Learning Beam Search: Utilizing Machine Learning to Guide Beam Search for Solving Combinatorial Optimization Problems

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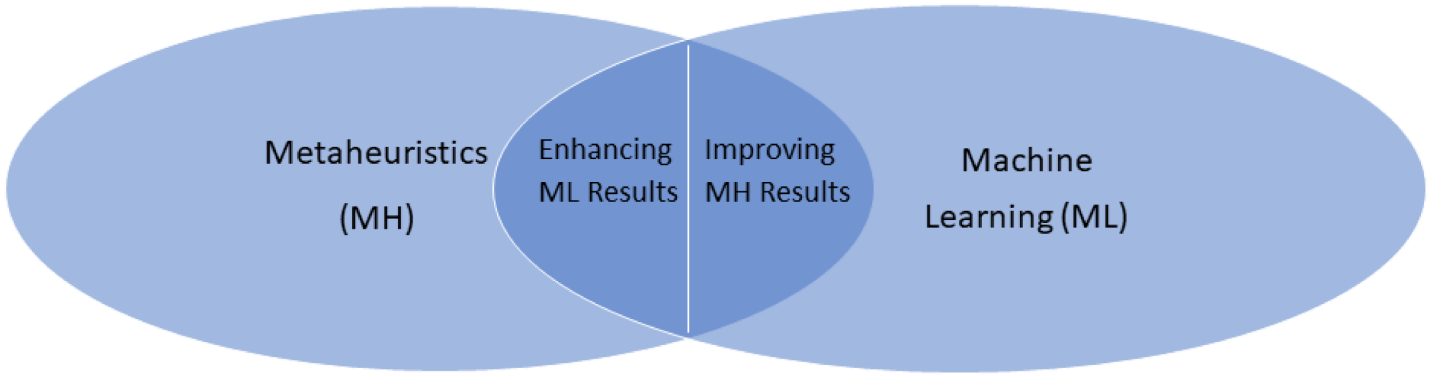
Combinatorial Optimization and Learning

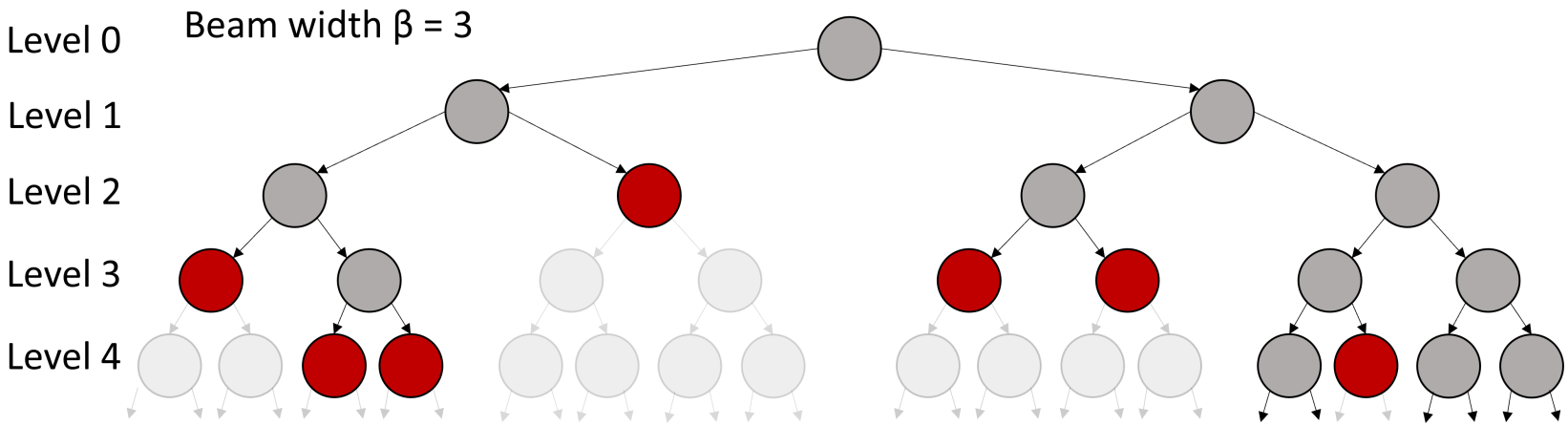
- AI/machine learning boom also hit the area of heuristic methods for combinatorial optimization



- Focus here:
  - utilize learning to better solve a combinatorial optimization problem
  - with **Beam Search (BS)**
- Let's keep it simple!

Beam Search (BS)

- Limited breadth first search
- Evaluates reached nodes at each level and only expands the β most promising nodes.



- Arcs have associated lengths (costs, rewards,. . .)
- Assume maximization
- Interested in longest path

Motivation

How to evaluate and select nodes?

- Evaluation function: $f(v) = g(v) + h(v)$, where
  - $g(v)$: length of a best path from the root r to node v.
  - $h(v)$: heuristic guidance function that estimates the further length-to-go from node v in the best case.

Guidance function:

- Typically developed manually in a highly problem-specific way.
- Often challenging as the function not only needs to deliver good estimates but also needs to be fast.

Idea:

- Use an ML model as guidance function $h(v)$ in BS.
- Train ML model offline by "self-play" on many representative randomly generated problem instances.

$\rightarrow$ **Learning Beam Search (LBS)**

Related Work

- **A general reinforcement learning algorithm that masters chess, shogi, and Go through self-play:**

  Silver et al. (2018)

  - Based on Monte Carlo Tree Search (MCTS) in which a Neural Network (NN) estimates for a current position
    - the expected outcome of the game ($\rightarrow$ "value")
    - and provides a policy (probability distribution) on next moves
  - Learning by self-play, i.e. reinforcement learning in which MCTS acts as a "quality amplifier".

- **Learning Beam Search Policies via Imitation Learning:**

  Negrinho et al. (2018)

  - Learn a BS policy for an abstract structured prediction problem to traverse the combinatorial search space of beams.
  - Pure theoretical work.

LBS: High-Level Procedure

ML model $= h(v)$:

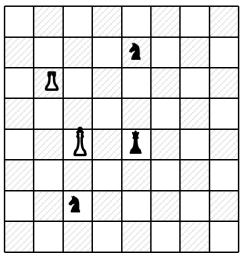
- Input: Problem-specific feature vector representing a node v (state) and possibly some problem instance features.
- Output: estimated further length to go from v.
- Randomly initialized

Repeat until stopping criterion fulfilled:

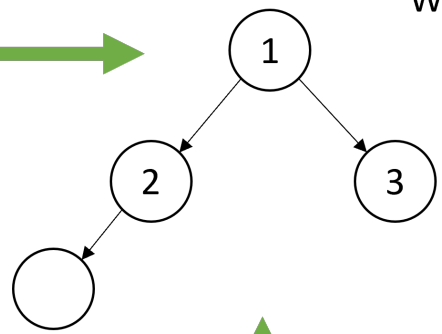
- Create representative random problem instance
- Perform a BS guided by the ML model
  - From each non-terminal node v with small probability:
    - **Perform a Nested BS (NBS)** to obtain approx. length-to-go
    - Store training sample in a limited size FIFO replay buffer
- Perform few training steps with batches of randomly sampled data from replay buffer

LBS: High-Level Procedure

Randomly generated problem instance

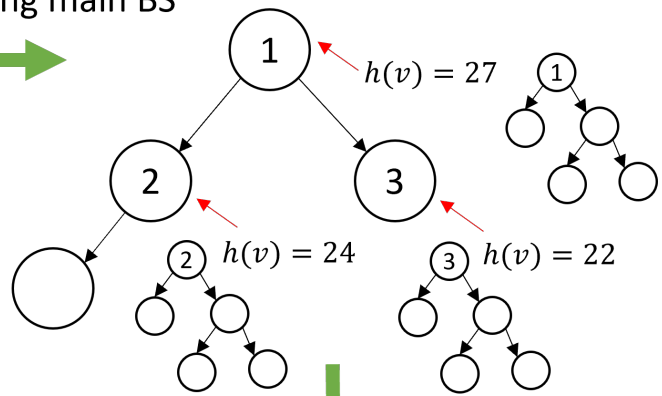


Main BS with beam width β
(solves problem instance)



While performing main BS

NBS calls from selected nodes
(generates α training data)

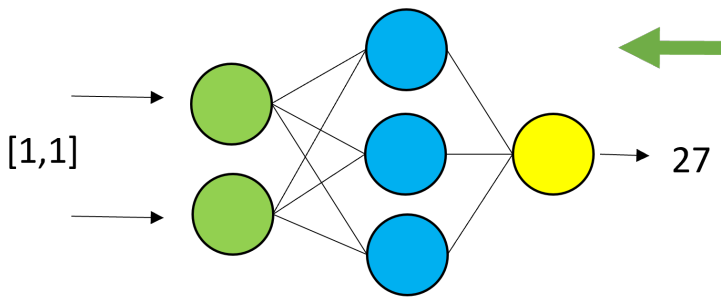


FIFO replay buffer of size γ
(stores training data,
removes older samples)

Feature Vectors	Targets
[1,1]	27
[1,4]	24
[3,5]	22
⋮	⋮

Train ML model

ML model (e.g. NN)
(guides BS)



Experiments on Longest Common Subsequence (LCS) Problem

- **Given:** set of m input strings $S = \{s_1, \ldots, s_m\}$ over alphabet Σ.
- **Goal:** Find a longest string that appears as subsequence in any string of S.

  Example: $m = 2$, $|\Sigma| = 3$

  s_1: ABBA
  s_2: CABA
  $\Rightarrow$ ABA.

Longest Common Subsequence Problem

- Applications in computational biology, text editing, etc.
  - e.g. to compare two DNA or protein sequences to learn how homologous they are.

- Can be solved efficiently in time $\mathcal{O}(n^2)$ for $m = 2$ strings by dynamic programming (n: string length).
- NP-hard for general m.
- State-of-the-art heuristic approach for large m and n based on BS with a theoretically derived expected solution length (EX) calculation (Djukanovic et al., 2020b).

Variant: Constrained LCS Problem (CLCS)

Extends LCS problem by a pattern string P that must appear as subsequence in a feasible solution.

Example:

P: CA

s_1: ABCBAB

s_2: CABBA

$\Rightarrow$ LCS: ABBA but CLCS: CAB

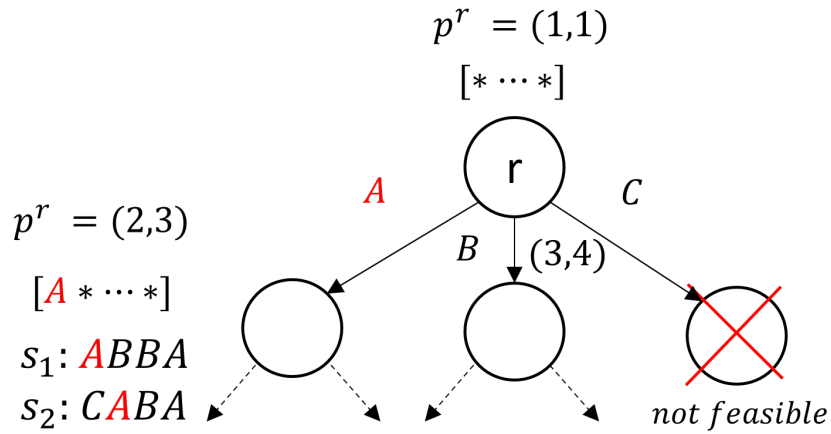
State Graph for LCS Problem

Directed acyclic graph $G = (V, A)$:

- States (nodes) in V are represented by position vectors, where root node r has position $\vec{1}$.

$$\begin{aligned} s_1\colon\ & ABBA \\ s_2\colon\ & CABA \end{aligned} \quad \Rightarrow (p_i^v)_{i=1,2} = \begin{bmatrix} 2 \\ 3 \end{bmatrix}.$$

- Actions (arcs) in A refers to transitioning from one to another state by appending a feasible letter to a partial solution.
- Actions in a state are feasible if the letter to append exists in each remaining string of $s_1, \ldots, s_m$.



State Graph for LCS Problem

Feature vectors (input for ML model):

- remaining string lengths:

$$q_i^v = |s_i| - p_i^v + 1, \quad \forall\, i = 1 \ldots, m.$$

$$\begin{matrix} s_1\colon\ AABA \\ s_2\colon\ CABA \end{matrix}, \ (p_i^v)_{i=1,2} = \begin{bmatrix} 2 \\ 3 \end{bmatrix} \Rightarrow (q_i^v)_{i=1,2} = \begin{bmatrix} 3 \\ 2 \end{bmatrix}.$$

sorted non-decreasingly to get rid of symmetries

- minimum letter appearances:

$$o_c^v = \min_{i=1,\ldots,m} |s_i[p_i^v, |s_i|]|_c, \quad c \in \Sigma.$$

$$\begin{matrix} s_1\colon\ AABA \\ s_2\colon\ CABA \end{matrix}, \ o_A^v = \min\{3, 2\} = 2$$

Experiments: LCS Benchmark Instances

- **`rat` instance set Shyu and Tsai (2009):**
  - 20 instances composed of sequences from rat genomes.
  - all differ in their combinations of values for
    - $n = 600$
    - $m \in \{10, 15, 20, 25, 40, 60, 80, 100, 150, 200\}$
    - $|\Sigma| \in \{4, 20\}$.
  - instances are close to independent random strings.
- **`BB` instance set Blum and Blesa (2007):**
  - 80 random instances.
  - ten instances per combination of values for
    - $n = 1000$
    - $m \in \{10, 100\}$
    - $|\Sigma| \in \{2, 4, 8, 24\}$.
  - strings of each instance exhibit large similarities.

Test setting:

- Julia 1.6 using the Flux package for the NN.
- Intel Xeon E5-2640 v4 2.40GHz, all runs single-threaded, memory limit of 20 GB.

Experiments: LCS Results on rat and BB Benchmark Instances

Compared LBS to the state-of-the-art methods from the literature Djukanovic et al. (2020b).

- All training with LBS was done with $\beta = 50$.
- Tests on the benchmark instances were performed with two different beam widths:
  - Low (computation) time with $\beta = 50$.
  - High quality with $\beta = 600$.

Achieved new best results for

- low time experiments: **13 out of 28**.
- high quality experiments: **7 out of 28**.

Runtimes similar to those of BS with EX.

Experimens: CLCS Benchmark Instances and Results

Benchmark set Djukanovic et al. (2020a):

- Ten instances for each combination of
  - $n \in \{100, 500, 1000\}$
  - $m \in \{10, 50, 100\}$
  - $|\Sigma| \in \{4, 20\}$
  - $\frac{n}{|P|} \in \{4, 10\}$, where P denotes the pattern string.

CLCS Results:

- All training with LBS was done with $\beta = 50$
- For tests on the benchmark instances $\beta = 2000$ was used.

Achieved new best results in 10 out of 36 cases
Scores worse in only 2 out of 36 cases.

ML Model: Simple Multilayer Perceptron

- Make the NN as small as possible.

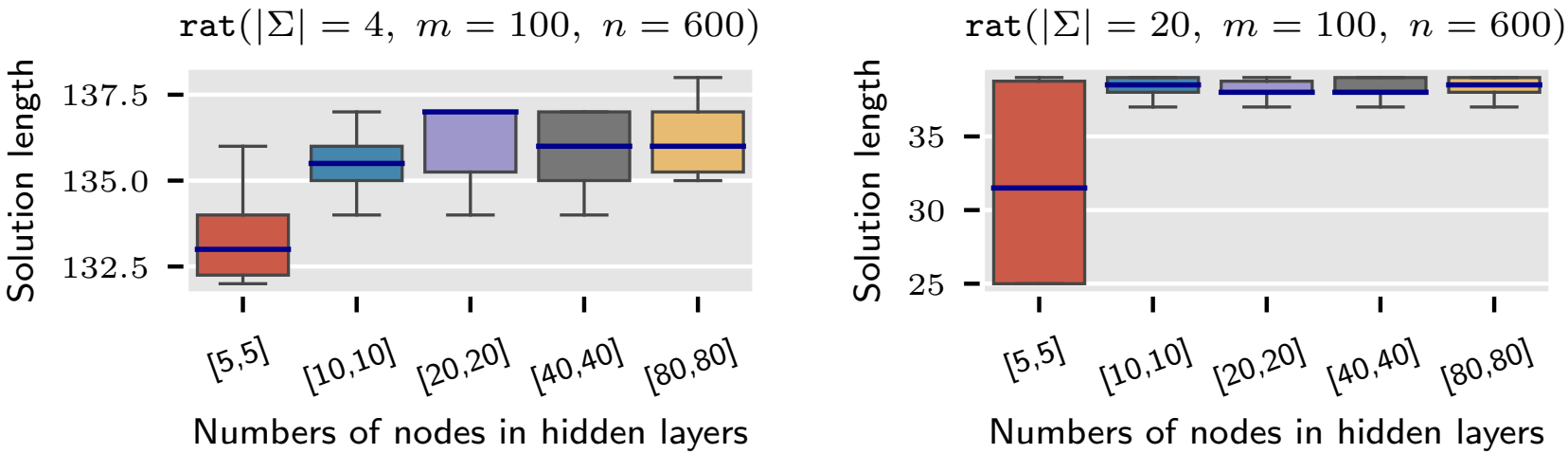


Figure: Impact of the numbers of nodes in the hidden layers on the solution length of LBS on `rat` benchmark instances.

Robust choice: 20 nodes in both hidden layers.

Impact of Beam Width on Solution Quality

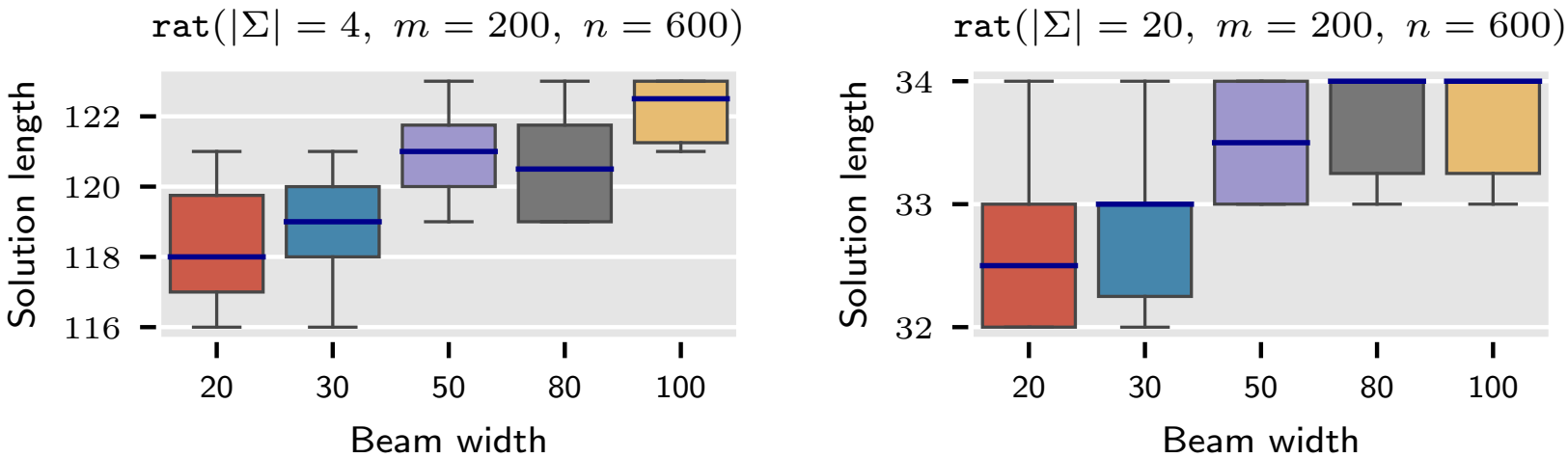


Figure: Impact of beam width β' in training and testing on `rat` instances.

Reasonable choice: $\beta = 50$.

Approximation of the Real LCS Length

How well does a NN trained by LBS predict the real LCS length?

- Approximate exact LCS lengths by applying the so far leading BS with EX guidance function Djukanovic et al. (2020b).

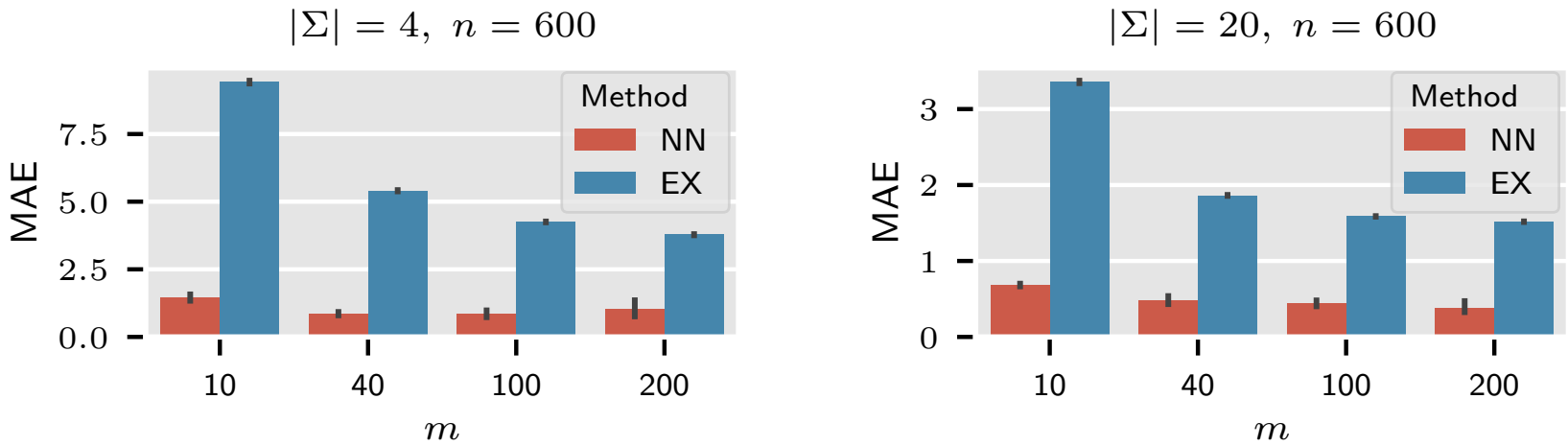


Figure: Mean absolute error of the trained NNs and EX on 10000 test samples, created by a BS with EX guidance function.

NNs approximate the LCS lengths much better than EX.

Nice!. . . But There are Still Weaknesses

- One has to train one model for each combination of m and Σ
- Long training times (hours per model) for large string lengths
- Weaker results for large string lengths n
  - Expected lengths-to-go differ only slightly within one beam

  $\rightarrow$ approximation must be very precise!

Observation:

- We do not need to approximate the length-to-go.
- Instead, we just need a scoring function to rank the nodes in the beam.

Relative Value Based Approach (RV-LBS)

Huber and Raidl (2022)

New Input Features:

Let $V_{\text{ext}} \subseteq V$ be the expanded set of nodes in the BS.

Cut-off value for remaining strings q_i^v, for $i = 1, \ldots, m$:

$$b^{\text{sl}} = \max(0, \overline{q_{\text{ext}}} - \lambda|\Sigma|), \tag{1}$$

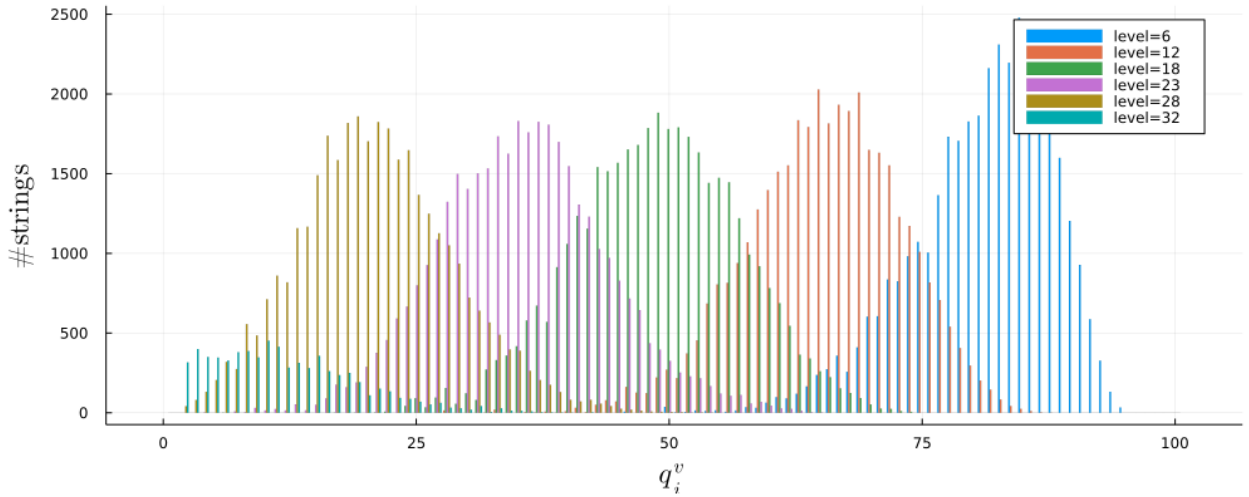
where

$$\overline{q_{\text{ext}}} = \frac{1}{m\,|V_{\text{ext}}|} \sum_{i=1}^{m} \sum_{v \in V_{\text{ext}}} q_i^v, \tag{2}$$

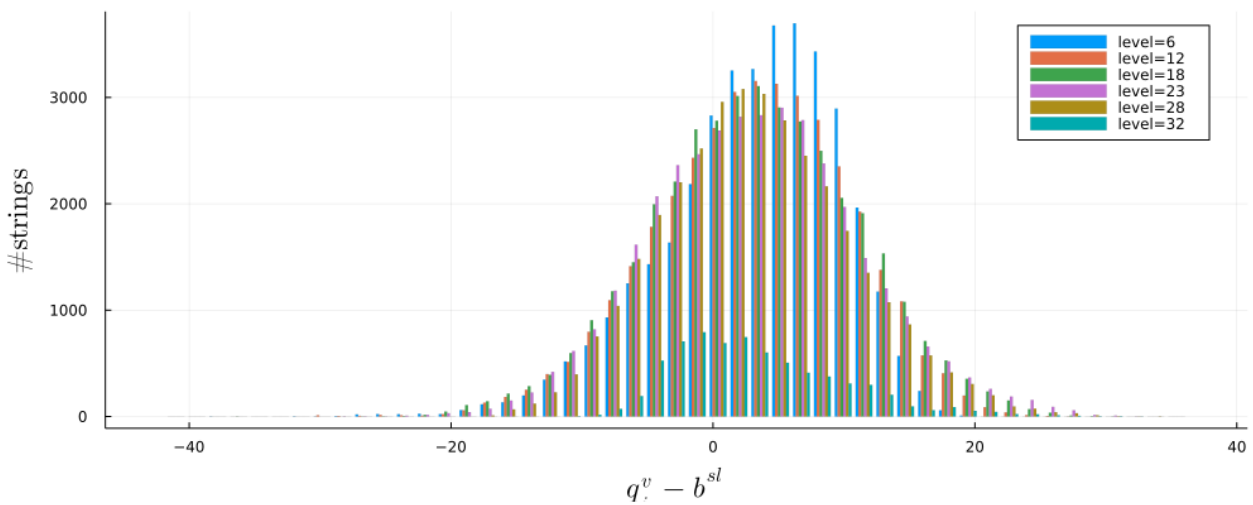
denotes the average length of all remaining input strings for all nodes in V_{ext}, and λ is a control parameter.

Relative Value Function Based Approach (RV-LBS)

Original remaining string lengths: $m = 10$, $n = 100$, $|\Sigma| = 4$



Cut remaining string lengths: $m = 10$, $n = 100$, $|\Sigma| = 4$, $\lambda = 1$



Relative Value Function Based Approach (RV-LBS)

Target Values:

Evaluate solutions in relation to other states at a current BS level.

- Approximation Goal:

$$h(v) \approx \mathrm{LCS}_{\mathrm{exp}}(v) - \frac{1}{|V_{\mathrm{ext}}|} \sum_{v' \in V_{\mathrm{ext}}} \mathrm{LCS}_{\mathrm{exp}}(v'), \tag{3}$$

$\mathrm{LCS}_{\mathrm{exp}}(v)$: expected solution length from node v.

Relative Value Function Based Approach (RV-LBS)

Obtaining Training Samples:

- Select whole levels of each BS run to create training data
- Utilize NBS to get a approximation of the expected solution length from a node v onward.
- Target value:

$$y^v = \mathrm{NBS}(v) - \frac{1}{|V_{\mathrm{ext}}|} \sum_{v' \in V_{\mathrm{ext}}} \mathrm{NBS}(v'), \tag{4}$$

Relative Value Function Based Approach (RV-LBS)

To get rid of number of the specific number of input strings: m

- Compress information of a remaining string lengths vector $q = (q_1, \ldots, q_m)$ into smaller vector of constant size $m' < m$ by downsampling through binning

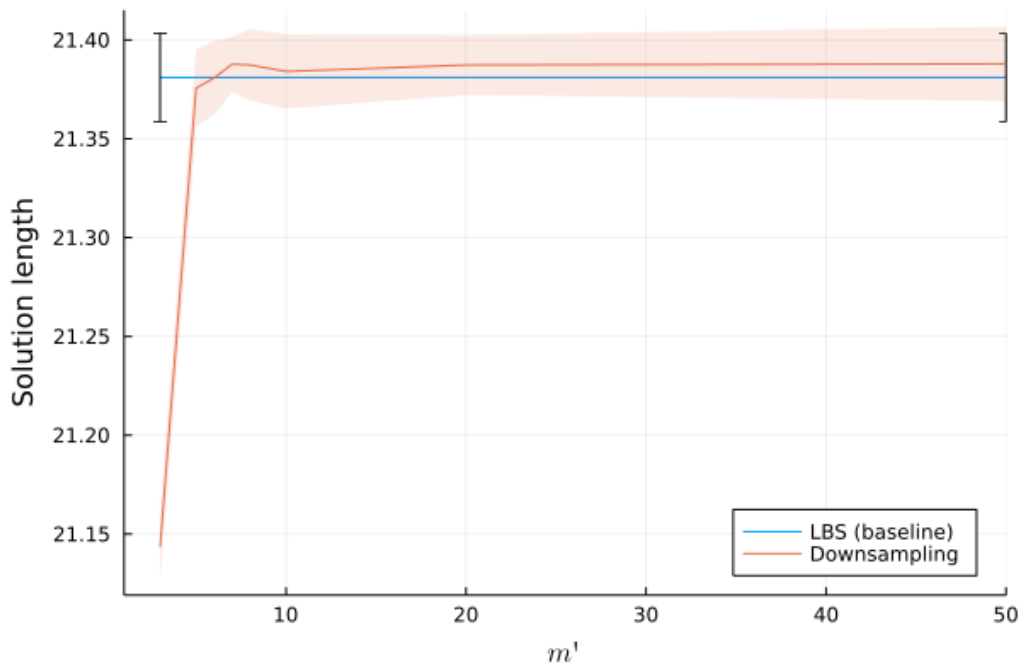


Figure: Previous LBS vs. downsampling approach $m = 100$, $n = 100$, $|\Sigma| = 4$.

Results

Training: $\lambda = 1$, $m' = 7$

m	n	Σ	s_RelVal	s_std
10	100	4	33.8	0.1054

Generalization: $\lambda = 1$, $m' = 7$

set	m	n	Σ	s_RelVal	s_std	s_LBS	s_Lit
rat	10	600	4	197.6	2.118	199	201
rat	100	600	4	132.7	2.869	135	133
BL	10	500	4	180.35	1.490	-	182.0
BL	10	1000	4	365.830	1.389	-	368.5

$\rightarrow$ RL-LBS trained on a small instance generalizes reasonably well to larger instances.

rat inst. set Shyu and Tsai (2009), BL inst. set Blum and Festa (2016)

Policy-Based Learning Beam Search

- Follows point-of-view from Negrinho et al. (2018):
  - ML model gets whole beam V_{ext} as input
  - Learn a scoring function for ranking the nodes, select β best nodes
- Special NN architecture
- Different loss functions considered and compared
- We again utilize Nested BS for obtaining training data
- Results comparable to LBS

Comparison to AlphaZero-like MCTS-based Approach

- Similar to Silver et al. (2018),
  but adapted to single-player scenario, normalization of values
- We did not obtain competitive results
- BUT: Learning works, because plugging trained NN into a BS yields almost competitive results!

Conclusions

- Built on BS because **simple is beautiful!**
- Learning with Nested BS works surprisingly well
- Only exploited a very limited number of features here
- Demonstrated on LCS/CLCS problem, but also nice results on
  - no-wait flowshop problem (Mayerhofer, 2022)
  - shortest common supersequence problem (ongoing work)
  - a quantum circuit design problem (ongoing work)
- Bootstrapping as in temporal difference learning also works here
- Evaluation on a wider-range of benchmark problems remains
- For some problems special NN structures (e.g., GNNs) required
- Well suited for parallelization

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