One-shot learning for MIPs with SOS1 constraints

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Charly Robinson La Rocca, Emma Frejinger, Jean-François Cordeau

Université de Montréal

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Background

- Goal: quickly find good quality solutions for MIPs with SOS1 constraints.
- One-shot learning (OSL): approach exploits data driven tools with focus on sample efficiency.
- Key results:
  - Locomotive assignment problem (LAP):
    - 10x speed up on small instance
    - Up to 1% relative gap improvement on real large instances
  - MIPLIB: improvement on 58% of selected instances with SOS1 constraints.

Outline

What is SOS1?

Special ordered sets of type 1 (SOS1) constraints are useful when a choice involves multiple options or resources, and only one can be selected.

$$\sum_{k \in K_v} x_v^k = 1 \qquad \forall v \in V \tag{1}$$

$$x_v^k \in \{0, 1\} \qquad \forall v \in V, \forall k \in K_v \tag{2}$$

Why SOS1?

SOS1 can be modelled as a classification problem. The solution vector for the binary variables is analogous to the one-hot encoding of the optimal class.

$$x_v = [0, 0, 1, 0] \rightarrow k = 3 \tag{3}$$

Structuring effect: SOS1 constraints can model *important* decisions in the problem.

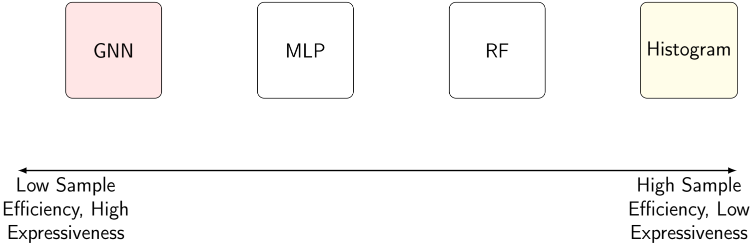
What is one-shot learning?

One-shot learning or few-shot learning aims to learn patterns where only one or a few training examples are available. Goal: Immitate the human ability to learn new concepts from one or a few examples. Examples: Matching Networks [Vinyals et al., 2016] and Prototypical Networks [Snell et al., 2017].

Why one-shot learning?

- Training data is expensive to obtain
- Easy to access and reproduce
- Act as a good baseline
- Can be used in combination with other methods: bagging or boosting
- Short improvement cycles

Efficiency vs expressiveness trade-off



Related works: Learning for MIPs

- MIP-GNN [Khalil et al., 2022]
- Entropic Branching (EB) [Gilpin and Sandholm, 2006]
- Rapid or Conflict Learning [Berthold et al., 2019]

Methodology: Probe and Freeze (PNF)

PNF is a one-shot learning heuristic that uses the probing data to build a model. It is composed of three routines:

- Probe
- Select
- Freeze

Probe

Hyperparameter: T_p is total probing time budget.
At every iteration, we compute the most likely class based on which variable has the highest value.

$$k_{vt} = \arg\max_{k \in K_v} \{x_{vt}^k\} \tag{4}$$

$$\mathrm{k}_v = [k_{v1}, k_{v2}, ..., k_{vn}] \tag{5}$$

Select

The selection strategy uses a scoring system to sort the SOS1 constraints based on the entropy H to infer uncertainty.

$$P(k|\mathrm{k}_v) = \frac{|\{z \in \mathrm{k}_v \mid z = k\}|}{|\mathrm{k}_v|} \tag{6}$$

$$H(\mathrm{k}_v) = -\sum_{k \in \mathrm{k}_v} P(k|\mathrm{k}_v) \log P(k|\mathrm{k}_v) \tag{7}$$

$$\mathrm{score}(v) = -H(\mathrm{k}_v) \tag{8}$$

Goal: Minimize potential assignment errors by selecting constraints with low entropy.

Predict

The predicted class k' is the most likely class in the probing vector k_v.

$$k' = \arg\max_k (P(k|\mathrm{k}_v)) \tag{9}$$

The underlying classifier uses the histogram method with discrete bins for each class.

Freeze

Hyperparameter: r is the ratio of constraints to freeze.
The freezing routine builds *freezing cuts* (FC) defined as follows:

$$FC(v, k') := \{x_v^{k'} = 1\}. \tag{10}$$

Goal: Create a reduced problem $\mathcal{P}'$ which is easier to solve.

Probe and Freeze (PNF)

1. **Probe**: Solve the problem with a probing time budget T_p.
2. **Select**: Sort the variables using the entropy.
3. **Freeze**: Freeze the variables based on the predicted class k'.
4. **Solve**: Solve the reduced problem $\mathcal{P}'$.

Notation: $PNF(r, T_p) == PNF\_r\_T_p$

Locomotive assignment problem (LAP)

Locomotive assignment problem (LAP) is a real-world problem that is used to assign locomotives to trains in a railway network.

$$Assignment\,(SOS1) : \sum_{c \in C_l} y_l^c = 1 \qquad \forall l \in L \qquad (11)$$

$$Flow : \sum_{l \in I[i]} x_l^q = \sum_{l \in O[i]} x_l^q \qquad \forall i \in N \qquad (12)$$

Metrics

Two metrics: runtime speed up (RS), and relative gap (RG).

$$\mathrm{RS} = \frac{\mathrm{runtime(CPLEX)}}{\mathrm{runtime(PNF)} + T_p} \tag{13}$$

$$\mathrm{RG} = \frac{c^T x' - c^T x_{\mathrm{CPLEX}}}{c^T x_{\mathrm{CPLEX}}} \times 100 \tag{14}$$

LAP CPLEX results

Table: Average summary metrics for LAP instances using CPLEX

Difficulty	Runtime (s)	Train count	Optimality gap (%)
E	206.42	141.77	0.01
M	2450.07	336.40	0.26
H	21600.20	5673.20	2.94

LAP speed up results

Table: Quantiles for runtime speed up in LAP instances

Scenario	Quantiles 0.25	Quantiles 0.75	Mean	Sample size
E+PNF_0.5_8	1.84	5.46	4.07	30.00
E+PNF_0.9_6	4.46	40.64	27.75	30.00
E+PNF_0.2_10	0.90	2.23	1.84	30.00
E+PNF_0.2_20	0.66	1.68	1.32	30.00
E+PNF_0.5_30	0.65	2.91	2.39	30.00
M+PNF_0.2_60	0.93	1.08	1.32	30.00
M+PNF_0.5_60	1.01	2.64	2.63	30.00
M+PNF_0.2_120	0.92	1.11	1.25	30.00
M+PNF_0.5_120	1.03	1.82	2.27	30.00
M+PNF_0.9_120	4.07	26.37	17.10	30.00
H+PNF_0.2_600	0.99	1.02	1.02	20.00
H+PNF_0.2_1800	0.99	1.02	1.00	20.00
H+PNF_0.5_1800	0.98	1.00	0.98	20.00

LAP gap results

Table: Quantiles for relative gap (%) in LAP instances

Scenario	Quantiles 0.25	Quantiles 0.75	Mean	Sample size
E+PNF_0.5_8	0.01	0.20	0.11	30.00
E+PNF_0.9_6	0.94	2.31	1.73	30.00
E+PNF_0.2_10	-0.00	0.02	0.02	30.00
E+PNF_0.2_20	-0.00	0.00	0.01	30.00
E+PNF_0.5_30	0.00	0.13	0.07	30.00
M+PNF_0.2_60	-0.12	0.00	-0.09	30.00
M+PNF_0.5_60	-0.11	0.04	-0.08	30.00
M+PNF_0.2_120	-0.05	0.00	-0.06	30.00
M+PNF_0.5_120	-0.03	0.03	-0.07	30.00
M+PNF_0.9_120	0.65	1.47	1.15	30.00
H+PNF_0.2_600	-1.09	-0.58	-0.10	20.00
H+PNF_0.2_1800	-0.99	-0.48	-0.52	20.00
H+PNF_0.5_1800	-1.16	-0.69	-1.03	20.00

Correlations

Table: Correlations with relative gap for LAP instances

Parameter	Spearman	Kendall	Average
Fixing ratio	0.61	0.51	0.56
Probing time budget (s)	-0.42	-0.33	-0.37

Gap over time

Table: Gap (%) for full LAP instances

Scenario	Time after probing (s)			
	1800	3600	5400	7200
cplex	nan	4.04	3.94	2.49
PNF_0.2_600	1.72	1.48	1.09	0.88
PNF_0.2_1800	2.01	1.67	1.18	1.17
PNF_0.5_1800	1.48	1.39	0.89	0.69

Table: Full LAP instances with feasible solution

Scenario	Time after probing (s)			
	1800	3600	5400	7200
cplex	0	6	7	7
PNF_0.2_600	7	9	9	9
PNF_0.2_1800	7	10	10	10
PNF_0.5_1800	8	9	9	9

MIPLIB 2017

The MIPLIB [Gleixner et al., 2021] dataset is an open source library of MIP instances. The instances in MIPLIB are generated independently and are not related to each other. This makes it a more challenging test bed for our approach.
Instance selection:

- Remove instance with high average entropy
- Remove instance with low sample size

MIPLIB summary results

Table: Number of solved MIPLIB instances

Scenario	Number of instances	Solved	Unsolved
E+PNF_0.2_1	68	67	1
E+PNF_0.2_2	68	57	11
M+PNF_0.2_60	44	39	5
M+PNF_0.2_120	44	37	7
H+PNF_0.2_300	76	61	15
H+PNF_0.2_600	76	58	18
Total	376	319	57

MIPLIB results

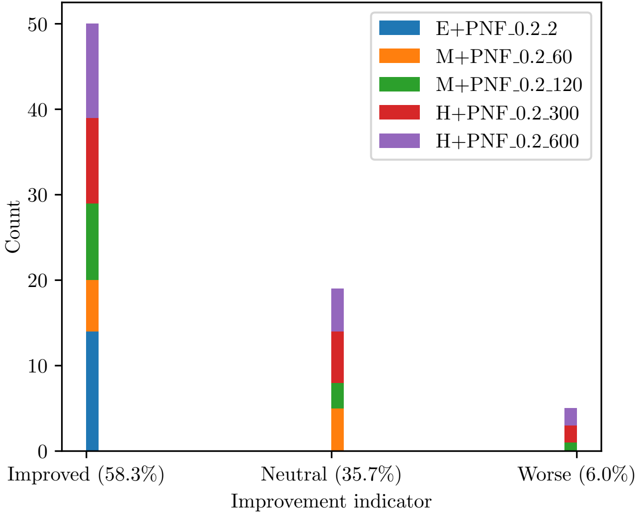
Table: Quantiles for runtime speed up in selected MIPLIB instances

Scenario	Quantiles 0.25	0.75	Mean	Sample size
E+PNF_0.2_2	1.07	1.24	1.19	14.00
M+PNF_0.2_60	0.38	3.62	2.80	11.00
M+PNF_0.2_120	0.30	1.34	1.23	13.00
H+PNF_0.2_300	0.29	1.01	1.32	18.00
H+PNF_0.2_600	0.38	1.31	1.22	18.00

Table: Quantiles for relative gap (%) in selected MIPLIB instances

Scenario	Quantiles 0.25	0.75	Mean	Sample size
E+PNF_0.2_2	-0.00	0.00	0.06	14.00
M+PNF_0.2_60	0.00	2.32	4.80	11.00
M+PNF_0.2_120	0.00	0.00	1.57	13.00
H+PNF_0.2_300	-0.06	0.00	-1.16	18.00
H+PNF_0.2_600	-0.00	0.06	-4.87	18.00

MIPLIB summary outcome results



Conclusion

Our results are consistant with Occam's razor principle which states that the simplest explanation is usually the best.

- Implication: Machine learning methods with *low expressiveness* can be used to accelerate the discovery of solutions for MIPs with SOS1 constraints.
- Limitation: PNF heuristic is unable to find a feasible solution for 11% of selected MIPLIB instances (21/188).
- Future work: risk management strategy to mitigate the risk of infeasibility.

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