

► L2O-MINLP

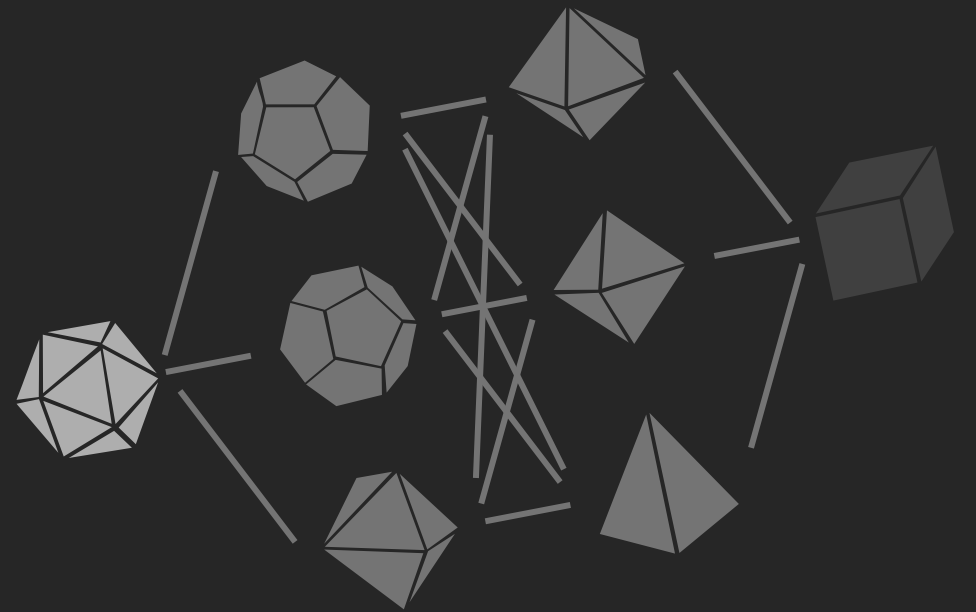
Learning to Optimize for
Mixed-Integer Non-Linear Programming



Mechanical & Industrial Engineering
UNIVERSITY OF TORONTO



Pacific Northwest
NATIONAL LABORATORY



Presented by Bo Tang
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Supply Chains

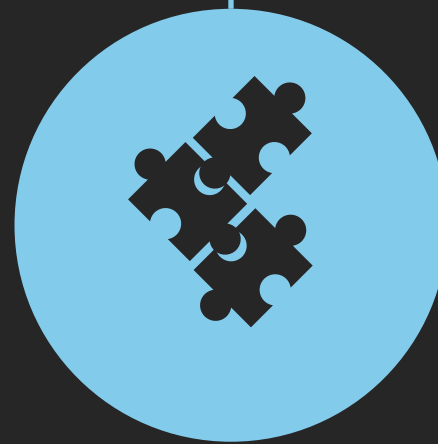


Ján Drgoňa

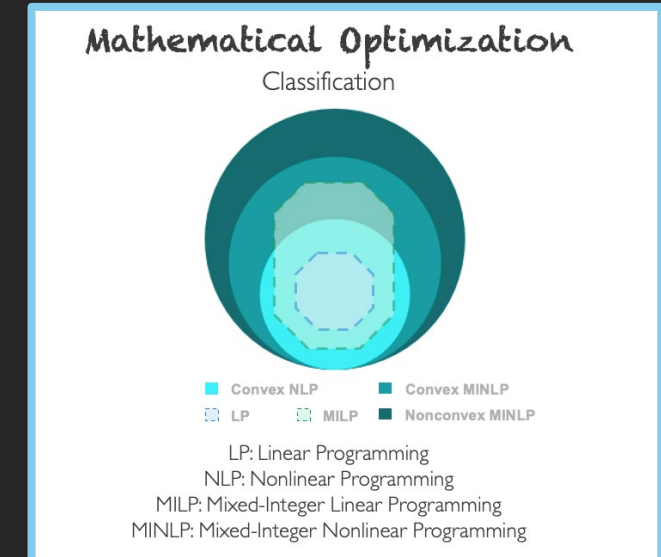
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Motivation

Why does MINLP matter?



MINLP is general but very hard:
Combinatorial Complexity + Non-Convexity.



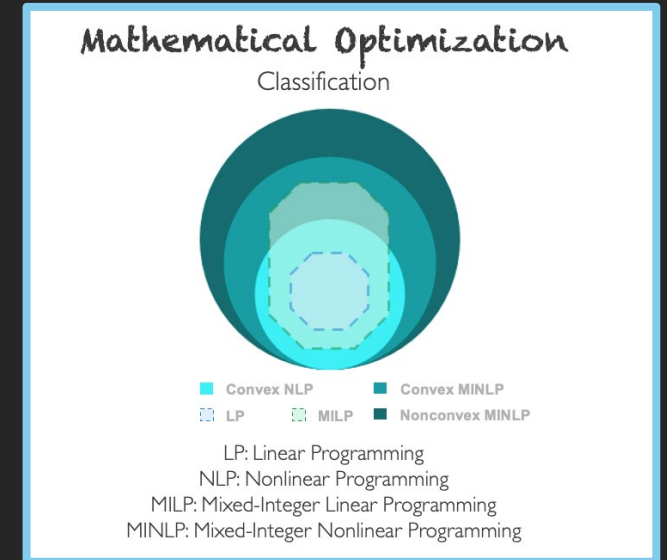
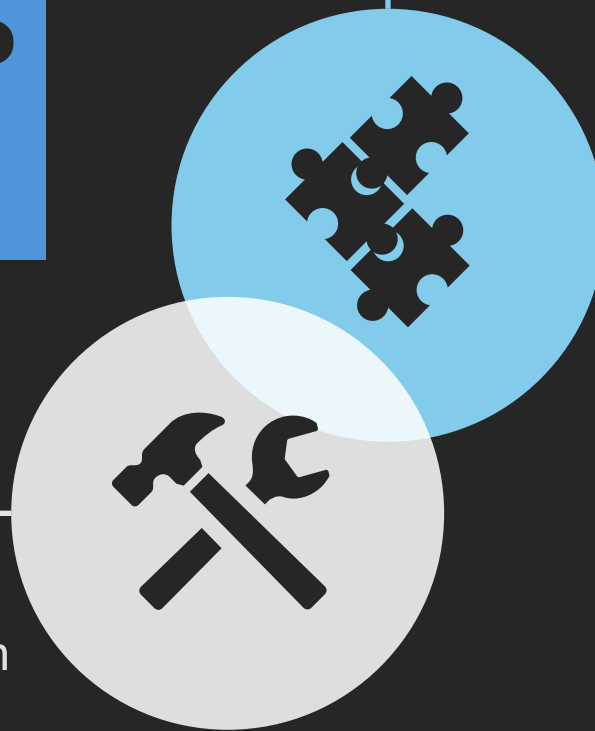
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Solvers are limited:

Traditional solvers struggle with large-scale MINLP problems.



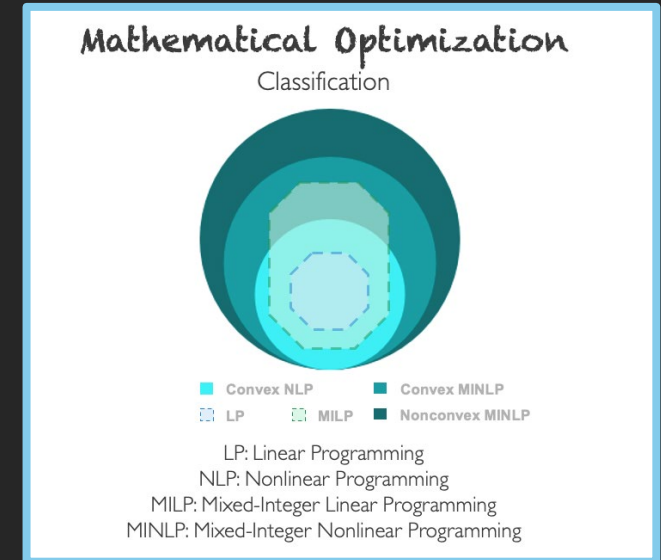
GUROBI
OPTIMIZATION



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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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Introduction to L2O

01 What is L2O?

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

L2O enables high-quality solutions with significantly reduced computational cost.

02 Why do we use L2O?

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!

03 How does L2O work?

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:

$$\min_x f(x)$$

$$\text{s. t. } g(x) \leq 0$$

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

Problem Formulation

Parametric MINLP Formulation:

$$\begin{aligned} \min_x \quad & f(x, \xi) \\ \text{s. t.} \quad & g(x, \xi) \leq 0 \\ & x \in \mathbb{R}^{n_r} \times \mathbb{Z}^{n_z} \\ & \xi \in \Xi \end{aligned}$$

Parameters ξ influence the objective and constraints of optimization problems.

$$\begin{array}{l} \text{Multiple} \\ \text{Instances} \end{array} \left\{ \begin{array}{l} \xi_1 \rightarrow x_1^* \\ \xi_2 \rightarrow x_2^* \\ \vdots \\ \xi_m \rightarrow x_m^* \end{array} \right.$$

Problem Formulation

Prediction for Parametric MINLP Formulation:

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

Expected objective function:

$$\text{s. t. } g(\hat{\mathbf{x}}_i, \xi_i) \leq 0$$

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

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

$$\xi_i \in \Xi$$

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

Solution prediction

$$\hat{\mathbf{x}}_i = \psi_{\Theta}(\xi_i)$$

Problem Formulation

Prediction for Parametric MINLP Formulation:

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

Minimize expected objective function:

IT SEEMS IDEAL:

What Prevents L2O from Extending to this MINLP?

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

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

$$\xi \in \Xi$$

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

Solution prediction

$$\hat{\mathbf{x}} = \psi_{\theta}(\xi)$$

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

01 Collecting Solutions as Training Label is Very Expensive



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

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Limitations of Existing L2O

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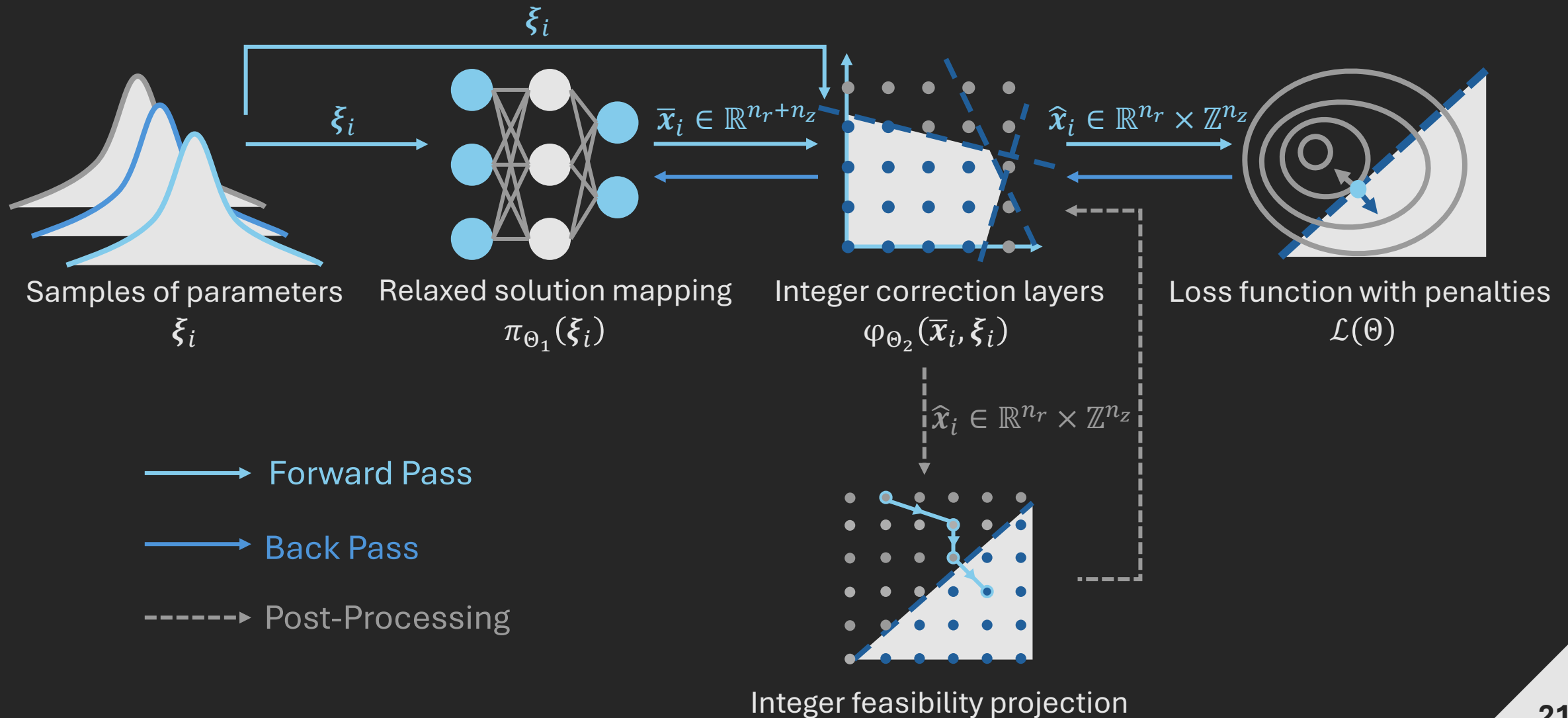
Our Solution: We introduce Integer Correction Layers to ensure integer feasibility.

03 It is Difficult to Ensure Feasibility, Especially in Integers

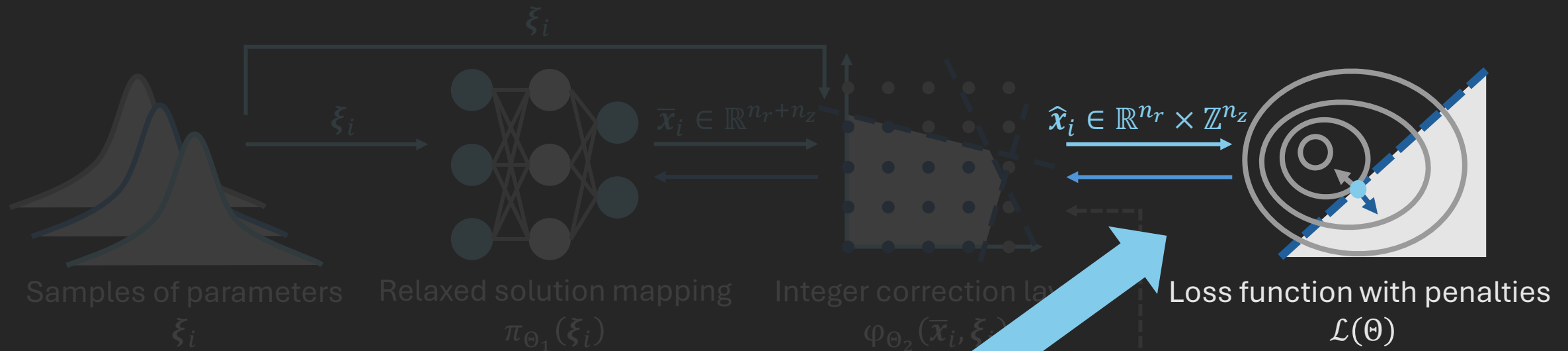


Our Solution: We introduce a gradient-based Feasibility Projection to adjust integer solutions.

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.

→ Forward

→ Backward

-----> Post-Processing

Integer feasibility projection

Loss Function

Loss Function with Penalty

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

Loss Function

Loss Function with Penalty

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

Loss Function

Loss Function with Penalty

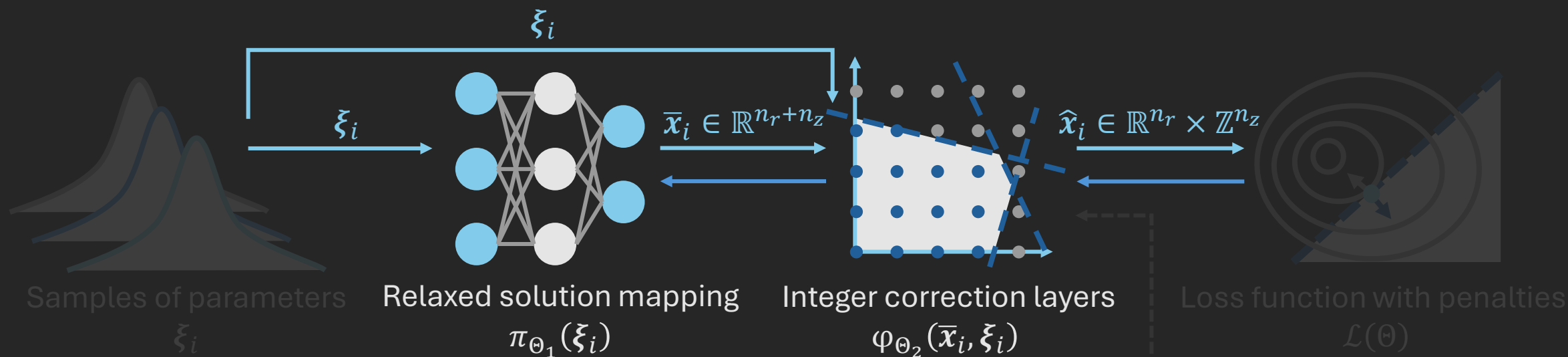
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Loss Function

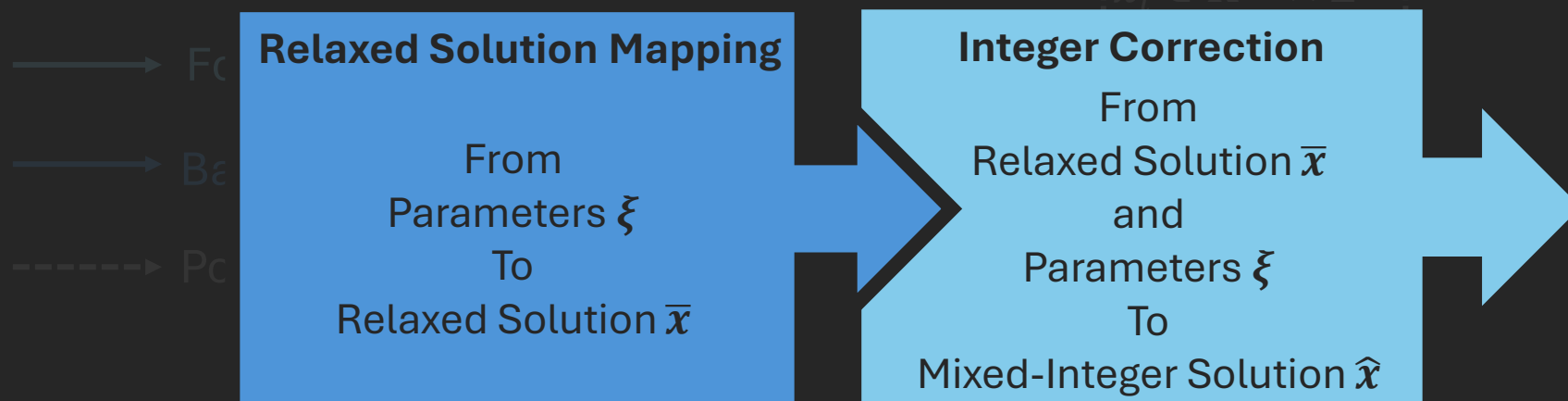
Loss Function with Penalty

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

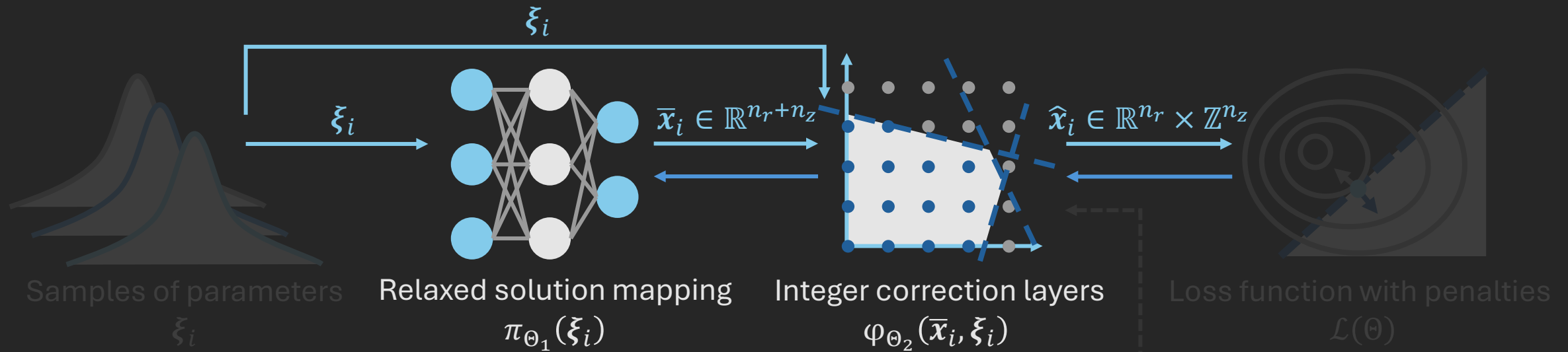
Integer Correction Layers



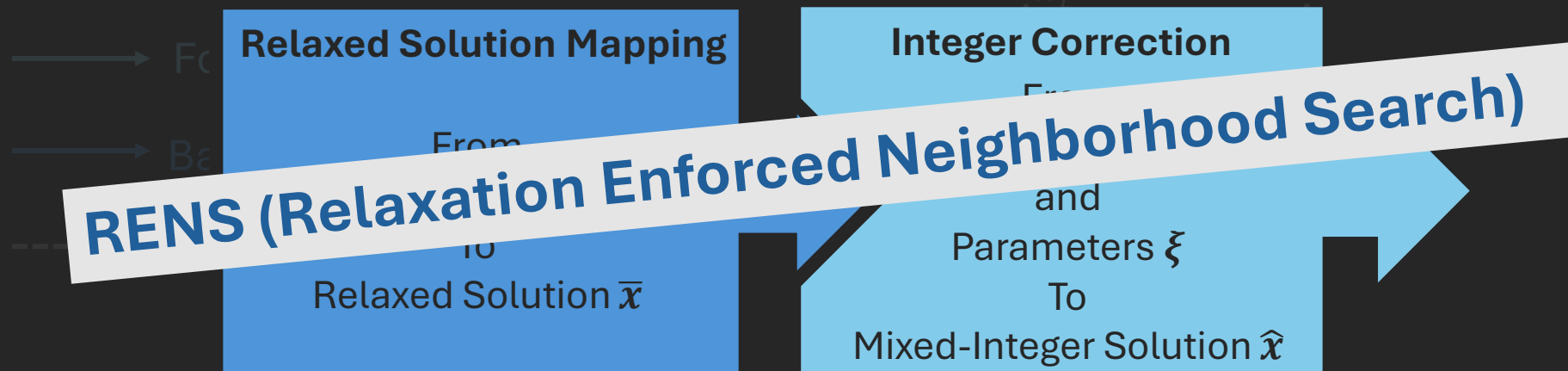
Bi-Level Neural Network Architecture



Integer Correction Layers

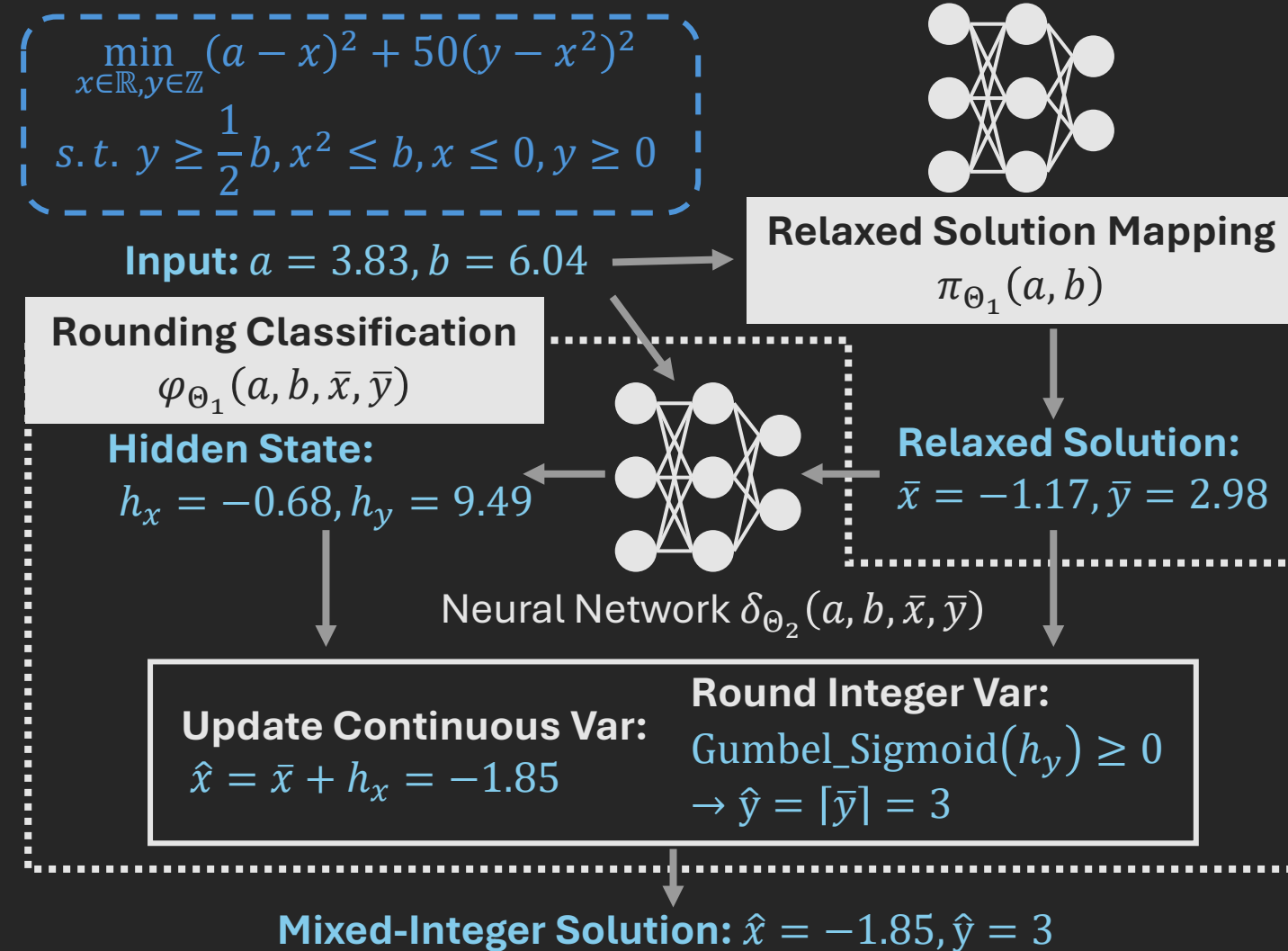


Bi-Level Neural Network Architecture



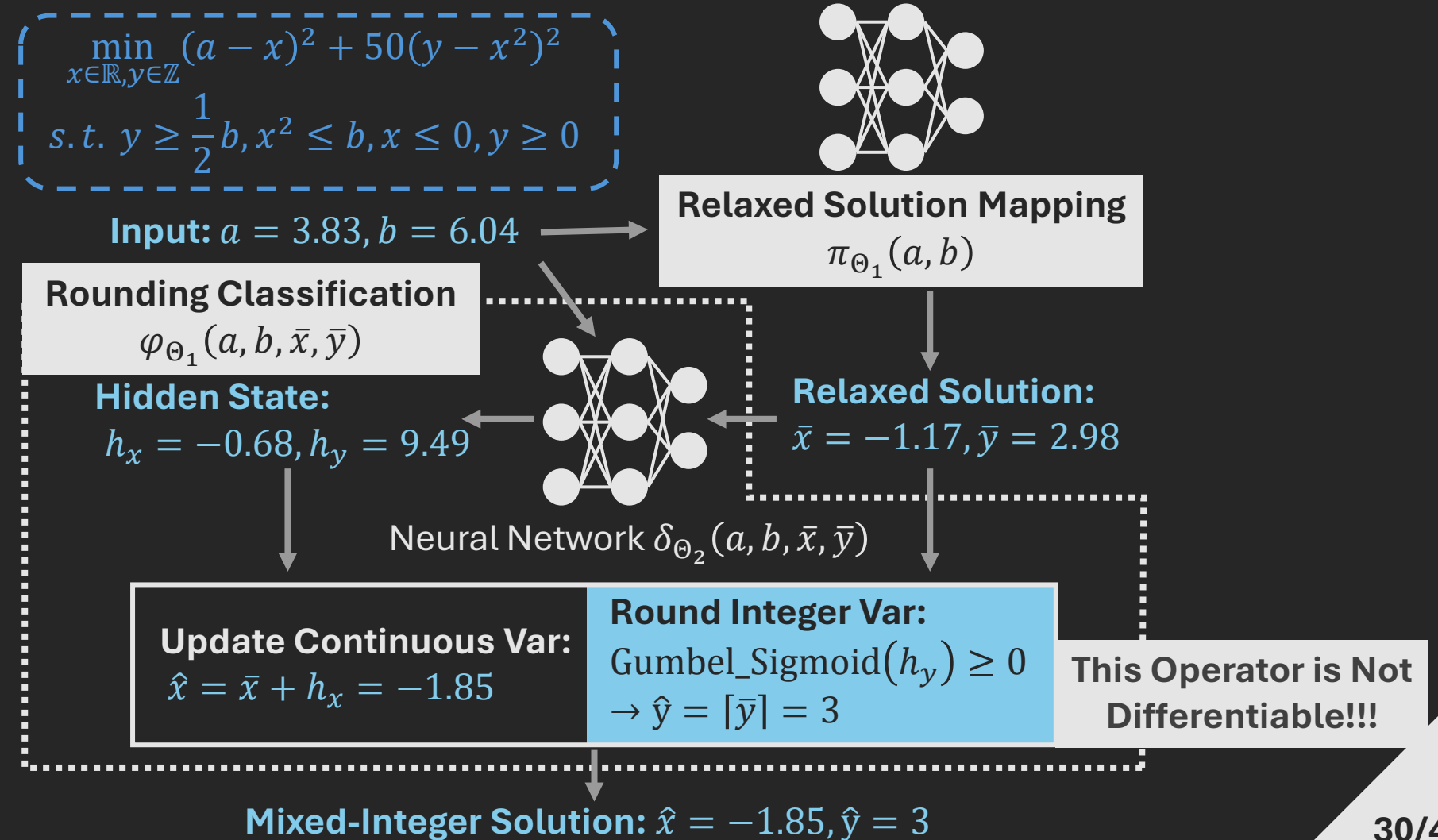
Integer Correction Layers

Example



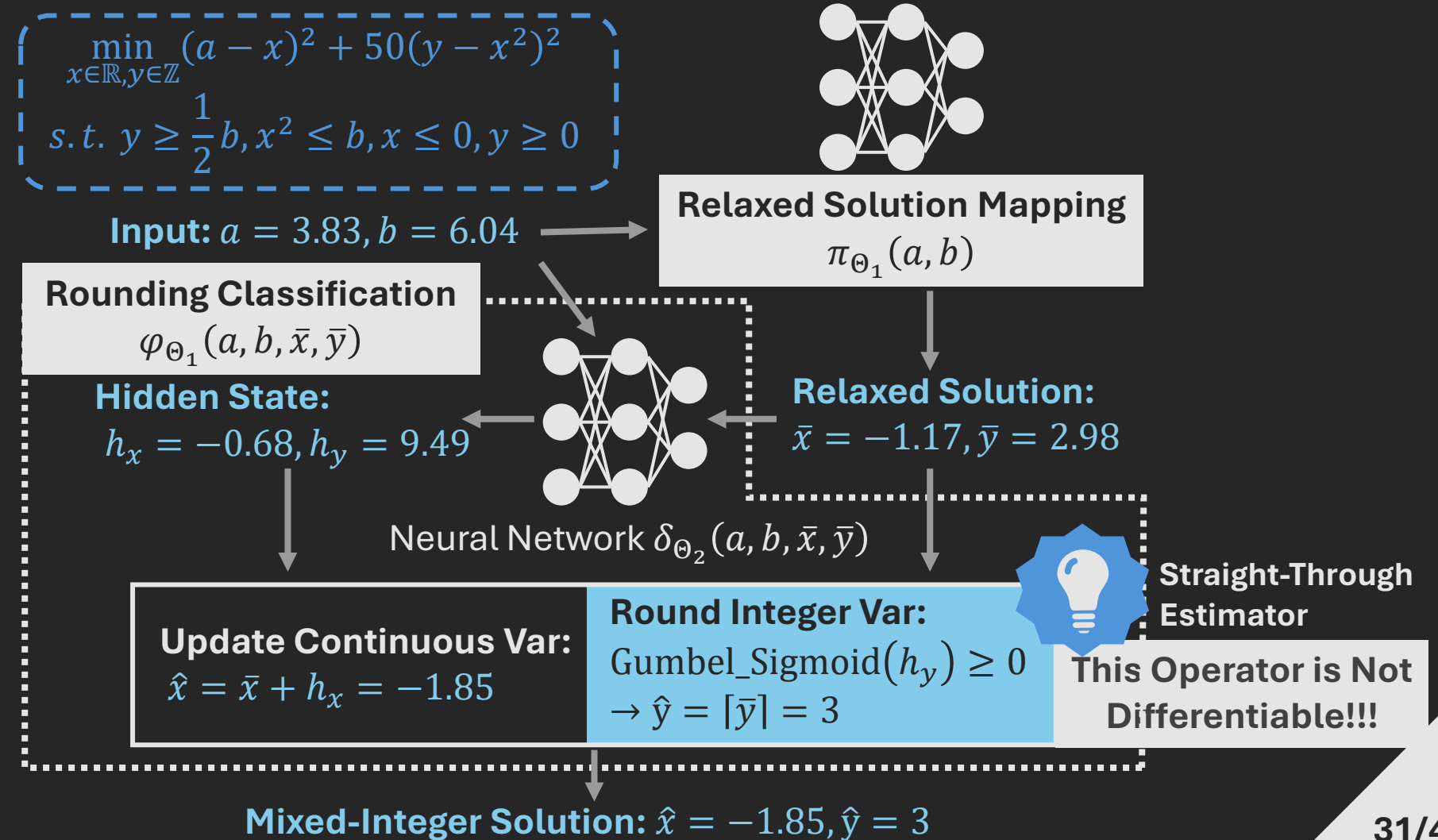
Integer Correction Layers

Example



Integer Correction Layers

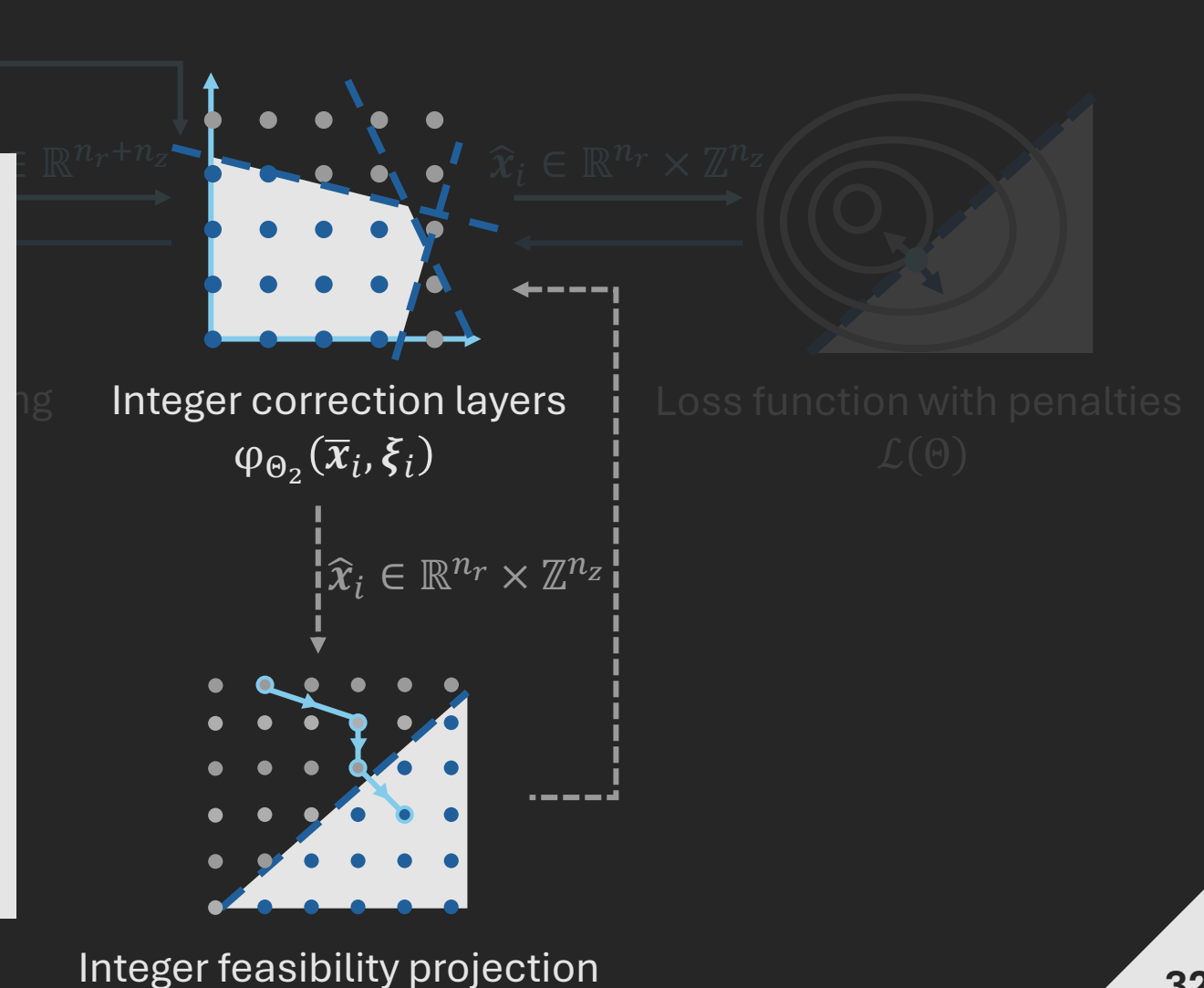
Example



Integer Feasibility Projection

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

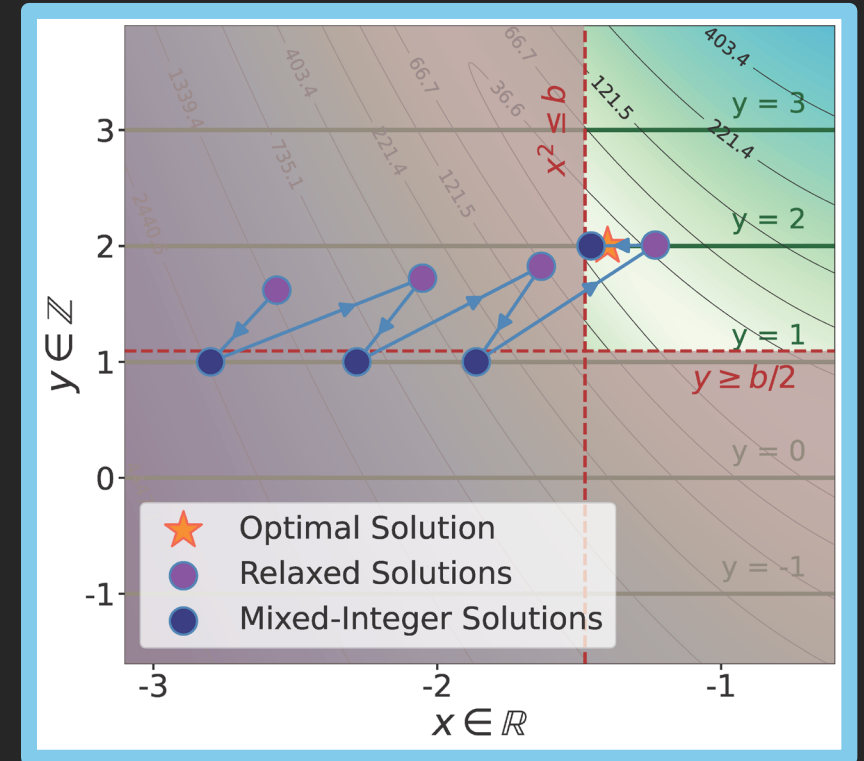
- **Computational Efficiency:** Avoids the need for repeated projections and second-order gradient computation during training.
- **Stable Training:** Keeps projection separate from training, preventing interference with the output of model.



Integer Feasibility Projection

Algorithm 2 Integer Feasibility Projection: Inference

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



Algorithm 2 Integer Feasibility Projection: Inference

```

1: Input: parameters  $\xi^i$ , layers  $\pi_{\Theta_1}(\cdot)$  and  $\varphi_{\Theta_2}(\cdot)$ , step size  $\eta$ 
2: Predict a continuously relaxed solution  $\bar{\mathbf{x}}^i \leftarrow \pi_{\Theta_1}(\xi^i)$ 
3: while True do    (1) Start from a relaxed solution
4:     Obtain a mixed-integer solution  $\hat{\mathbf{x}}^i \leftarrow \varphi_{\Theta_2}(\bar{\mathbf{x}}^i, \xi^i)$ 
5:     Compute feasibility violation  $\mathcal{V}(\hat{\mathbf{x}}^i, \xi^i) \leftarrow \|\mathbf{g}(\hat{\mathbf{x}}^i, \xi^i)_+\|_1$ 
6:     if  $\mathcal{V}(\hat{\mathbf{x}}^i, \xi^i) = 0$  then
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10:    end if
11: end while
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```



Algorithm 2 Integer Feasibility Projection: Inference

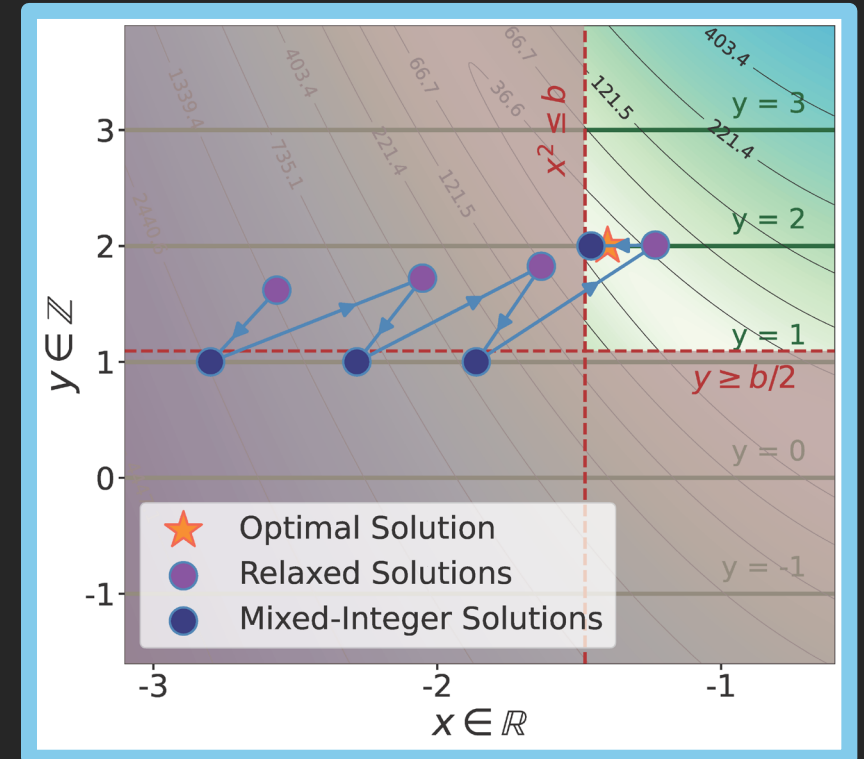
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- 2: Predict a continuously relaxed solution $\bar{\mathbf{x}}^i \leftarrow \pi_{\Theta_1}(\xi^i)$
- 3: **while** True **do** (2) Differentiable integer correction
- 4: **Obtain a mixed-integer solution** $\hat{\mathbf{x}}^i \leftarrow \varphi_{\Theta_2}(\bar{\mathbf{x}}^i, \xi^i)$
- 5: Compute feasibility violation $\mathcal{V}(\hat{\mathbf{x}}^i, \xi^i) \leftarrow \|\mathbf{g}(\hat{\mathbf{x}}^i, \xi^i)_+\|_1$
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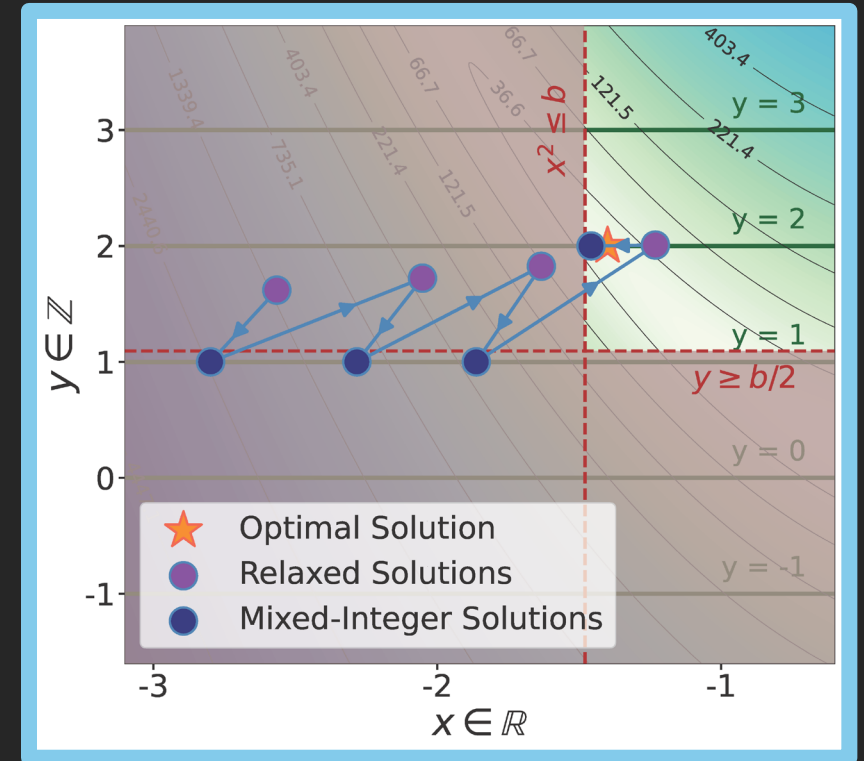
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- 5: **Compute** feasibility violation $\mathcal{V}(\hat{\mathbf{x}}^i, \xi^i) \leftarrow \|\mathbf{g}(\hat{\mathbf{x}}^i, \xi^i)_+\|_1$
- 6: **if** $\mathcal{V}(\hat{\mathbf{x}}^i, \xi^i) = 0$ **then** (3) **Compute** constraint violation
 Break based on mixed-integer solution
- 8: **else**
- 9: Update relaxed solution $\bar{\mathbf{x}}^i \leftarrow \bar{\mathbf{x}}^i - \eta \nabla_{\bar{\mathbf{x}}} \mathcal{V}(\hat{\mathbf{x}}^i, \xi^i)$
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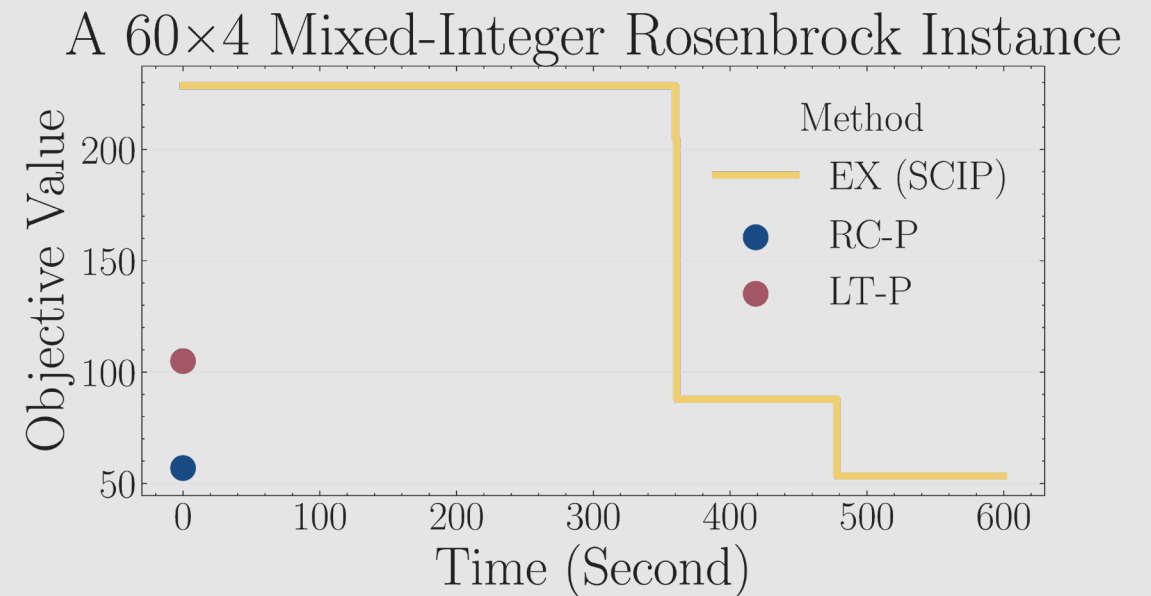
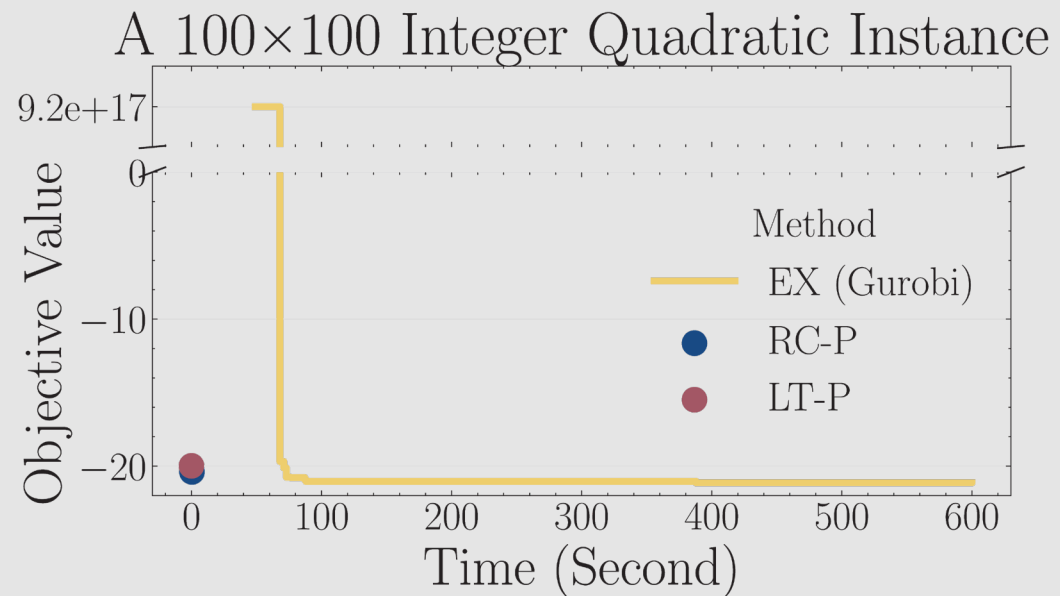
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- 10: **end if** (4) Update relaxed solution to reduce violation
- 11: **end while**
- 12: **Output:** a mixed-integer solution $\hat{\mathbf{x}}^i$



Key Methods in Comparison

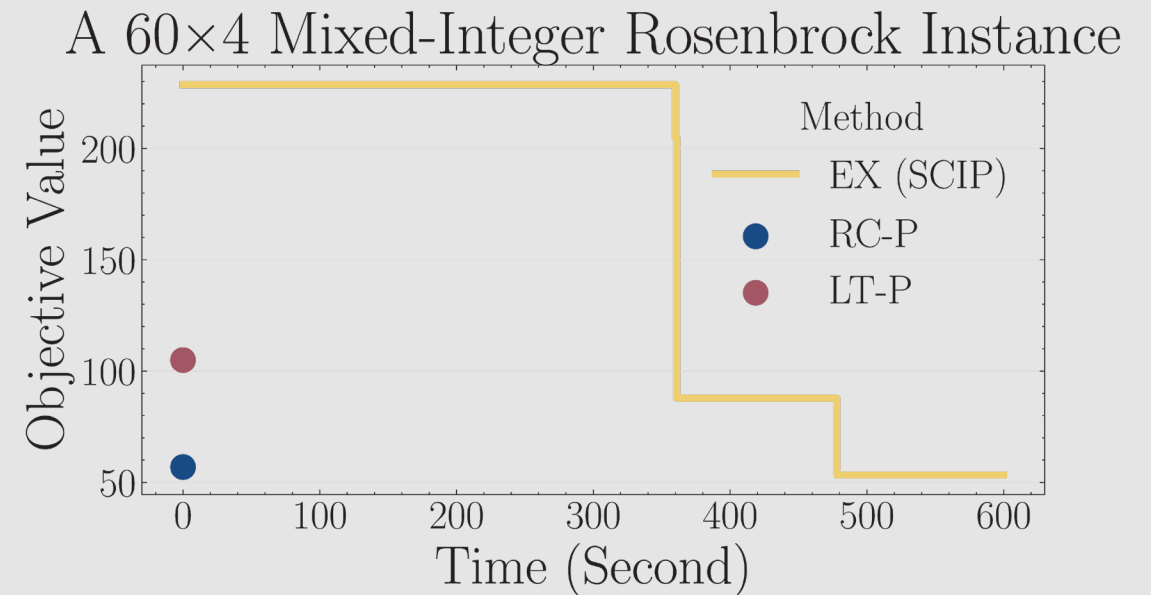
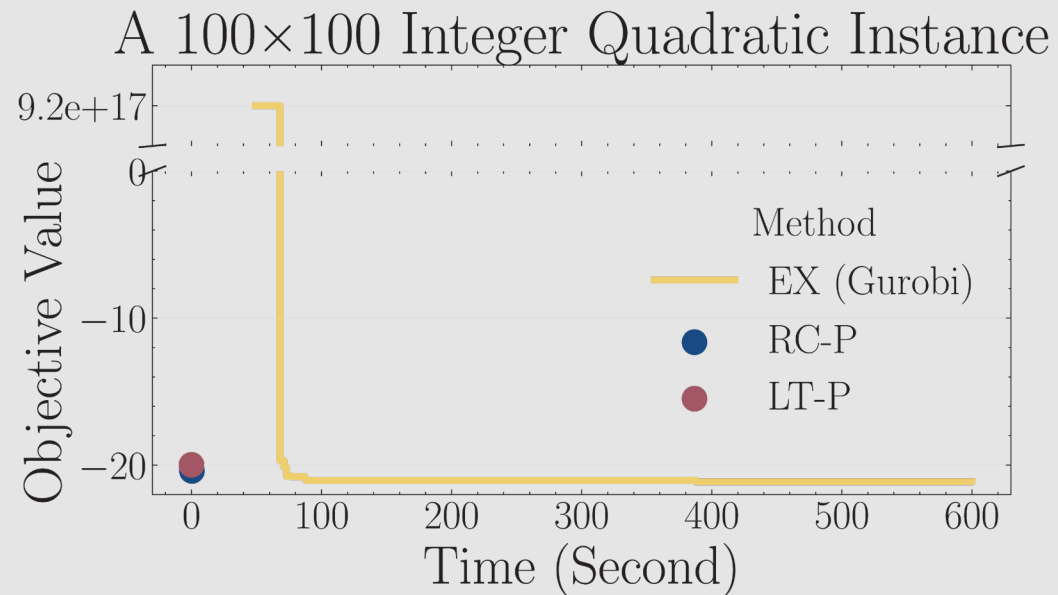
Method	Description
EX (Exact Solver)	Solves problems exactly using traditional solver with 1000-sec time-limit as a benchmark.
N1 (Root Node Solution)	Finds the first feasible solution from the root node of the solver, combining various heuristics.
RC (Rounding Classification)	A neural network-based 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.

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.

Training time is about 100 second!

More Experiments

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

Method	RC				RC-P				LT			
	Obj	Obj	%	Time	Obj	Obj	%	Time	Obj	Obj	%	Time
Metric	Mean	Median	Feasible	(Sec)	Mean	Median	Feasible	(Sec)	Mean	Median	Feasible	(Sec)
100×100	-13.54	-13.6	96%	0.0022	-13.54	-13.57	100%	0.0050	-13.65	-13.77	93%	0.0023
200×200	-31.62	-31.71	97%	0.0021	-31.62	-31.71	100%	0.0050	-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			
	Obj	Obj	%	Time	Obj	Obj	%	Time	Obj	Obj	%	Time
Metric	Mean	Median	Feasible	(Sec)	Mean	Median	Feasible	(Sec)	Mean	Median	Feasible	(Sec)
100×100	-13.65	-13.77	100%	0.0100	-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

**Gurobi
Fails to
Find a
Solution!**

Result for IQPs. Each method evaluated on a test set of 100 instance

Method	RC				RC-P				LT			
	Obj	Obj	%	Time	Obj	Obj	%	Time	Obj	Obj	%	Time
Metric	Mean	Median	Feasible	(Sec)	Mean	Median	Feasible	(Sec)	Mean	Median	Feasible	(Sec)
100×100	-13.54	-13.6	96%	0.0022	-13.54	-13.57	100%	0.0050	-13.65	-13.77	93%	0.0023
200×200	-31.62	-31.71	97%	0.0021	-31.62	-31.71	100%	0.0050	-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			
	Obj	Obj	%	Time	Obj	Obj	%	Time	Obj	Obj	%	Time
Metric	Mean	Median	Feasible	(Sec)	Mean	Median	Feasible	(Sec)	Mean	Median	Feasible	(Sec)
100×100	-13.65	-13.77	100%	0.0100	-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

**Milliseconds
Inference
(with 100sec
Training)**

Result for IQPs. Each method evaluated on a test set of 100 instance

Method	RC				RC-P				LT			
	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%	0.0050	-13.65	-13.77	93%	0.0023
200×200	-31.62	-31.71	97%	0.0021	-31.62	-31.71	100%	0.0050	-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%	0.0090	-142.6	-142.6	100%	0.0047
Method	LT-P				EX				N1			
	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%	0.0100	-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

**100%
Feasibility
With
Projection**

Result for IQPs. Each method was evaluated on a test set of 100 instance

Method	RC				RC-P				LT			
	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%	0.0050	-13.65	-13.77	93%	0.0023
200×200	-31.62	-31.71	97%	0.0021	-31.62	-31.71	100%	0.0050	-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%	0.0090	-142.6	-142.6	100%	0.0047
Method	LT-P				EX				N1			
	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%	0.0100	-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

We can
even
achieve
better!

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

Method	RC				RC-P				LT			
	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%	0.0050	-13.65	-13.77	93%	0.0023
200×200	-31.62	-31.71	97%	0.0021	-31.62	-31.71	100%	0.0050	-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			
	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%	0.0100	-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

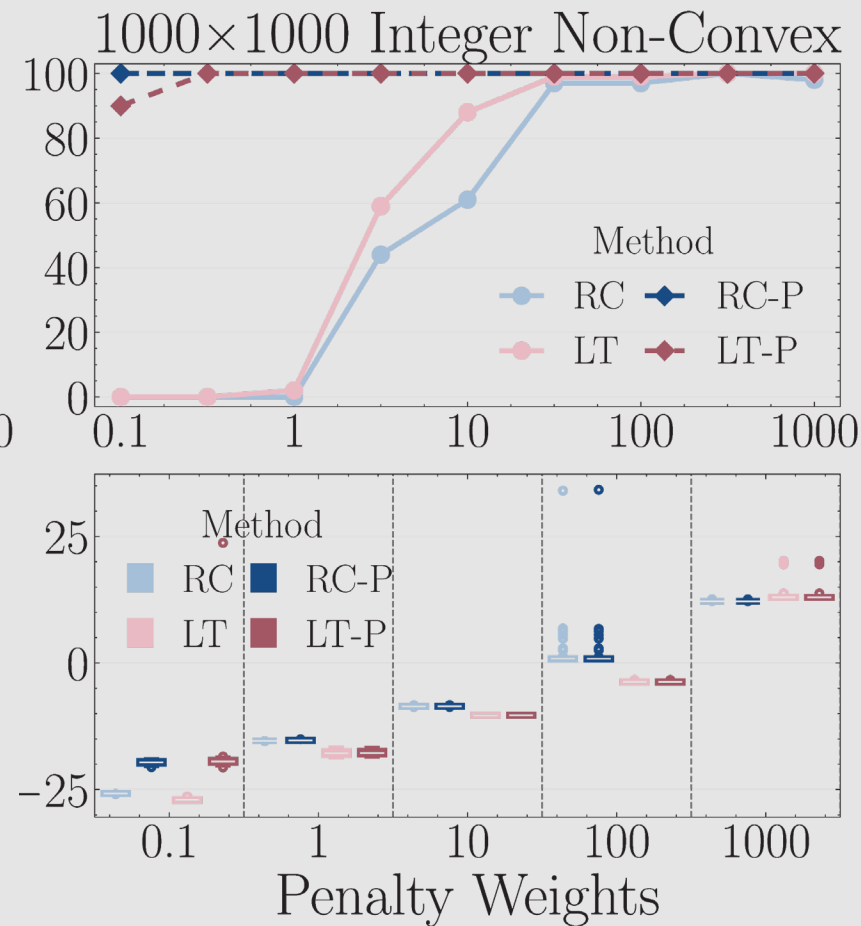
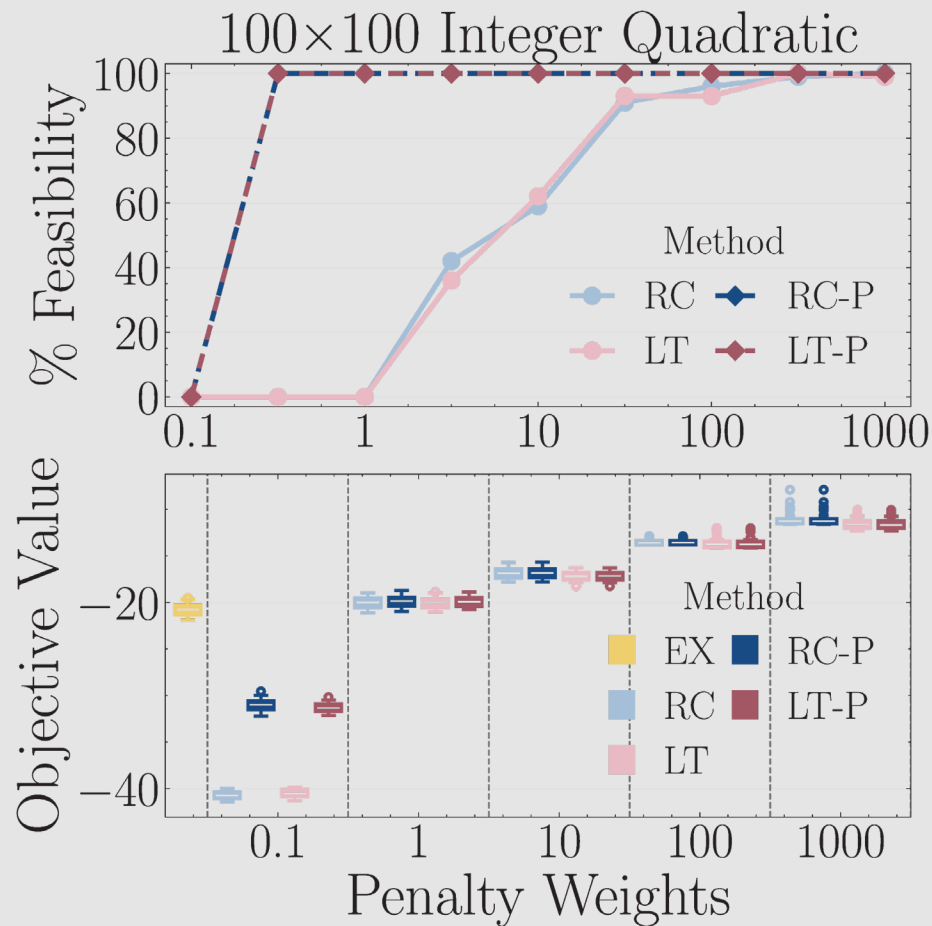
Method	RC				RC-P				LT			
	Obj	Obj	%	Time	Obj	Obj	%	Time	Obj	Obj	%	Time
Metric	Mean	Median	Feasible	(Sec)	Mean	Median	Feasible	(Sec)	Mean	Median	Feasible	(Sec)
100×100	1.664	1.594	100%	0.0022	1.664	1.594	100%	0.0060	0.669	0.649	96%	0.0021
200×200	1.472	1.436	99%	0.0022	1.471	1.436	100%	0.0054	-0.356	-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			
	Obj	Obj	%	Time	Obj	Obj	%	Time	Obj	Obj	%	Time
Metric	Mean	Median	Feasible	(Sec)	Mean	Median	Feasible	(Sec)	Mean	Median	Feasible	(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			
	Obj	Obj	%	Time	Obj	Obj	%	Time	Obj	Obj	%	Time
Metric	Mean	Median	Feasible	(Sec)	Mean	Median	Feasible	(Sec)	Mean	Median	Feasible	(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			
	Obj	Obj	%	Time	Obj	Obj	%	Time	Obj	Obj	%	Time
Metric	Mean	Median	Feasible	(Sec)	Mean	Median	Feasible	(Sec)	Mean	Median	Feasible	(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%	782

Effect of Penalty Weight

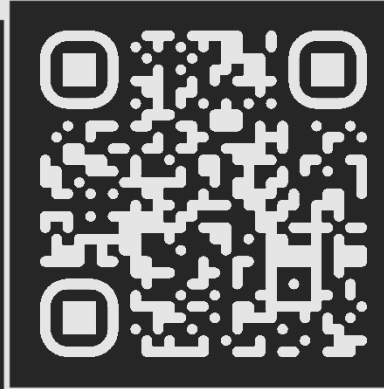


There is an inherent trade-off between achieving more feasible solutions and lower objective values prior to the integer feasibility projection (RC and LT).

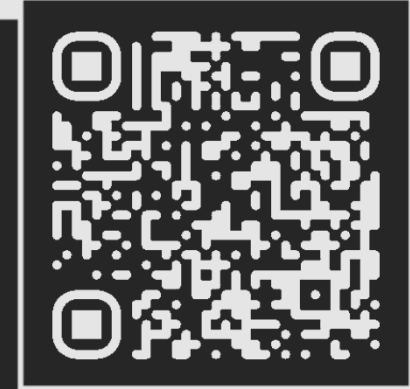
After applying the integer feasibility projection (RC-P and LT-P), the high infeasibility rates observed even with smaller penalty weights.

Thank You

Paper



GitHub



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