Teaching Transformers to Solve Combinatorial Problems through Efficient Trial & Error

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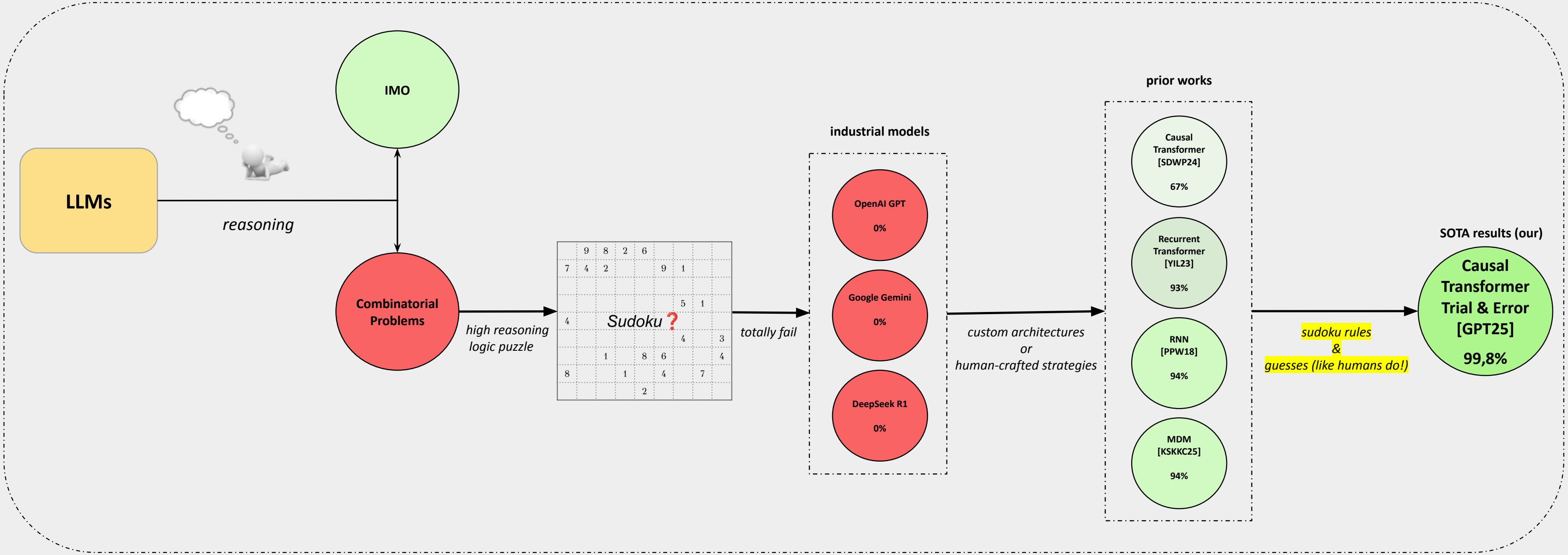
Presented at NeurIPS 2025, San Diego, USA — December 2025.

Motivation

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



Key Contributions

- A generalized framework for NP-class problems that have an efficient verifier
    - Sudoku is NP-complete problem
- 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 puzzles beyond those solvable by human-crafted strategies
    - 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
    - In combinatorial problems, an efficient generator enables live-stream training without relying on static datasets, helping to avoid overfitting
    - Ensures that the model is exposed randomly to the full distribution of Sudoku puzzle difficulties, rather than a limited subset

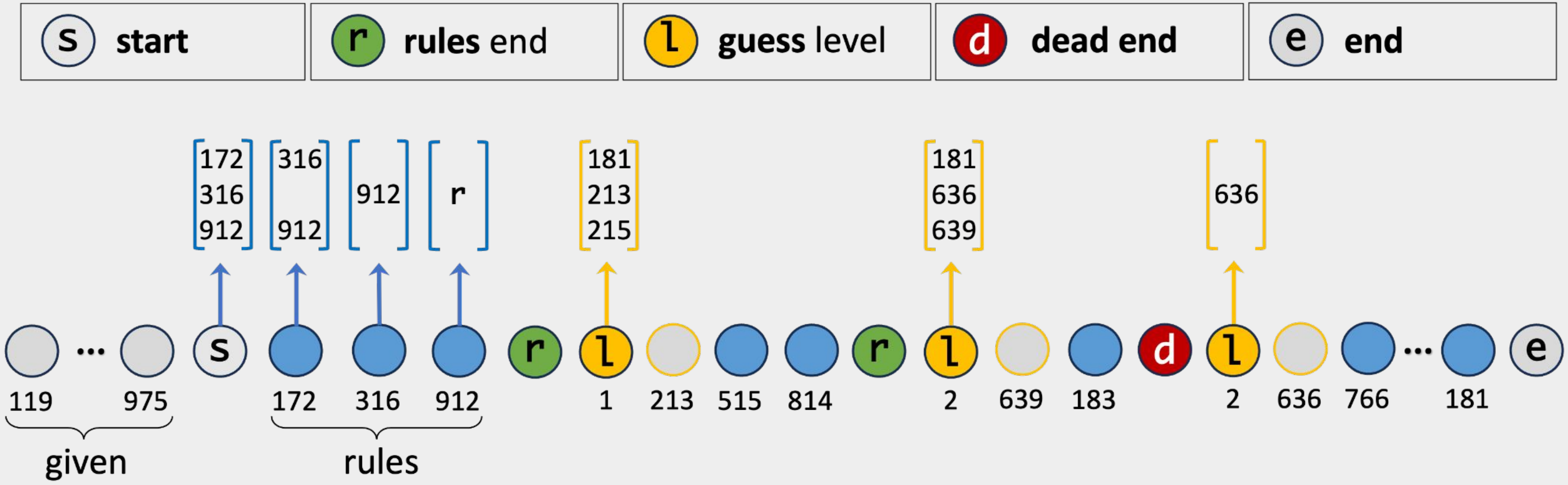
(1/2) Imitation Learning

Sudoku rules + informed multiple guesses

- Encoding: Each move encoded as a 3-digit number rcv (111 → 999); row_column_value
- Multiple Targets: 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
- Results: 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

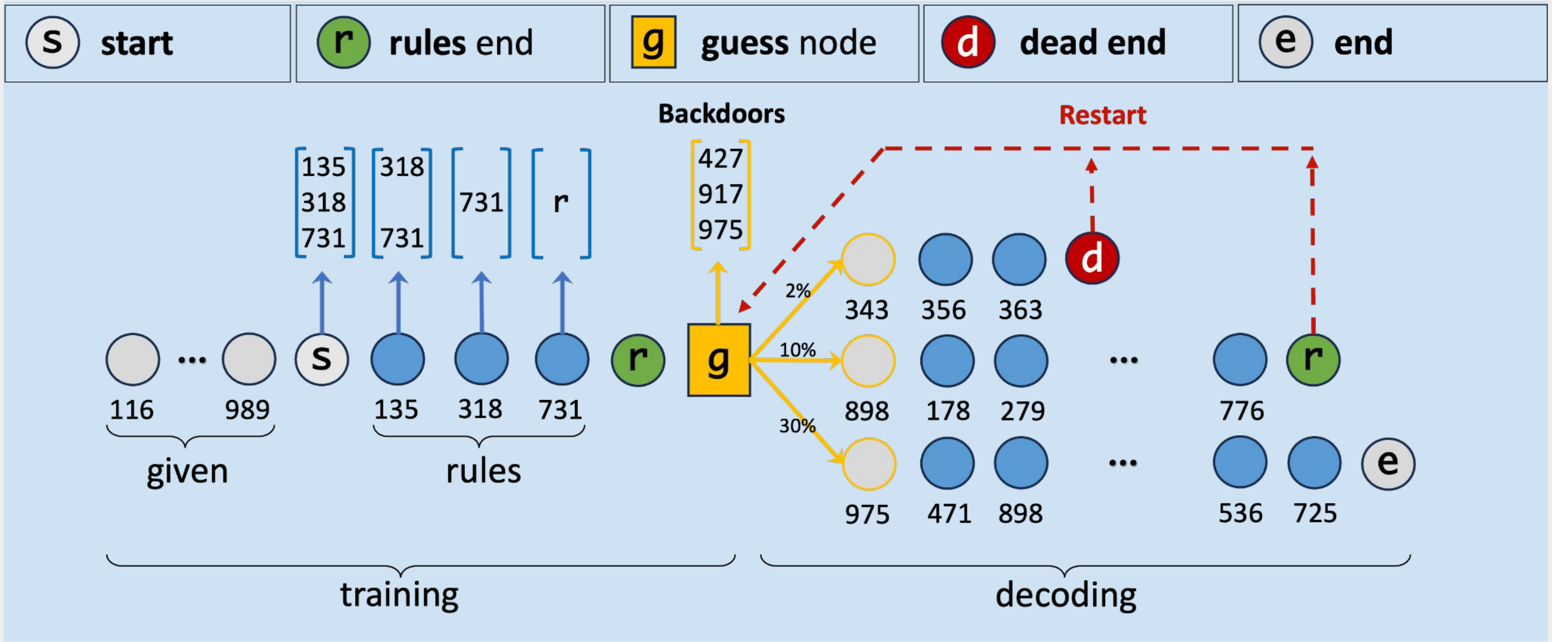
Sudoku rules + a single guess

- Encoding & Multiple Targets: Same as Imitation Learning
- Guesses: A single guess (backdoor; once identified, applying simple rules leads to the full solution)
- Loss Function: 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)
- Results: Accuracy 99.8%; new SOTA, outperforming even our previous best results
- Insights: This approach shows empirically that 99.8% of Sudoku can be solved by using only one guess (backdoor)

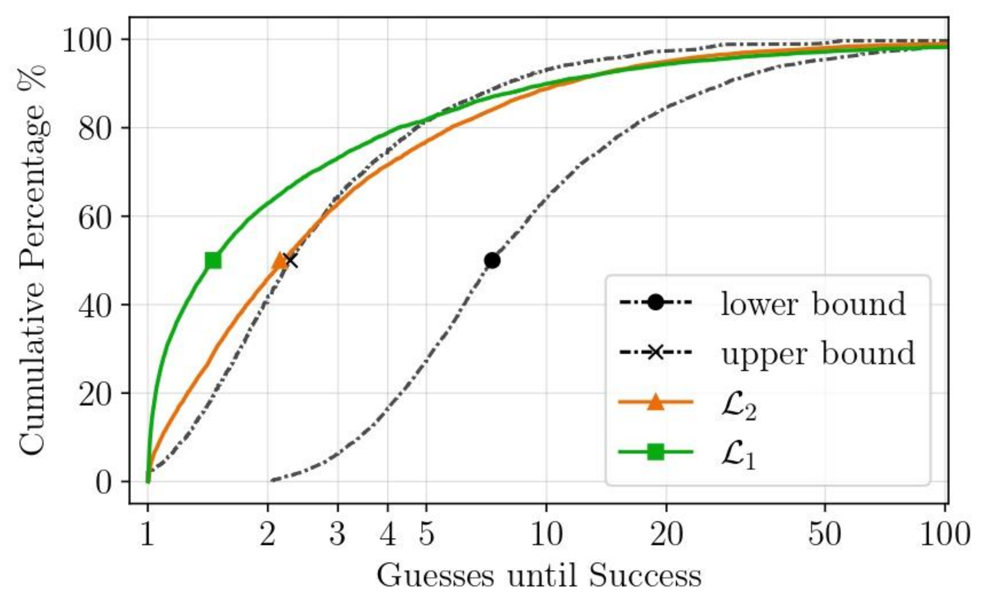
(2/4) Beyond Imitation Learning

Sudoku rules + a single guess



(3/4) Beyond Imitation Learning

Sudoku rules + a single guess



Remark: For half of all Sudoku, the backdoor guess can be found in about 1,5 guesses

(4/4) Beyond Imitation Learning

Mathematical insights

- <u>Assumptions</u>: depth-1 of search and non adaptive policy
- <u>Challenge</u>:
  - 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
- <u>Goal</u>: 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.

<u>Remark</u>: 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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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!