Teaching Transformers to Solve Combinatorial Problems through Efficient Trial & Error

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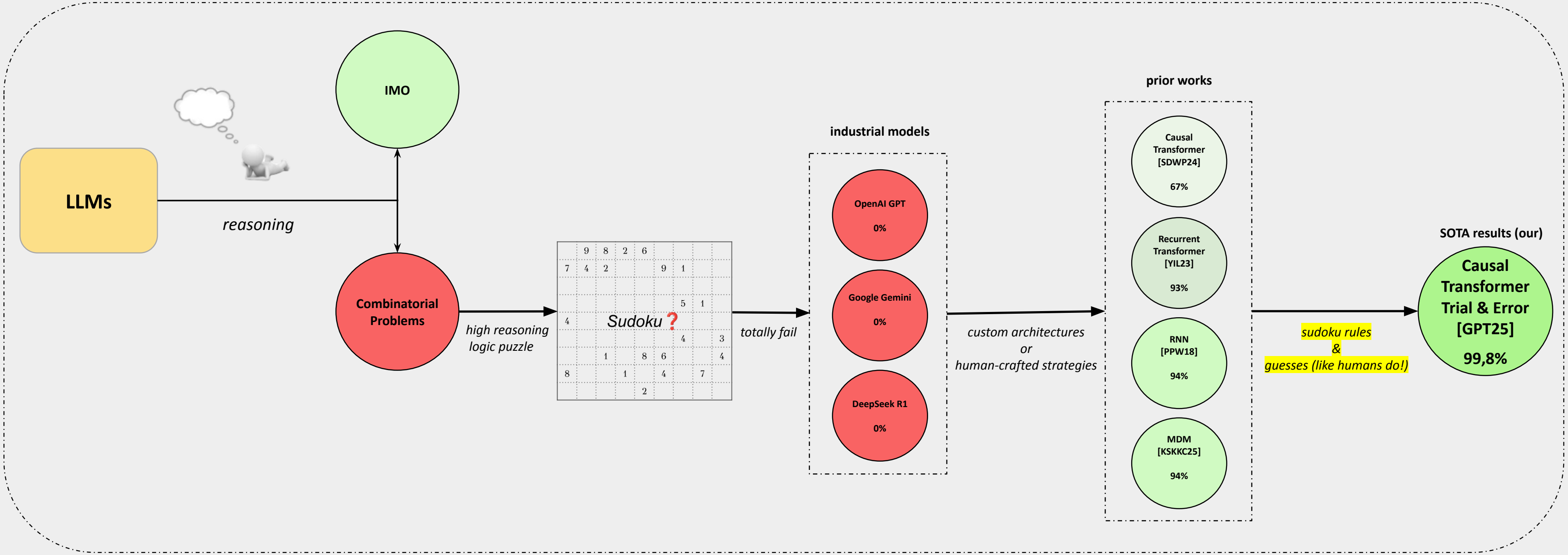
Motivation

LLMs have shown surprisingly strong results in mathematical tasks, but…



Key Contributions

- A generalized framework for NP-class problems
- No custom architecture: valina-decoder only GPT-2 with 42M parameters
- Training transcripts solely based on Sudoku rules (DFS method) and guesses
  - An approach that can solve Sudoku which we do not know yet deterministic strategies to solve them
  - Close related approach to human nature!
- Minimization of guesses via a novel loss inspired by Min-Sum Set Cover problem
- SOTA results; accuracy 99.8% on randomly generated Sudoku
- SudokuPy: a Python library for generating random Sudoku puzzles

(1/2) Imitation Learning

Sudoku rules + informed multiple guesses

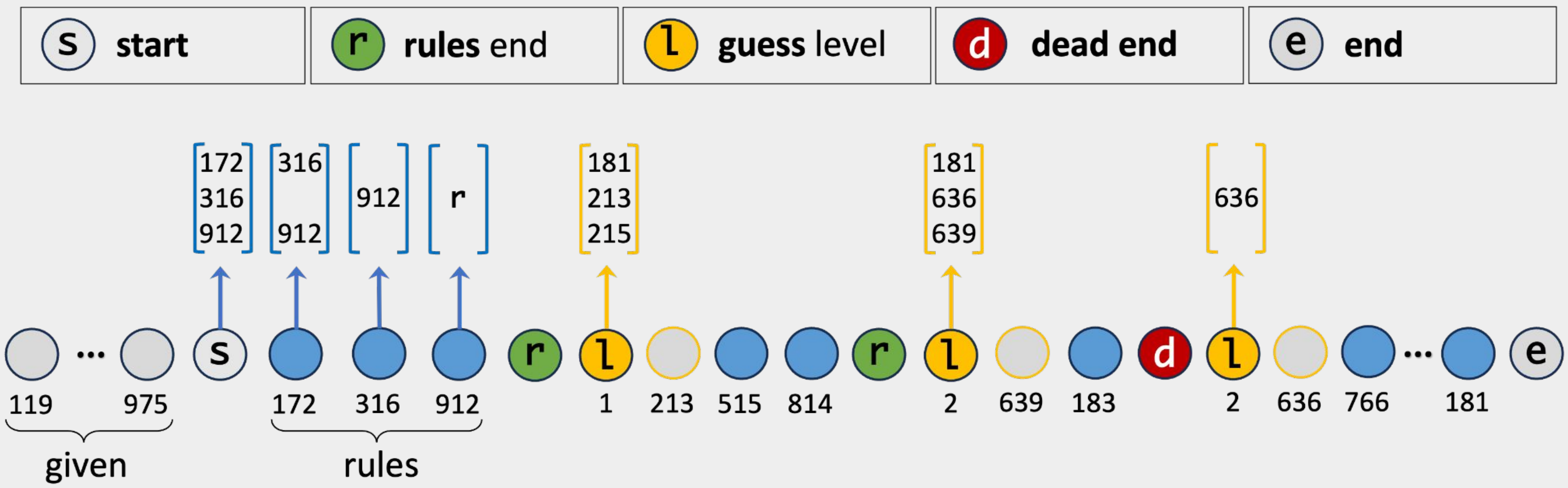
- <u>Encoding</u>: Each move encoded as a 3-digit number rcv (111 → 999); row_column_value

- <u>Multiple Targets</u>: Combinatorial puzzles allow multiple valid next moves
  - Instead of a single deterministic label, we support multiple next-token predictions
    Cross Entropy loss: $-\log p_i$ → Multiple target loss: $-\sum \log p_i$ over all valid next tokens

- <u>Results</u>: Accuracy 98,9%; SOTA compared to other prior works
  Accuracy 99,1% in 1-3 SAT problem (NP-complete problem)

(2/2) Imitation Learning

Sudoku rules + informed multiple guesses



(1/4) Beyond Imitation Learning

Sudoku rules + a single guess

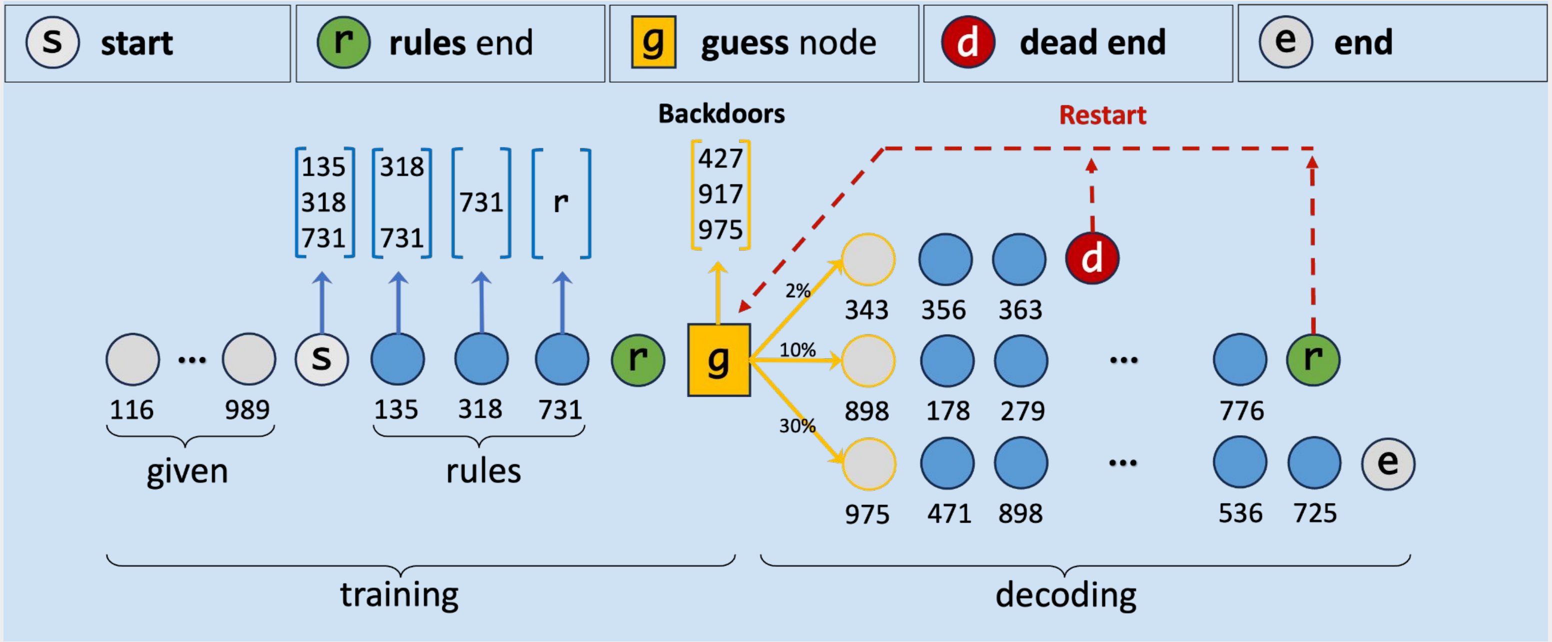
- <u>Encoding & Multiple Targets</u>: Same as Imitation Learning
- <u>Guesses</u>: A single guess (backdoor; once identified, applying simple rules leads to the full solution)
- <u>Loss Function</u>: We still support multiple next-token predictions and a new loss formulation for guesses

  Multiple target loss: $-\log p_i$ & Guesses loss: $1/\sum p_i$ over all valid guesses (1)

- <u>Results</u>: Accuracy 99.8%; new SOTA, outperforming even our previous best results
- <u>Insights</u>: This approach shows empirically that 99.8% of Sudokus can be solved by using only one guess (backdoor)

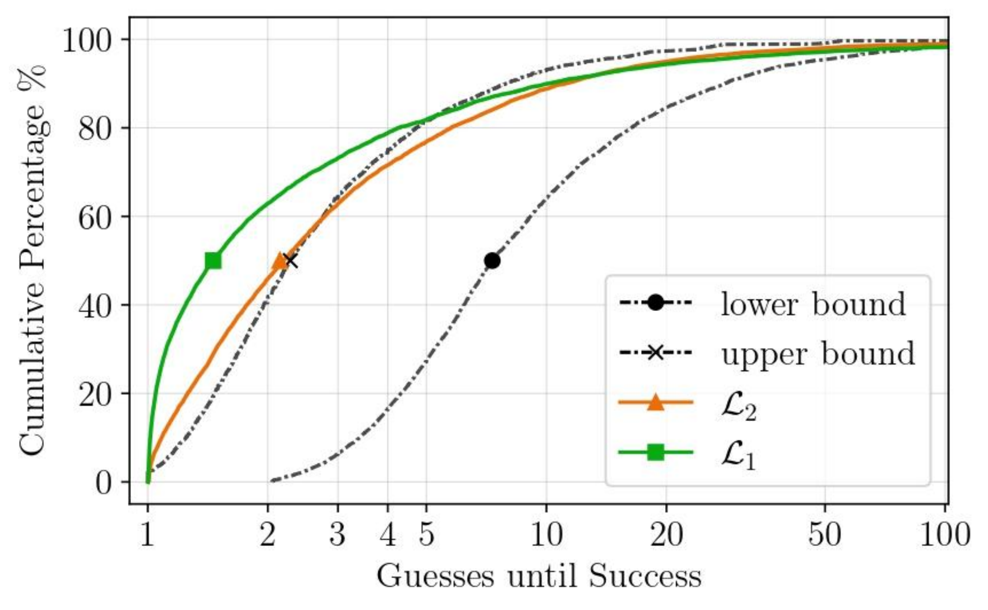
(2/4) Beyond Imitation Learning

Sudoku rules + a single guess



(3/4) Beyond Imitation Learning

Sudoku rules + a single guess



<u>Remark</u>: For half of all Sudokus, the backdoor guess can be found in about 1,5 guesses

(4/4) Beyond Imitation Learning

Mathematical insights

- Assumptions: depth-1 of search and non adaptive policy
- Challenge:
  - You face *n* possible choices, but only a hidden subset *S* is valid
  - Subset *S* is drawn from a known distribution *D*
  - Each test costs 1 time unit and once it is made you only learn if it is valid
- Goal: Find a policy *π* that minimizes the expected time to discover a valid choice

Theorem. *For any distribution $\mathcal{D}$ over sets $S \subseteq [n]$, it holds that for any permutation τ:*

$$\min_{\pi \in \Delta(n)} \mathbb{E}_{S \sim \mathcal{D}} \left[\frac{1}{\sum_{i \in S} \pi_i} \right] \leq H_n \cdot \mathbb{E}_{S \sim \mathcal{D}} \left[\arg \min_{i=1}^{n} \{ \tau_i \in S \} \right]$$

where $H_n = 1 + \frac{1}{2} + \frac{1}{3} + \cdots + \frac{1}{n} = \Theta(\log n)$ is the n-th harmonic number.

Remark: Loss function (1) yields solutions with a bounded approximation to the optimal policy, whereas treating the problem as a multi-class classification task (e.g., weighted Cross-Entropy Loss) leads to much worse approximations

References

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- K. Shah, N. Dikkala, X.Wang, R.Panigrahy. Causal language modeling can elicit search and reasoning capabilities on logic puzzles. NeurIPS’24.
- J.Kim, K. Shah, V. Kontonis, S. Kakade, S. Chen. Train for the worst, plan for the best: Understanding token ordering in masked diffusions. ICML’25.

Questions & Answers

For questions, feel free to reach us via email

or

visit us in San Diego, USA!

For more details, read our full paper:

Thank you for your time!