Machine Learning-guided optimization of energy systems

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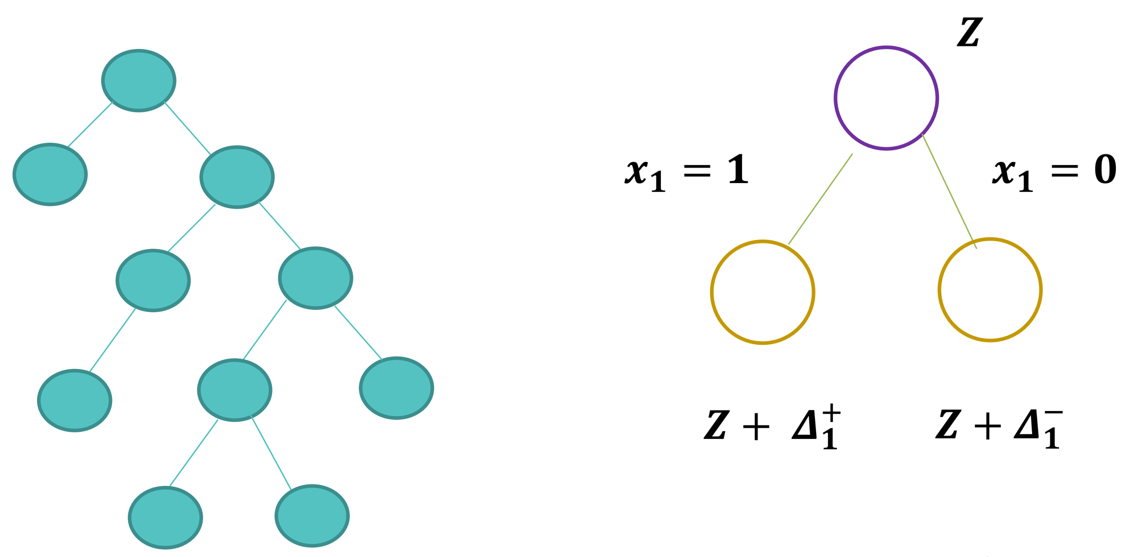
Motivation: Speed up a MIP Solver

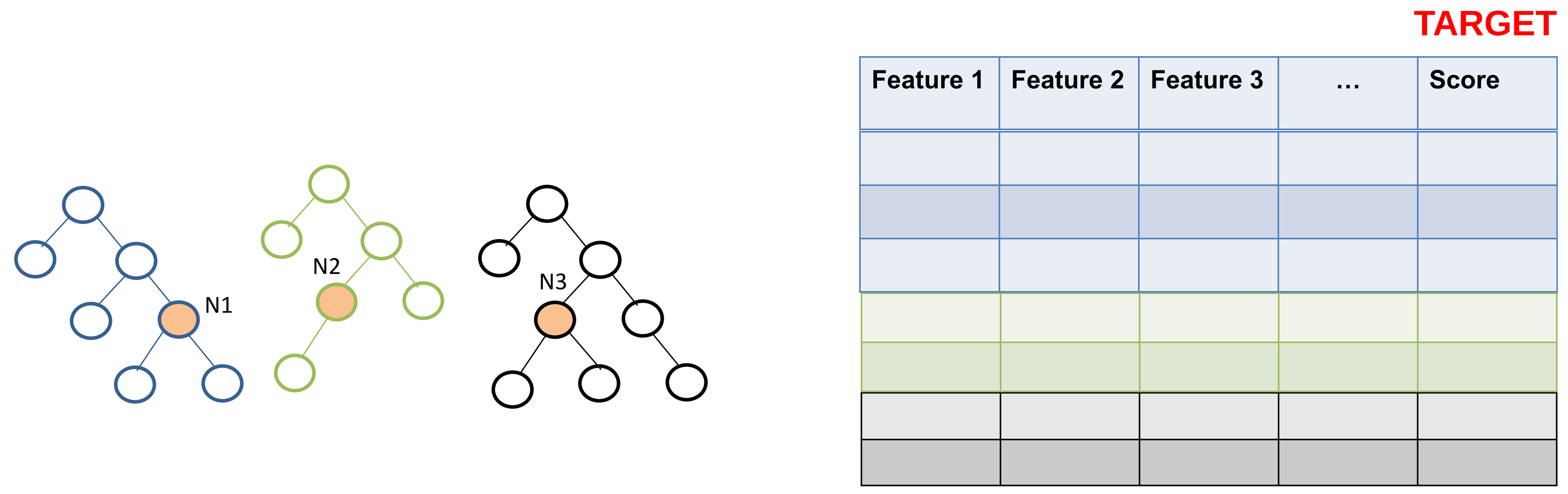
- Energy systems optimization requires the solution of challenging mixed-integer linear and mixed-integer nonlinear optimization problems (MIPs and MINLPs)
- MIPs and MINLPs are solved by branch-and-bound algorithms that involve a number of heuristics in their branching step
- This research aims to develop ML-guided branching algorithms and demonstrate them in energy systems optimization

Machine Learning Task



$$\text{score}_1 = f(\Delta_1^+, \Delta_1^-)$$

- Given a large set of measurements of branching scores collected by solving many instances of a problem type, learn a function to predict **strong branching scores** so that strong branching can be applied to other instances without having to solve strong branching LPs
- Regression problem: Predict (normalized) strong branching scores



- Score ≈ β_1 Solution value + β_2 Objective coefficient + β_3 Number of rows the variable is in + …
- Past work: Neural networks, tree-based ensemble methods
- This work: Sparse models based on the LASSO, L0L1, and L0L2
- Problems: Set covering, combinatorial auctions, facility location

Features

- Each branching candidate at a node in the search tree has a set of features:
  1. Aggregated Graph Neural Network features (Gasse et al., 2019)
  2. Khalil et al., 2016 features
- Ecole library (Prouvost et al., 2020) is used for extracting features
- This work uses quadratic transformations of features

Sparse Regression

- Sparse models are solutions to

$$\hat{\beta} \in \underset{\beta \in \mathbb{R}^p}{\arg\min} \; \frac{1}{2}\|y - X\beta\|_2^2 + \lambda_0\|\beta\|_0 + \lambda_q\|\beta\|_q^q$$

- Penalizing number of nonzero coefficients and the norm of the solution vector
- The LASSO $\quad \lambda_0 = 0, \lambda_1 > 0 \quad$ using *glmnet* package (Friedman et al., 2010)
- L0L1 model $\quad \lambda_0 > 0, \lambda_1 > 0 \quad$ using *l0learn* package (Hazimeh, 2022)
- L0L2 model $\quad \lambda_0 > 0, \lambda_2 > 0 \quad$ using *l0learn* package

Training Results

Implemented and compared several ML-based branching rules

Model	# of Trainable Parameters Across All Models
LASSO	143–1,123
L0L1	41–50
L0L2	41–50
GNN	64,000

Existing algorithms are based on Graph Neural Networks (GNNs) that involve tens of thousands of parameters. As a result, they require hundreds of thousands of training data and their implementation is very slow in the absence of Graphics Processing Units (GPUs). On the contrary, the models we propose involve a few tens or hundreds of parameters, no more than a few hundreds or a few thousands of training data, and are computationally efficient on standard CPUs.

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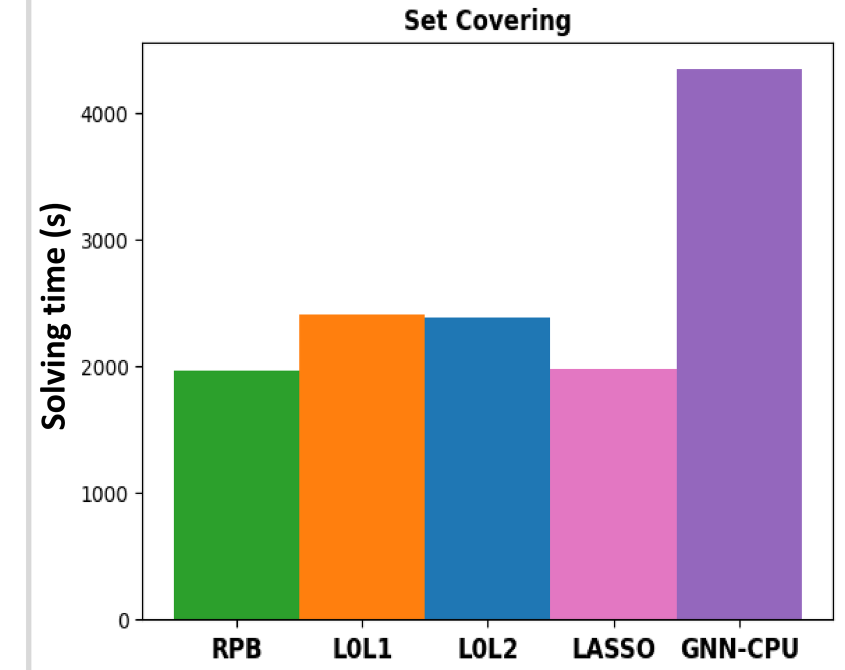
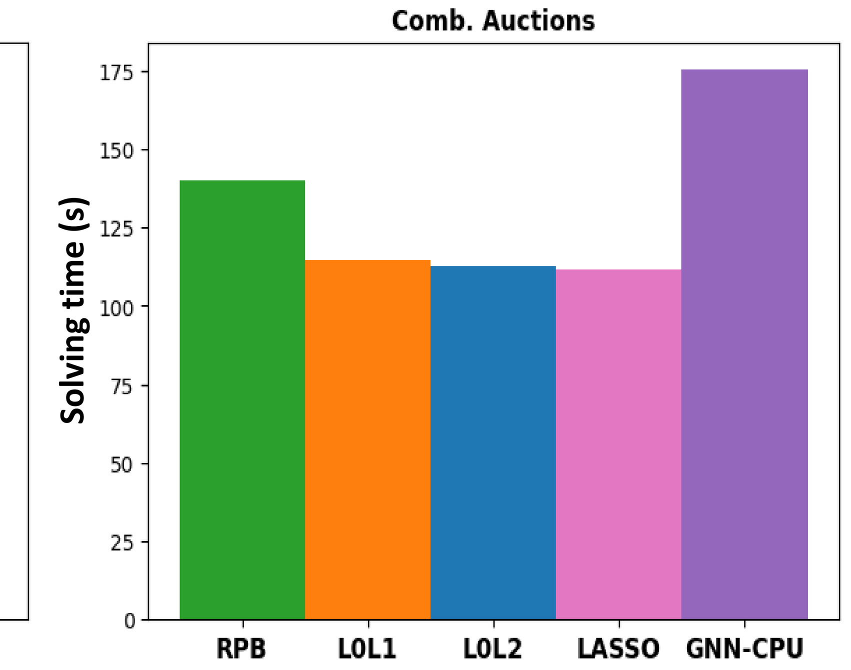
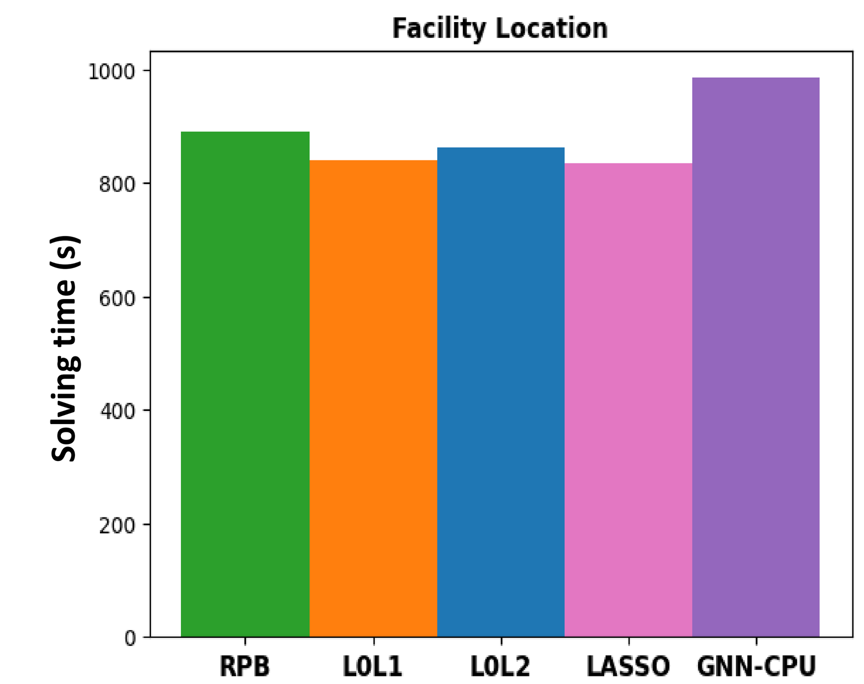
CPU Times

The figures below show CPU times for different problem classes and different learning algorithms. RPB is the default SCIP and GNN is based on previous literature. The others are the proposed algorithms. Our algorithms speed up SCIP, a state-of-the-art MIP solver (the best open-source MIP solver.)







Conclusions

- Sparse models have < 2% of the parameters in the GNN model
- On average, sparse models are faster than the default SCIP rule (RPB) in large combinatorial auctions (the LASSO is 20% faster) and facility location (the LASSO is 6% faster) problems. L0Lq models are significantly sparser than the LASSO models and their performance is comparable

Future Work

- Increase speedups of our algorithm by:
  - Increasing predictive ability of our models through new features
  - Predicting which variables lead to infeasible nodes in the search tree
- Application to various energy models
  - Currently working on large-scale security-constrained unit commitment problems