Heuristic approach with machine learning alongside for the resource-constrained shortest path problem

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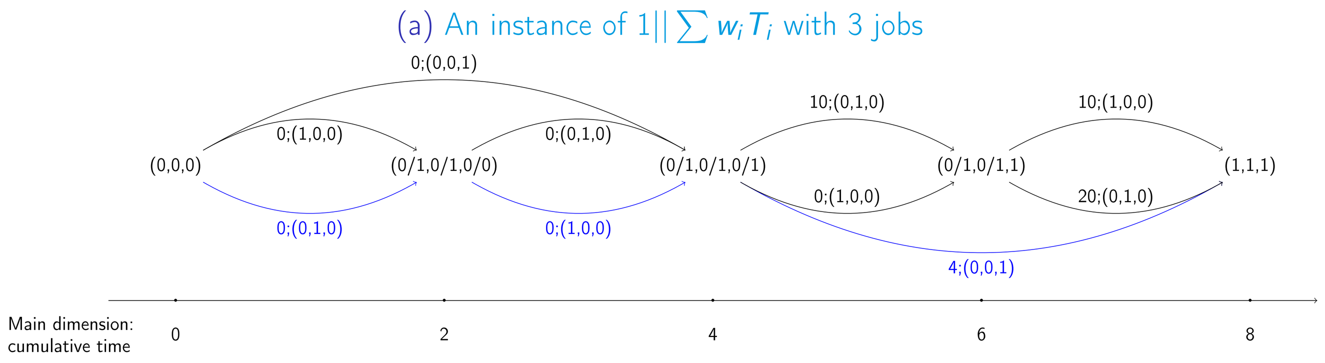
Problem introduction

- We study the problem that can be formulated partially or completely as a sequential decision process with additional linear constraints related to the resource consumption in the whole decision sequence.
  - Many combinatorial optimization problems can be expressed as sequential decision processes (SDP) such as planning, knapsack, scheduling, véhicule routing.
  - In the SDP formalism, a representation of the problem (or a sub-problem thereof) is associated with a acyclic directed multi-graph representing the states of the system and the possible transitions between these states.
  - Network-flow formulations [de Lima et al., 2022].
  - We study a special case of network formulations: resource-constrained shortest path problem (RCSPP).

Job	processing time	due time	weight
1	2	7	10
2	2	4	6
3	4	6	10

(a) An instance of $1||\sum w_i T_i$ with 3 jobs



(b) The associated graph

Figure: An example of reformulating one single machine weighted total tardiness problem $1||\sum w_i T_i$ as RCSPP

Research objectives

- The present study investigates the following objectives:
  - Develop a generic heuristic tree-search approach with machine learning models alongside to produce useful information for RCSPP.
  - Train machine learning models to produce useful information.
  - Compare the performance to classical tree search without learning and to problem-specific heuristics.

Arc-flow formulation for RCSPP

- $\mathcal{G}(\mathcal{V},\mathcal{A})$ be a directed acyclic multi-graph, where $s \in \mathcal{V}$ represents the source and $t \in \mathcal{V}$ represents the sink.
- Each arc $a \in \mathcal{A}$ has a tail $v^-(a)$ and a head $v^+(a)$.
- For each arc $a \in \mathcal{A}$, c_a represents the cost of a.
- Let $\mathcal{R}$ be the set of resource constraints. For each resource constraint indexed by $k \in \{1 \dots, |\mathcal{R}|\}$, we have the resource capacity denoted by r^k, and each arc a is also assigned a resource consumption r_a^k.
- A arc-flow formulation of RCSPP is given as follows in (1) - (4):

$$\min \sum_{a\in\mathcal{A}} c_a x_a \tag{1}$$

$$\text{s.t.} \sum_{a\in\mathcal{A}|v^+(a)=v} x_a - \sum_{a'\in\mathcal{A}|v^-(a')=v} x_{a'} = \begin{cases} -1, & \text{if } v = s,\\ 1, & \text{if } v = t,\\ 0, & \text{otherwise,}\end{cases} \quad \forall v \in \mathcal{V}, \tag{2}$$

$$\sum_{a\in\mathcal{A}} r_a^k x_a \le (\text{or} =) r^k, \quad \forall k \in \{1,\dots,|\mathcal{R}|\}, \tag{3}$$

$$x_a \in \{0,1\}, \quad \forall a \in \mathcal{A} \tag{4}$$

Beam search

- A constructive heuristic, which starts with an empty solution and repeatedly extends the current partial solution until a complete solution is obtained.
- Vocabulary:
  - $\ell \in \mathcal{L}$ label: a partial solution
  - β beam size: the maximum number of labels to keep at each level
  - $\psi : \mathcal{L} \to \mathbb{R}$ heuristic criterion: a function to score $\ell \in \mathcal{L}$.
  - g_ℓ: value of the partial solution ℓ
  - $\mathcal{B}^n \subset \mathcal{L}$: a set of labels at level n of the beam search.
  - $\mathcal{F}^n \subset \mathcal{L}$: a set of complete solutions at level n of the beam search
- Choice of ψ:
  - Many classical tree-search based algorithms use ν_ℓ the dual bound of solutions that complete ℓ as the score $\psi(\ell)$ [Kuroiwa and Beck, 2023].
  - The dual bound quality impact directly to the solution quality of the beam search.

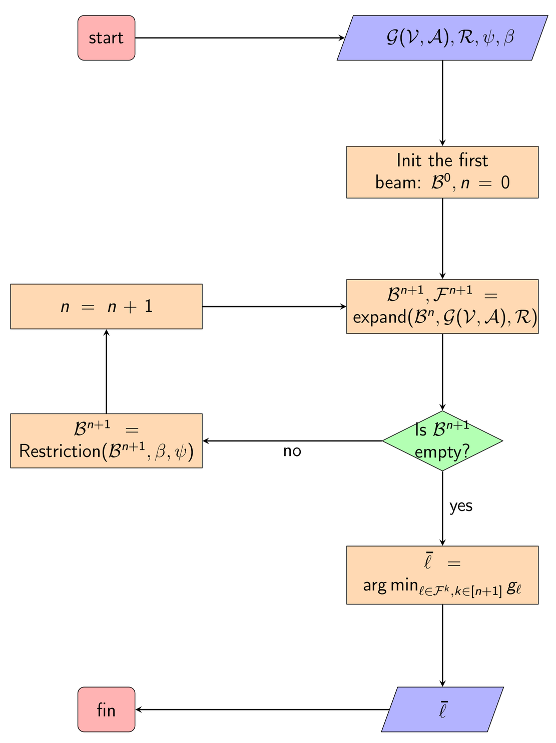


Figure: Flowchart of Beam search

Beam search with machine learning alongside

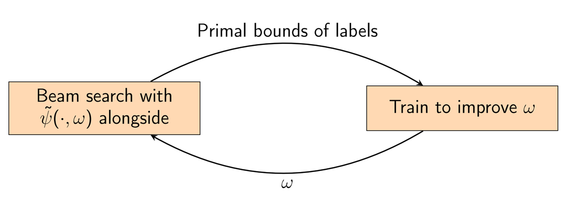
- Using a machine learning model to estimate the scoring function ψ.
- Let ϕ be a mapping from a label to a vector of m features representing the label.

$$\phi : \mathcal{L} \to \mathbb{R}^m$$
$$\ell \to \phi(\ell)$$

- Let $\tilde{\psi}(\cdot;\omega)$ be a function parameterized by ω such that $\psi(\ell;\omega) = \tilde{\psi}(\phi(\ell);\omega)$

$$\tilde{\psi}(\cdot;\omega) : \mathcal{R}^m \to \mathbb{R}$$
$$\phi(\ell) \to \psi_\ell(\omega) = \tilde{\psi}(\phi(\ell);\omega)$$

- The objective is to train $\tilde{\psi}(\cdot;\omega)$ such that $\psi_\ell(\omega)$ estimates the primal bound of solutions completing ℓ. [Huber and Raidl, 2022]



Exploration phase

- The exploration phase uses beam search to generate diverse labels with primal bounds.
- The generated labels should be diverse enough to improve the training efficiency.
- Generate as many labels as we can v.s. generate "good" labels?

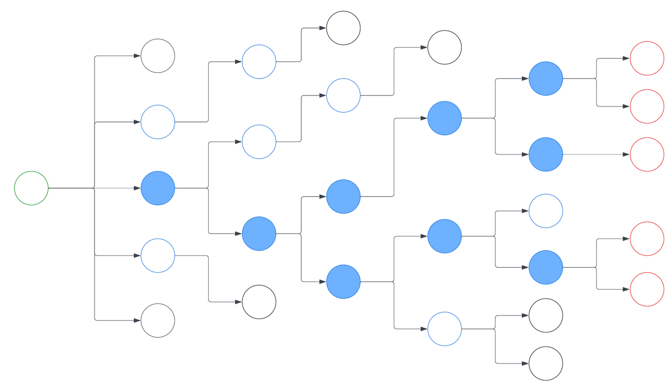


Figure: Lack of diversity for labels with primal bounds in beam search. An example with $\beta = 3$. Nodes represent labels. Nodes filled in blue are labels with primal bound generated by the beam search.

- Perform a greedy rollout on each label $\ell \in \mathcal{B}^{n+1}$
- If the completion of ℓ is optimal proven by its dual bound, the best primal bound of solutions completing ℓ is found. No need to further expand ℓ. Move label ℓ into $\mathcal{U}^{n+1}$.
- Labels in $\mathcal{U}^{n+1}$ are concatenated with the associated rollout solution and are added into $\mathcal{F}^{n+1}$.

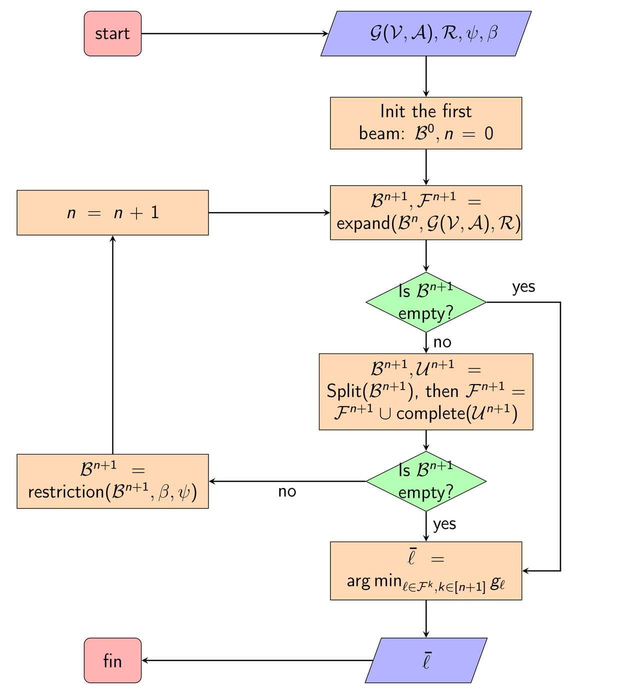


Figure: Flowchart of Beam search with greedy rollout

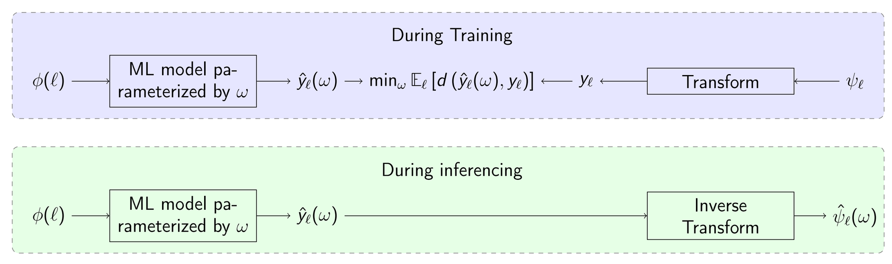
Features of labels

- The number of resources varies as the instance size varies.
- Cost of labels ($\boldsymbol{\lambda}^a = 0$)
- Cost of labels ($\boldsymbol{\lambda} = \boldsymbol{\lambda}^{*\,b}$)
- Dual completion of labels ($\boldsymbol{\lambda} = 0$)
- Dual completion of labels ($\boldsymbol{\lambda} = \boldsymbol{\lambda}^*$)
- Sum of resource consumption over $\boldsymbol{r}^T\boldsymbol{\lambda}^* > 0$
- Sum of resource consumption over $\boldsymbol{r}^T\boldsymbol{\lambda}^* < 0$
- Sum of resource consumption over $\boldsymbol{r}^T\boldsymbol{\lambda}^* \in [\min, \max]$
- Sum of resource consumption over a quantile for some indicator
- Sum of resource slack over ...
- Main dimension value
- ...

[a] $\boldsymbol{\lambda}$: the Lagrangian multipliers of the resource constraints (3)
[b] $\boldsymbol{\lambda}^*$: the best Lagrangian multipliers of constraints (3)

Transformations and inverse transformations

- The scale of ψ_ℓ primal bounds of labels varies between instances. Transforming them into the same scale is vital for the convergence of machine learning models.
- The transformation must be bijective.

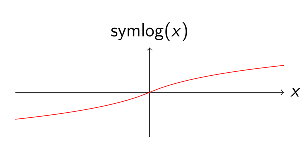


- Alternatives of transformations
  - Normalize by ν_ℓ the dual bound of the label

$$y_\ell = \frac{\nu_\ell}{\psi_\ell}, \quad \hat{\psi}_\ell(\omega) = \frac{\nu_\ell}{\hat{y}_\ell(\omega)}$$

  - Symlog transformation [Hafner et al., 2023]

$$\text{symlog}(x) = \text{sign}(x)\log(1+|x|), \quad \text{symexp}(y) = \text{sign}(y)(\exp(|y|) - 1)$$
$$y_\ell = \text{symlog}(\psi_\ell), \quad \psi_\ell(\omega) = \text{symexp}(\hat{y}_\ell(\omega))$$



Preliminary numerical results

- 125 instances of $1||\sum w_i T_i$ with 100 jobs.
- The preliminary results show the solution quality of beam search (BS) using ν_ℓ as heuristic criterion without ML model alongside compared to the baseline.
- Baseline: early due date (EDD) + shortest processing time (SPT) + local search (LS)

Heuristic	beam size	meanGap(%)	stdGap(%)
EDD+SPT+LS	-	-	-
EDD	-	55.11	18.52
SPT	-	62.42	29.40
BS	10	2.23	3.41
	20	1.57	2.67
	100	1.00	1.90
	200	0.86	1.76
	500	**0.66**	**1.39**

Conclusions

- Machine learning alongside heuristic methods remains a relatively novel research area, with limited achievements thus far.

Perspectives

- Converge machine learning models.
- Generalize models for $1||\sum w_i T_i$ problem.
- Study more complex problems like the disjunctive knapsack problem.

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