MACHINE LEARNING FOR OPTIMIZATION

January 24, 2025

Today (session 4/5)
Overview of ML techniques for MILP solves

Monday (Lab): End lab 2 + (MI)LPs and GNNs

Exam: Feb. 7, 10 am - 12 pm
- Open book (written/printed documents allowed)
- Will consist of
  - ↳ Questions about what we saw in class
  - ↳ (Guided) questions about a short research paper related to the course

MACHINE LEARNING FOR MIXED-INTEGER LINEAR PROGRAMS

Goal:
- → Overview of the learning tasks and the techniques used to perform these tasks
- → Following review papers: details are scattered among individual papers/codes
- → Focus: Use of graph neural networks to represent LP-related learning tasks

(1) MILPs

a) Problem and branch-and-bound

$$(MILP) \quad \underset{x \in \mathbb{R}^n}{\text{minimize}} \; c^T x \quad \text{s.t.} \quad Ax \geq b$$
$$x_j \in \mathbb{Z}_{\geq 0} \quad \forall j \in A$$
$$x_j \in \{0,1\} \quad \forall j \in B$$
$$x_j \geq 0 \quad \forall j \in \mathcal{E}$$

$A \in \mathbb{Q}^{m \times n}$
$b \in \mathbb{Q}^m$
$c \in \mathbb{Q}^n$

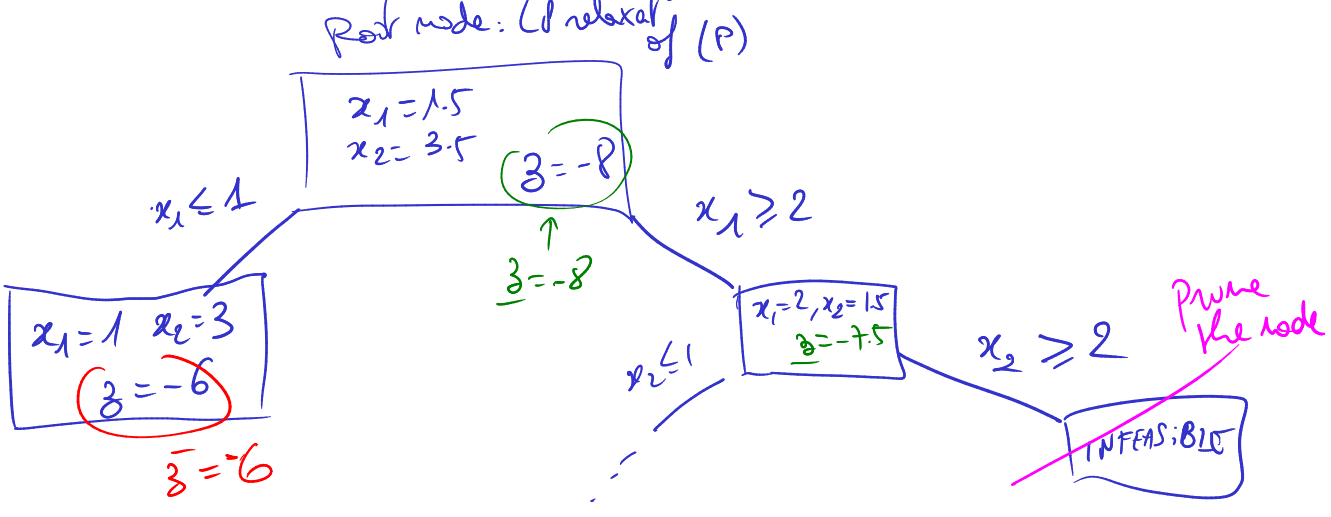
$A \cup B = I$: set of discrete (integer + binary) variables
$A, B, \mathcal{E}$ partition of $\{1, \dots, n\}$

LP relaxation: Replace $x_j \in \mathbb{Z}_{\geq 0}$ $j \in A$ $\Rightarrow$ $x_j \geq 0$ $j \in A$
$x_j \in \{0,1\}$ $j \in B$ $\Rightarrow$ $x_j \in [0,1]$ $j \in B$

⇒ Most state-of-the-art solvers for MILP are based on (variants) of the branch-and-bound technique

- Build a search tree of LP relaxations based on adding bounds on variables one at a time
- At every iteration, have
  - → an upper bound on the optimal value (from an integer feasible solution) : $\bar{z}$
  - → a lower bound for the best optimal value obtained by the LP relaxations $\underline{z}$
- Stops
  - when $\underline{z} = \bar{z}$
  - when all nodes have been processed
  - when timeout

Ex) (P) minimize $-(3x_1 + x_2)$ s.t. $-x_1 + x_2 \leq 2$
$x \in \mathbb{R}^2$ $8x_1 + x_2 \leq 19$
$x_1, x_2 \geq 0$
$x_1, x_2 \in \mathbb{Z}$



b) MILP solvers

In addition to the Branch-and-Bound algorithm, many heuristics and many degrees of freedom in designing the method

* Preprocessing

Goal: Reduce the size of problem (both in terms of constraints and variables)

→ Fundamental in practice but heuristic/empirical nature

* Branching and node selection

At every node, solve the LP relaxation. and when one integer variable is given a fractional value ($x_j^{LP} \in \mathbb{Q} \setminus \mathbb{Z}$) can branch on $x_j \leq \lfloor x_j^{LP} \rfloor$ or $x_j \geq \lceil x_j^{LP} \rceil$

⇒ Numerical studies have shown that branching strategies, but often it is possible to branch on several variables, no generic rule.

* Cutting planes

Idea: Strengthen the LP relaxation by adding new inequality constraints ("cuts") that reduce the size of the feasible set without eliminating integer feasible solutions.

Two approaches: Cuts at the root node only (standard)

Cuts at every node (Branch-and-cut)

⊖ Having too many cuts slows down the solve of the LP relaxation

⇒ Solvers have a cut management strategy

* Primal heuristics

Idea: Methods to find integer feasible solutions quickly without theoretical guarantees of success

Applying ML to these heuristic components requires:

→ To specify a learning task

→ To find data

→ To design a model to learn from the data

② Learning tasks

a) Learning paradigms

→ Supervised learning: Data $\{(x_i, y_i)\}_{i=1..N}$ with $x \in \mathcal{X}$, $y \in \mathcal{Y}$

Goal: Learn $f(\cdot, \theta) : \mathcal{X} \to \mathcal{Y}$ Model

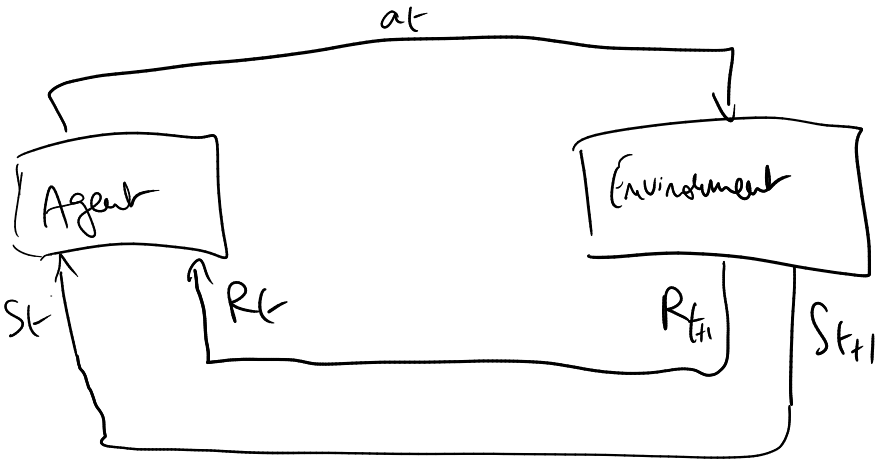
by solving $\underset{\theta \in \Theta}{\text{minimize}} \frac{1}{n} \sum_{i=1}^{n} \ell(f(x_i, \theta), y_i)$ (loss function)

→ Reinforcement learning

* Based on Markov Decision Processes

a_t: Action at time t

s_t: state at time t



* Goal: Learn a policy $\pi : S \rightarrow A$ that maps states to actions in the best possible way

$$\underset{\pi}{\text{maximize}} \; \mathbb{E}\left[\sum_{t=1}^{T} \gamma^{t-1} R_t\right]$$

T: time horizon

$\gamma \in [0,1]$

$$R_t = R_t(\pi, A_t, S_t, \ldots)$$

→ Standard RL setup: the agent only has access to a reward, not to the best action

→ Imitation learning: Get the best action at every step from an expert

⇒ Equivalent to having some data $\{(s_i, a_i^*)\}$

s_i: state; a_i^*: best action for that state

+ Distinction between online and offline

Offline setting: Learn once and for all (training)
Then run the solver with what you have learned (inference)

Online setting: Do training during the run
⊕ Adaptive
⊖ Cost (running time implementation)

b) Learning tasks for MILP

→ Solver configurations

Ex) SCIP has more than 2000 user-tunable parameters.

Approach: Tune one parameter at a time through learning

One example: (Bonami et al 2018) Predict whether an MIQP (Quadratic objective) should be linearized before solving with CPLEX or not

⇒ Huge impact on preprocessing
⇒ Now implemented in CPLEX

Other example: MIP 2023 challenge
Given past instances, can you learn efficient solver configurations for subsequent instances?

→ Branching strategies

Well-known: strong branching

At node i, suppose the optimal value of the LP relaxation is z^{LP_i}. and that by branching on x_h, get two other optimal values $z^{LP_i^-}$ and $z^{LP_i^+}$

Scores of x_h : $z^{LP_i^+} - z^{LP_i}$ and $z^{LP_i^-} - z^{LP_i}$

⊕ Can drastically reduce the size of B&B tree
⊖ Requires to solve several LPs.

Approaches * Learn to predict strong branching scores
offline (past instances)
or online (as you run B&B)

→ Can learn the scores themselves or just the ranking of the variables according to their scores

* Learn (by imitation) branching rules from scratch

→ Node selection

Classical: Best first search (use best known lower bound)

→ Research from the mathematical programming has been scarce for the past decades
→ New effort due to ML (typically supervised learning / offline)

→ Cutting planes

In a solver: given an LP relaxation, generate a number of cuts of different kinds, select some of them and add them to the relaxation so that the fractional solution of the relaxation becomes infeasible

Approach: Learn cut selection from imitation learning or (standard) RL

(One-cut selection seems easier to learn than multiple-cut selection)

→ Primal heuristics

4 tasks:

offline
- → Given a family of heuristics: learn how to schedule them for a specific instance
  - ↓ which heuristics to run, and for how long
- → Predict a reference solution, i.e. a partial assignment of the integer variables (e.g. by supervised learning on known feasible sets)

(also by supervised learning on known optimal values)

(2) Datasets / Software

Recent developments:
- Ecole → ML (RL) + SCIP solver (≃ Gym for RL)
- MIPLearn

→ Need instance generators and instance distributions
→ Highly dependent on the task
(ex) Learning branching rules should be done in instances for which proving optimality is difficult

→ In construction!

(3) Graph neural networks for (MI)LP

a) Graph Neural Network (GNN)

→ $G = (V, E)$ undirected graph
$\forall$ vertex $v \in V$, $N(v)$: set of neighbors of v

→ Graph embedding $\xi : (G, v) \mapsto \xi(G, v) \in \mathbb{R}^d$
($v \in V$)

$\Rightarrow$ Represents some "features" of v within G

Definition A GNN takes as inputs a graph G and an embedding ξ^0 on G, then defines a recursive embedding by

$$\forall v \in V, \forall t \in \mathbb{N}, \quad \xi^{t+1}(G,v) = \text{comb}\left(\xi^t(G,v), \sum_{u \in N(v)} \xi^t(G,u)\right)$$

comb: combination function, e.g. sum, a layer of a neural network

"Message passing"

Variant based on edge and vertex information

$\rightarrow$ Suppose we have in addition to ξ^0 (embedding on vertices) an embedding $\bar{\xi}$ on edges $\bar{\xi}: (G, e \in E) \mapsto \bar{\xi}(G,e) \in \mathbb{R}^d$

$\rightarrow$ Recursive embedding becomes

$$\xi^{t+1}(G,v) = \text{comb}\left(\xi^t(G,v), \sum_{u \in N(v)} \text{aggr}\left(\xi^t(G,u), \bar{\xi}(G,(u,v))\right)\right)$$

aggr: aggregation function (sum, NN layer, etc.)

Goal: Use GNNs to process MILP data

Challenges: should represent and process data while respecting invariants

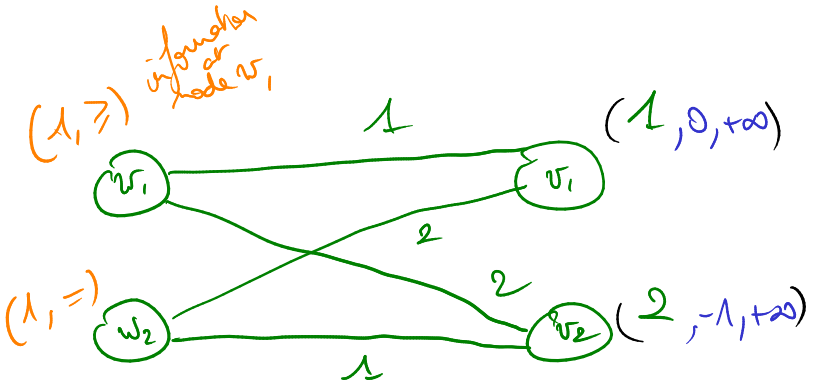
Ex) Permutation of variables / constraints

b) Representation and GNNs for (continuous) linear programs

Key idea: LPs can be represented as bipartite graphs with weighted edges and node information

$$\begin{aligned} \text{minimize}_{x \in \mathbb{R}^2} \quad & 1x_1 + 2x_2 \quad \text{s.t.} \quad x_1 + 2x_2 \geq 1 \\ & 2x_1 + x_2 = 1 \\ & x_1 \geq 0 \\ & x_2 \geq -1 \end{aligned}$$

Bounds



$v_1 \equiv x_1$
$v_2 \equiv x_2$
$w_1 \equiv x_1 + 2x_2 \geq 1$
$w_2 \equiv 2x_1 + x_2 = 1$

Generally

Graph $G = (V \cup W, E)$ bipartite
$|V| = n$ $|W| = m$

Every node is equipped with a feature vector

$$\forall i \in \{1, \dots, n\}, \quad h_i^V \in \underbrace{\mathbb{R}}_{\text{weight of variable } i \text{ in the objective}} \times \underbrace{(\mathbb{R} \cup \{-\infty\}) \times (\mathbb{R} \cup \{+\infty\})}_{\text{bounds on variable } i}$$

$$\forall j \in \{1, \dots, m\}, \quad h_j^W \in \underbrace{\mathbb{R}}_{\text{right-hand side}} \times \underbrace{\{\leq, \geq, =\}}_{\text{nature of the constraint}}$$

↳ Based on this representation, can define a GNN using learnable embedding functions

$\xi^{0,V}: R_i^V \mapsto \xi_i^{0,V} \in \mathbb{R}^{d_0^V}$ $\xi^{0,W}: h_j^W \mapsto \xi_j^{0,W} \in \mathbb{R}^{d_0^W}$

learnable = parameterized functions on which you can apply learning techniques (e.g. NN layers)

= will be learned by training

Every layer l involves learnable functions

comb_l^V, comb_l^W,

and computes

$$h_i^{l,V} = \text{comb}_l^V\left(h_i^{l-1,V}, \sum_{j\in N(i)} E_{ij}\, \text{comb}_l^W\left(h_j^{l-1,W}\right)\right)$$

(E_{ij}: weight of edge (i,j))

$$h_j^{l,W} = \text{comb}_l^W\left(h_j^{l-1,W}, \sum_{i\in N(j)} E_{ij}\, \text{comb}_l^V\left(h_i^{l-1,V}\right)\right)$$

Two sorts of outputs (after L layers)

- Single output $f_{out}\left(\sum_{i=1}^m h_i^{L,V}, \sum_{j=1}^m h_i^{L,W}\right)$
- One output per vertex in V ($\equiv$ variable)

$$\left[f_{out}\left(\sum_{i=1}^m h_i^{L,V}, \sum_{j=1}^m h_j^{L,W}, h_k^{L,W}\right)\right]_{k=1\ldots m}$$

One use case

Want a GNN that given an instance outputs
0 if the problem is infeasible
1 otherwise

in reality, we have a continuous output $\in [0,1]$

Theorem (2023, informal)

Under some assumptions, there exists a GNN such that, if $F(G) \in [0,1]$ is the output of the GNN, then $F(G)$ $\begin{cases} > 1/2 & \text{if the problem is feasible} \\ \leq 1/2 & \text{otherwise} \end{cases}$

c) More advanced use of GNNs in B&B

(Gasse et al '19)

Goal: Learn (strong) branching rules from an expert

LP model $\Leftrightarrow$ LP relaxation at the current node

NB: If the solver only add cuts at the root node, then all the other LP relaxations have same structure

Imitation learning: State: state of the solver: current node and LP relaxation, $\bar{x}, \bar{z}, \ldots$

Actions: strong branching

GNN: 3 layers, mix of convolution + fully connected + ReLU

Output: $\pi \in \mathbb{R}^n$, n number of variables

π probability vector π_i: proba of branching on variable i

Training: Done with GPUs

=> One drawback of GNNs: computational cost

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For more in the future

→ Papers in ML conferences: NeurIPS, ICLR

→ Papers in optimization/OR journals:
- Mathematical Programming
- European Journal of Operations Research
- INFORMS Journals on { Computing / Optimization