	0.0021
200×200	1.472	1.436	99%	0.0022	1.471	1.436	100%	0.0054	-0.356	-0.373	100%	0.0023
500×500	0.526	0.526	96%	0.0029	0.524	0.526	100%	0.0061	-1.374	-1.594	98%	0.0029
1000×1000	1.423	0.809	97%	0.0040	1.423	0.809	100%	0.0115	-3.744	-3.716	99%	0.0050

Method	LT-P				EX				N1			
Metric	Obj Mean	Obj Median	% Feasible	Time (Sec)	Obj Mean	Obj Median	% Feasible	Time (Sec)	Obj Mean	Obj Median	% Feasible	Time (Sec)
100×100	0.669	0.649	100%	0.0058	256.93	134.62	14%	1001	4411	155.2	14%	940.4
200×200	-0.356	-0.373	100%	0.0056	-	-	-	-	-	-	-	-
500×500	-1.374	-1.594	100%	0.0072	-	-	-	-	-	-	-	-
1000×1000	-3.744	-3.716	100%	0.0117	-	-	-	-	-	-	-	-

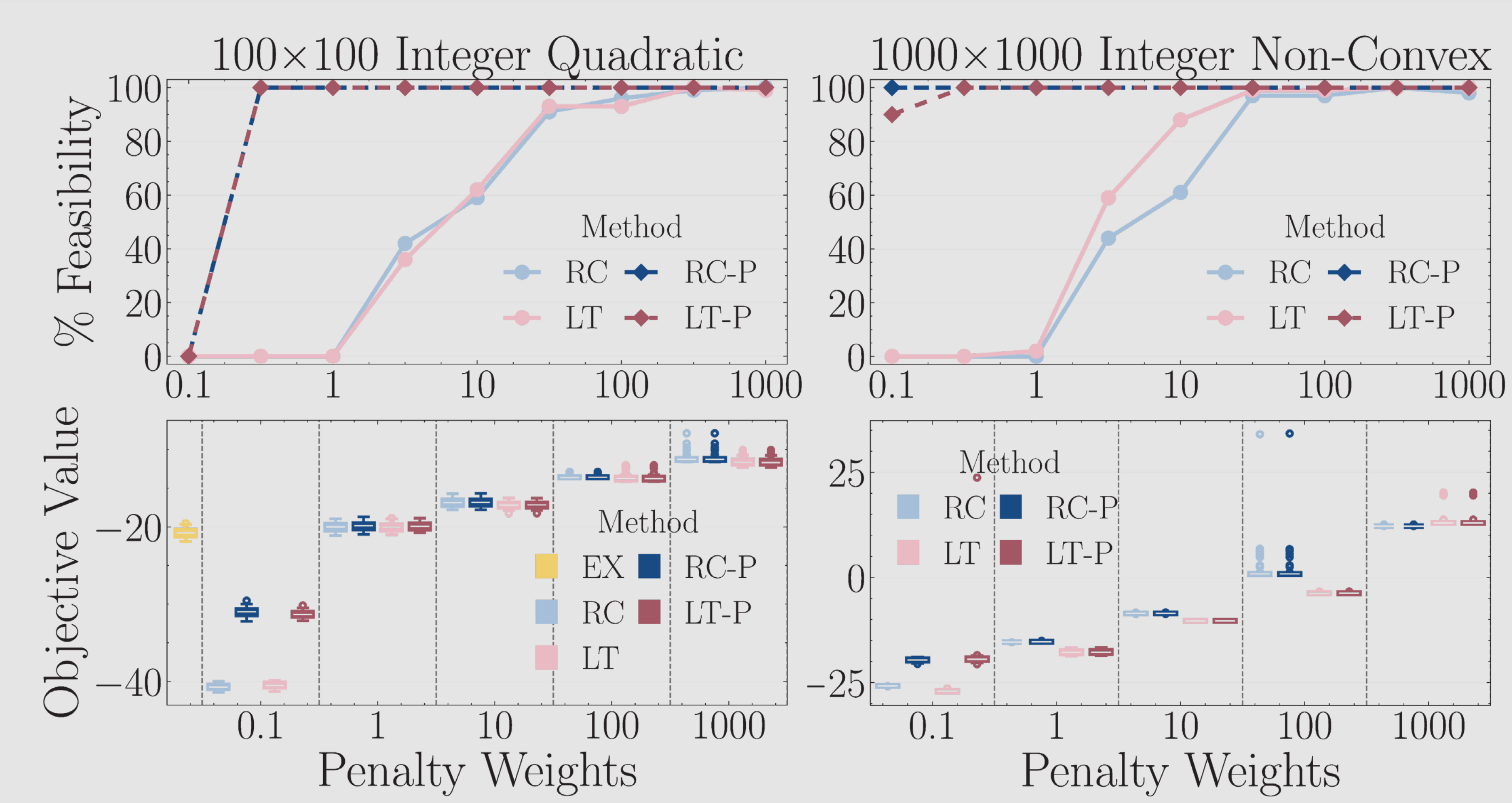
More Experiments

Result for MIRBs. Each problem size is evaluated on a test set of 100 instance

Method	RC				RC-P				LT			
Metric	Obj Mean	Obj Median	% Feasible	Time (Sec)	Obj Mean	Obj Median	% Feasible	Time (Sec)	Obj Mean	Obj Median	% Feasible	Time (Sec)
20×4	59.39	48.86	100%	0.0019	59.39	48.86	100%	0.0048	62.51	63.40	100%	0.0020
200×4	503.5	461.7	99%	0.0021	504.2	461.7	100%	0.0052	622.8	626.0	100%	0.0026
2000×4	5938	5792	99%	0.0033	5942	5792	100%	0.0070	5612	5558	97%	0.0030
20000×4	6.7E+4	6.7E+4	76%	0.0121	9.8E+4	7.3E+4	100%	0.0824	4.8E+4	3.5E+4	66%	0.0127

Method	LT-P				EX				N1			
Metric	Obj Mean	Obj Median	% Feasible	Time (Sec)	Obj Mean	Obj Median	% Feasible	Time (Sec)	Obj Mean	Obj Median	% Feasible	Time (Sec)
20×4	62.51	63.40	100%	0.0055	64.67	59.16	100%	1005	87.83	77.34	100%	0.0813
200×4	622.8	626.0	100%	0.0062	8.4E+5	908.8	100%	1002	3.7E+8	957.4	100%	0.2608
2000×4	5615	5558	100%	0.0071	4.7E+10	9262	96%	1002	8.3E+12	9379	95%	71.91
20000×4	8.0E+4	4.5E+4	100%	0.0639	1.1E+15	1.0E5	78%	1040	1.2E+15	1.0E5	78%	78[illegible]

Effect of Penalty Weight



There is an inherent trade-off between achieving more feasible solutions and lower objective values prior to the integer feasibility projection (RC and LT).

After applying the integer feasibility projection (RC-P and LT-P), the high infeasibility rates observed even with smaller penalty weights.

Thank You

Paper

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