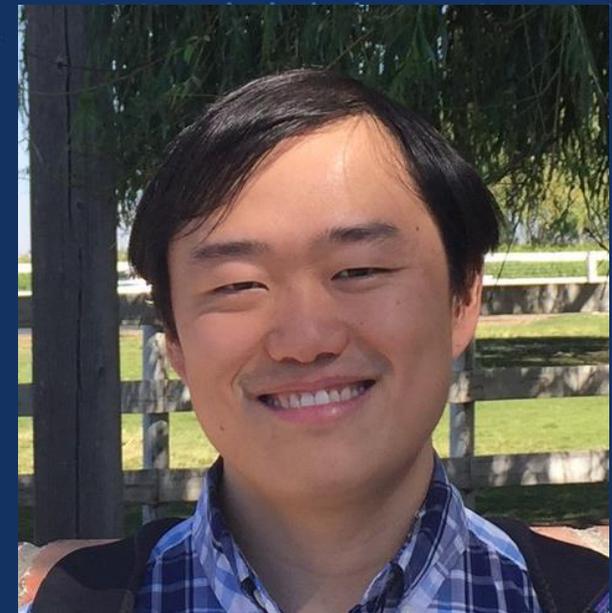


Towards a unified framework of Neural and Symbolic Decision Making

Yuandong Tian
Research Scientist Director

Meta AI (FAIR)



Large Language Models (LLMs)



Conversational AI



Content Generation



AI Agents

Standard Prompting

Input

Q: Roger has 5 tennis balls. He buys 2 more cans of tennis balls. Each can has 3 tennis balls. How many tennis balls does he have now?

A: The answer is 11.

Q: The cafeteria had 23 apples. If they used 20 to make lunch and bought 6 more, how many apples do they have?

Model Output

A: The answer is 27. ❌

Chain of Thought Prompting

Input

Q: Roger has 5 tennis balls. He buys 2 more cans of tennis balls. Each can has 3 tennis balls. How many tennis balls does he have now?

A: Roger started with 5 balls. 2 cans of 3 tennis balls each is 6 tennis balls. $5 + 6 = 11$. The answer is 11.

Q: The cafeteria had 23 apples. If they used 20 to make lunch and bought 6 more, how many apples do they have?

Model Output

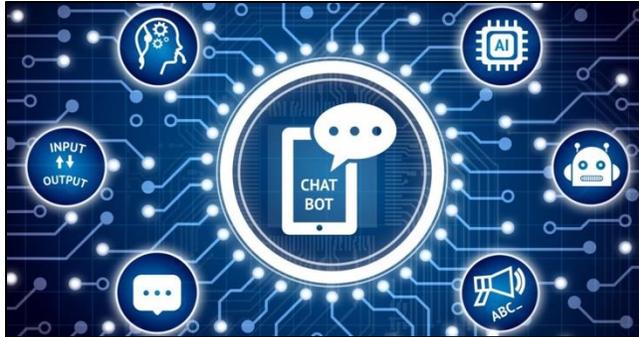
A: The cafeteria had 23 apples originally. They used 20 to make lunch. So they had $23 - 20 = 3$. They bought 6 more apples, so they have $3 + 6 = 9$. The answer is 9. ✅

Reasoning



Planning

Large Language Models (LLMs)



Conversational AI



Content Generation



AI Agents

Standard Prompting	Chain of Thought Prompting
<p>Input</p> <p>Q: Roger has 5 tennis balls. He buys 2 more cans of tennis balls. Each can has 3 tennis balls. How many tennis balls does he have now?</p> <p>A: The answer is 11.</p> <p>Q: The cafeteria had 23 apples. If they used 20 to make lunch and bought 6 more, how many apples do they have?</p>	<p>Input</p> <p>Q: Roger has 5 tennis balls. He buys 2 more cans of tennis balls. Each can has 3 tennis balls. How many tennis balls does he have now?</p> <p>A: Roger started with 5 balls. 2 cans of 3 tennis balls each is 6 tennis balls. $5 + 6 = 11$. The answer is 11.</p> <p>Q: The cafeteria had 23 apples. If they used 20 to make lunch and bought 6 more, how many apples do they have?</p>
<p>Model Output</p> <p>A: The answer is 27. ❌</p>	<p>Model Output</p> <p>A: The cafeteria had 23 apples originally. They used 20 to make lunch. So they had $23 - 20 = 3$. They bought 6 more apples, so they have $3 + 6 = 9$. The answer is 9. ✅</p>

Reasoning

Planning

What LLMs cannot do well yet?



User

I'm going from **Seattle to California** from **November 6 to 10, 2023**. I have a **budget of \$6,000**. For lodging, I prefer an **entire room** and the accommodations must be **pet-friendly**.

Travel planning

What LLMs cannot do well yet?



I'm going from **Seattle to California** from **November 6 to 10, 2023**. I have a **budget of \$6,000**. For lodging, I prefer an **entire room** and the accommodations must be **pet-friendly**.



Information Collection

[Tool] **CitySearch**[California]
 [Result] San Francisco, Los Angeles, ..., San Diego



[Tool] **FlightSearch**[Seattle, San Francisco, 2023-11-06]
 [Result] No Flights.

[Tool] **FlightSearch**[Seattle, Los Angeles, 2023-11-06]
 [Result] Flight Number: F123, 13:40-16:12, Cost: \$120

[Tool] **DistanceMatrix**[Los Angeles, San Diego, taxi]
 [Result] Duration: 1 hour 57 mins, Distance: 193 km, Cost: \$200

Planning

The plan must adhere to certain **constraints**, e.g., **user needs** and **commonsense**. It's also vital to ...



User Needs (Hard Constraints)

1. Budget: \$6000
2. Room Type: Entire Room
3. Room Rule: Pet-friendly



Commonsense Constraints

1. Reasonable City Route
2. Diverse Restaurants
3. Diverse Attractions
4. Non-conflicting Transportation
5. Accommodation meets Minimum Night



Delivery Plan

2023-11-06	2023-11-07	2023-11-08	2023-11-09	2023-11-10
Seattle -> Los Angeles • Flight: F123 (13:40-16:12), Cost: \$120 • Accommodation: Luxury building studio • Dinner: The Attraction	Los Angeles • Breakfast: Chicken Minar • Lunch: Rajdhani Restaurant • Dinner: Domino's Pizza • Accommodation: Santa Monica Pier, Griffith Park • Accommodation: Luxury building studio	Los Angeles -> San Diego • Take taxi to San Diego • Breakfast: Open Yard • Lunch: The Lost Mughal • Dinner: Burger King • Attractions: Cabrillo Monument • Accommodation: East Side Apartment	San Diego • Breakfast: Baskin Robbins • Lunch: Harry's Bar • Dinner: Dragon Way • Attractions: La Jolla Shores Park, California Tower • Accommodation: East Side Apartment	San Diego -> Seattle • Flight: F789 (7:59-10:56), Cost: \$300



2023-11-06

Seattle -> Los Angeles

- Flight: F123, (13:40-16:12), Cost: \$120
- Accommodation: Luxury building studio
- Dinner: The Attraction

Using SoTA LLMs for Travel Planning (not great)

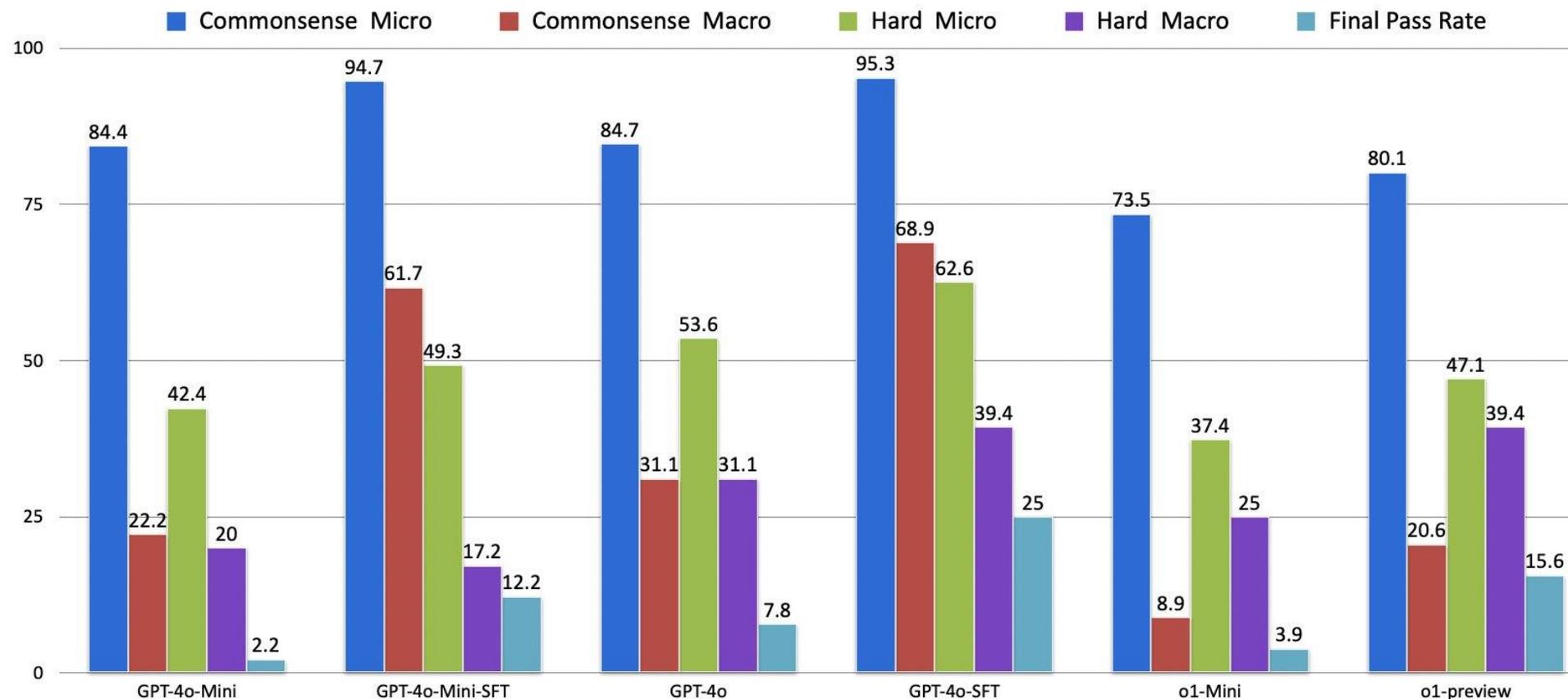
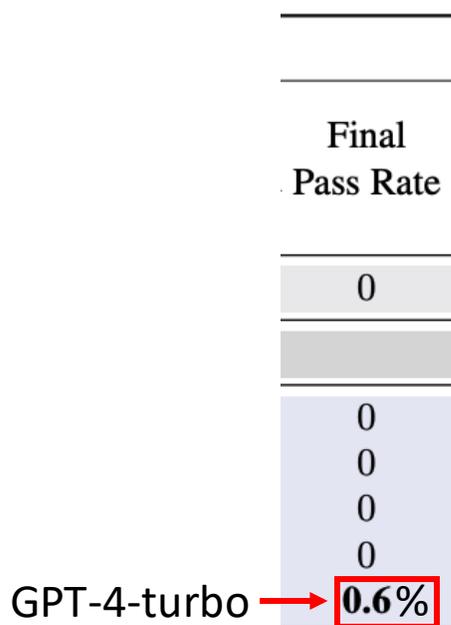
Even SoTA LLMs struggle for such hard planning problems

	Validation (#180)						Test (#1,000)					
	Delivery Rate	Commonsense Pass Rate		Hard Constraint Pass Rate		Final Pass Rate	Delivery Rate	Commonsense Pass Rate		Hard Constraint Pass Rate		Final Pass Rate
		Micro	Macro	Micro	Macro			Micro	Macro	Micro	Macro	
Greedy Search	100	74.4	0	60.8	37.8	0	100	72.0	0	52.4	31.8	0
Two-stage												
Mistral-7B-32K (Jiang et al., 2023)	8.9	5.9	0	0	0	0	7.0	4.8	0	0	0	0
Mixtral-8x7B-MoE (Jiang et al., 2024)	49.4	30.0	0	1.2	0.6	0	51.2	32.2	0.2	0.7	0.4	0
Gemini Pro (G Team et al., 2023)	28.9	18.9	0	0.5	0.6	0	39.1	24.9	0	0.6	0.1	0
GPT-3.5-Turbo (OpenAI, 2022)	86.7	54.0	0	0	0	0	91.8	57.9	0	0.5	0.6	0
GPT-4-Turbo (OpenAI, 2023)	89.4	61.1	2.8	15.2	10.6	0.6	93.1	63.3	2.0	10.5	5.5	0.6
Sole-planning												
Direct _{GPT-3.5-Turbo}	100	60.2	4.4	11.0	2.8	0	100	59.5	2.7	9.5	4.4	0.6
CoT _{GPT-3.5-Turbo}	100	66.3	3.3	11.9	5.0	0	100	64.4	2.3	9.8	3.8	0.4
ReAct _{GPT-3.5-Turbo}	82.2	47.6	3.9	11.4	6.7	0.6	81.6	45.9	2.5	10.7	3.1	0.7
Reflexion _{GPT-3.5-Turbo}	93.9	53.8	2.8	11.0	2.8	0	92.1	52.1	2.2	9.9	3.8	0.6
Direct _{Mixtral-8x7B-MoE}	100	68.1	5.0	3.3	1.1	0	99.3	67.0	3.7	3.9	1.6	0.7
Direct _{Gemini Pro}	93.9	65.0	8.3	9.3	4.4	0.6	93.7	64.7	7.9	10.6	4.7	2.1
Direct _{GPT-4-Turbo}	100	80.4	17.2	47.1	22.2	4.4	100	80.6	15.2	44.3	23.1	4.4

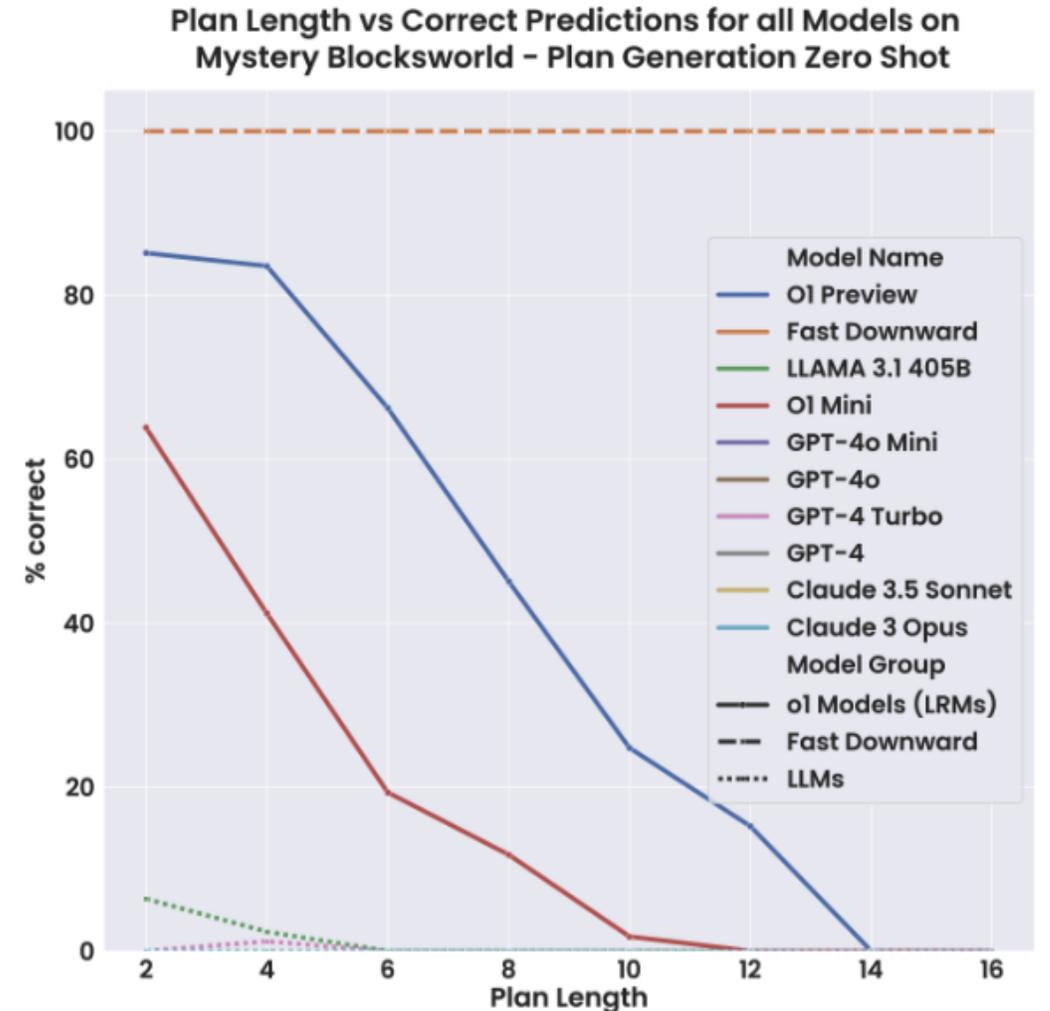
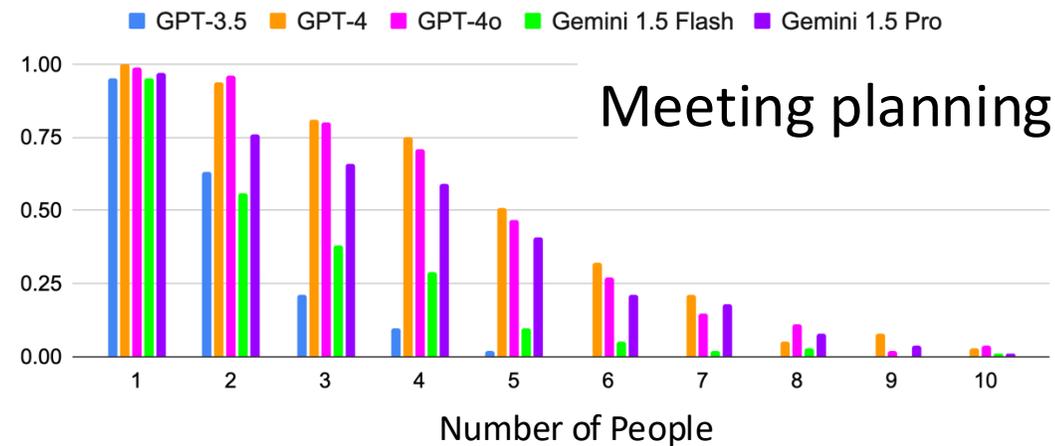
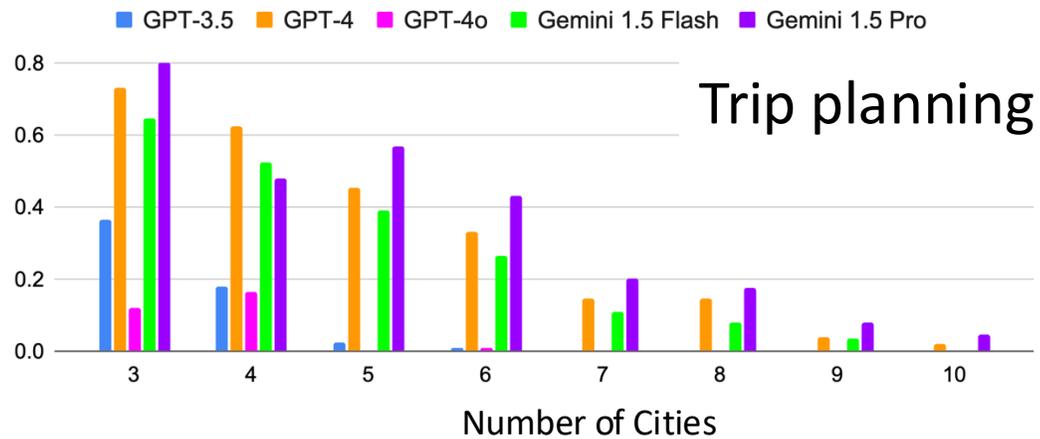
First tool use,
Then plan the travel

Ground-truth tool use,
Then plan the travel

How about o1?

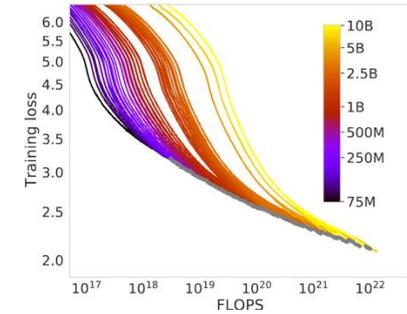


LLM planning is still a hard problem

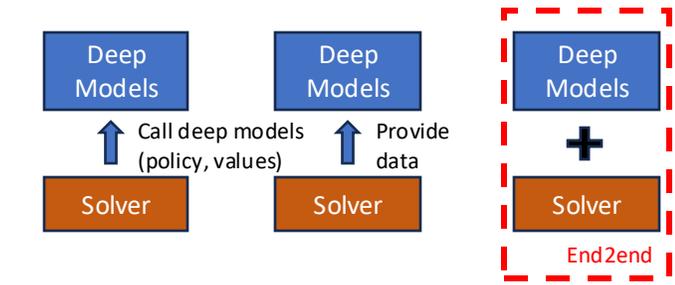


What are the Solutions?

What are the Solutions?



Option **One**: Scaling Law

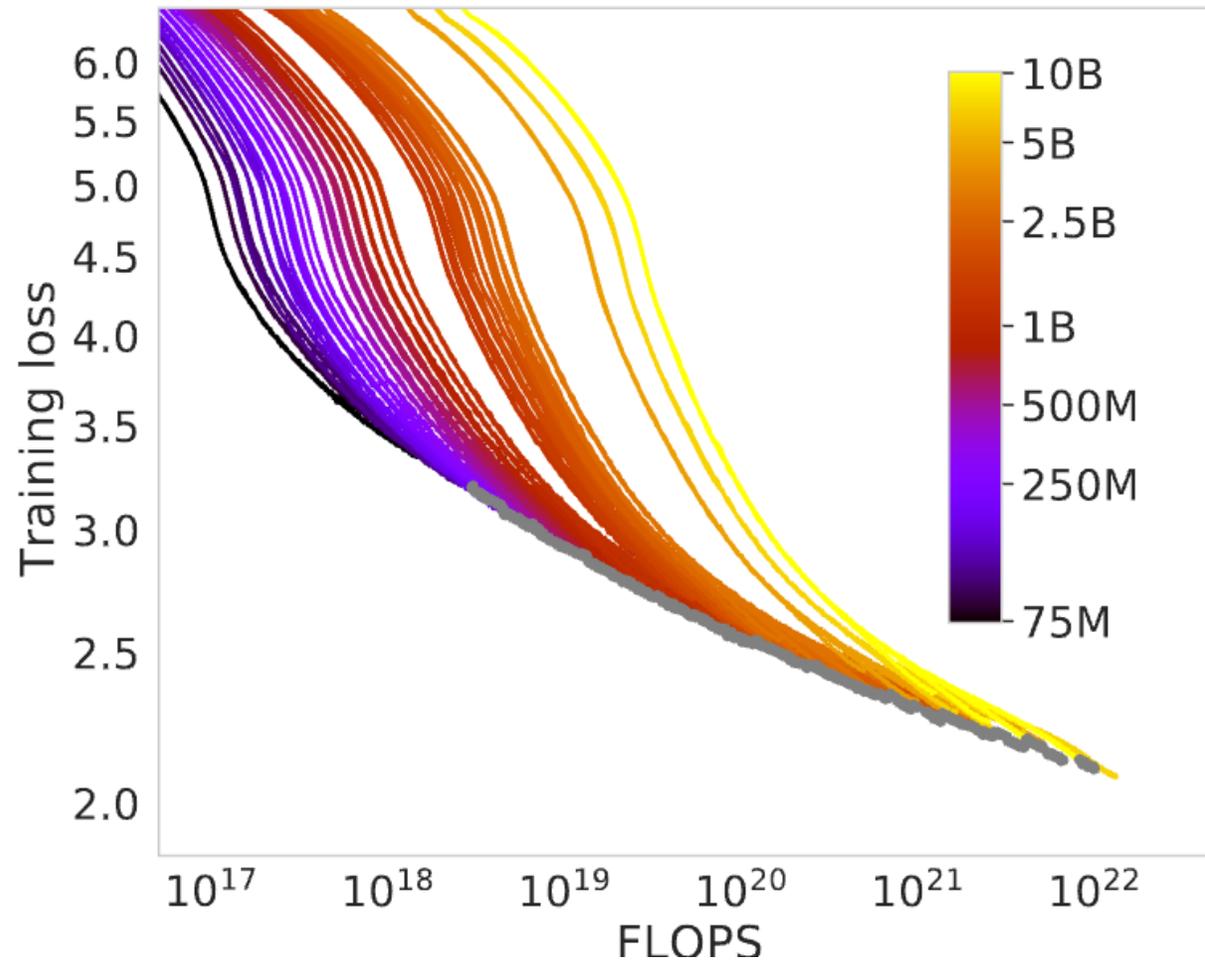


Option **Two**: Hybrid System



Option **Three**: Emerging Symbolic Structure from Neural network

Option One: The Scaling Law



More data
More compute
Larger models

Very expensive

**Does that work for
reasoning/planning?**

Option **Two**: Hybrid Systems

Deep Models



Tool use

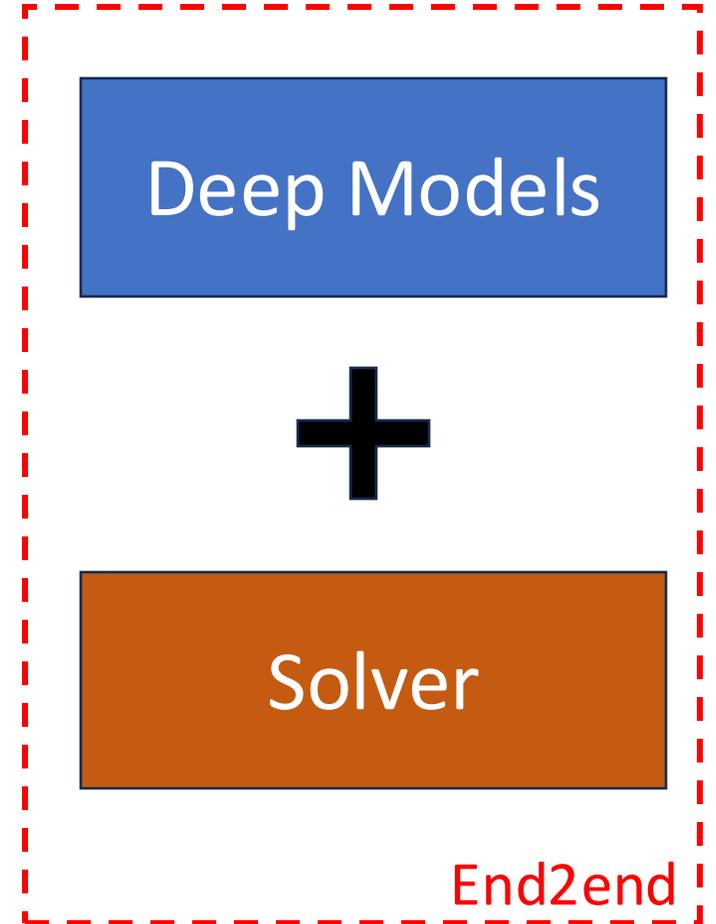
Solver

Deep Models



Provide data

Solver



Option **Two**: Hybrid Systems

Deep Models



Tool use

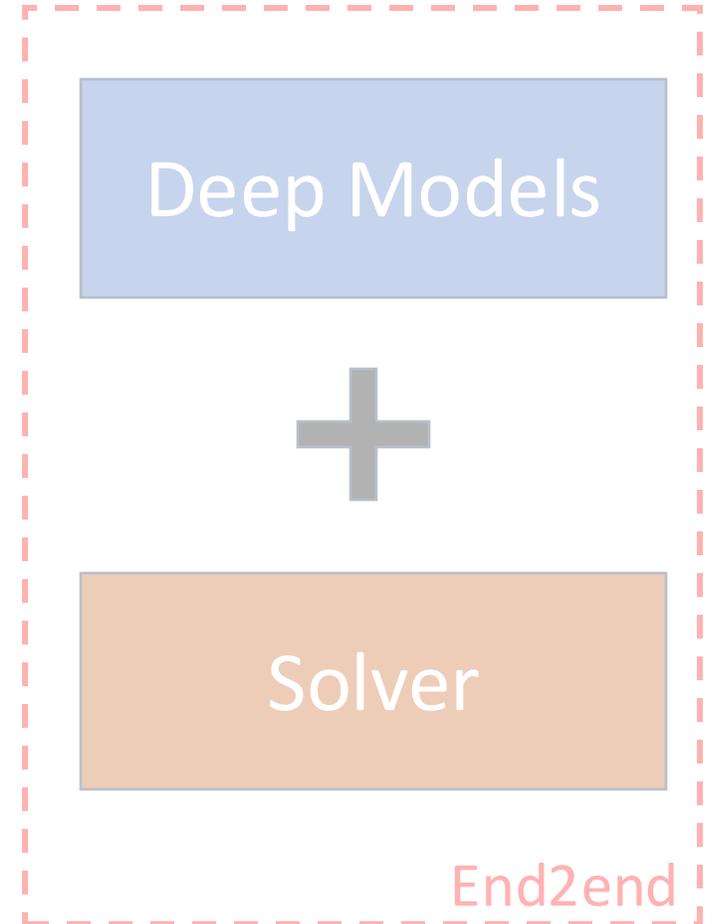
Solver

Deep Models



Provide data

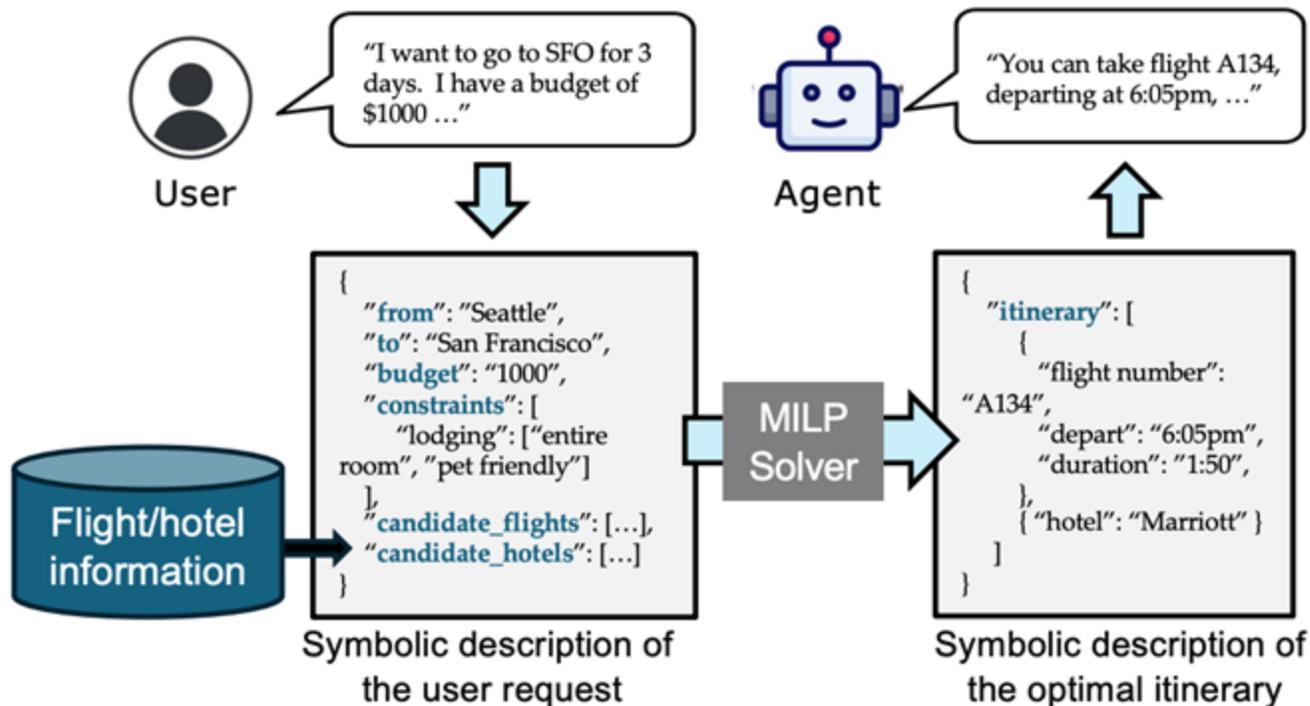
Solver



Language-Driven Guaranteed Travel Planning

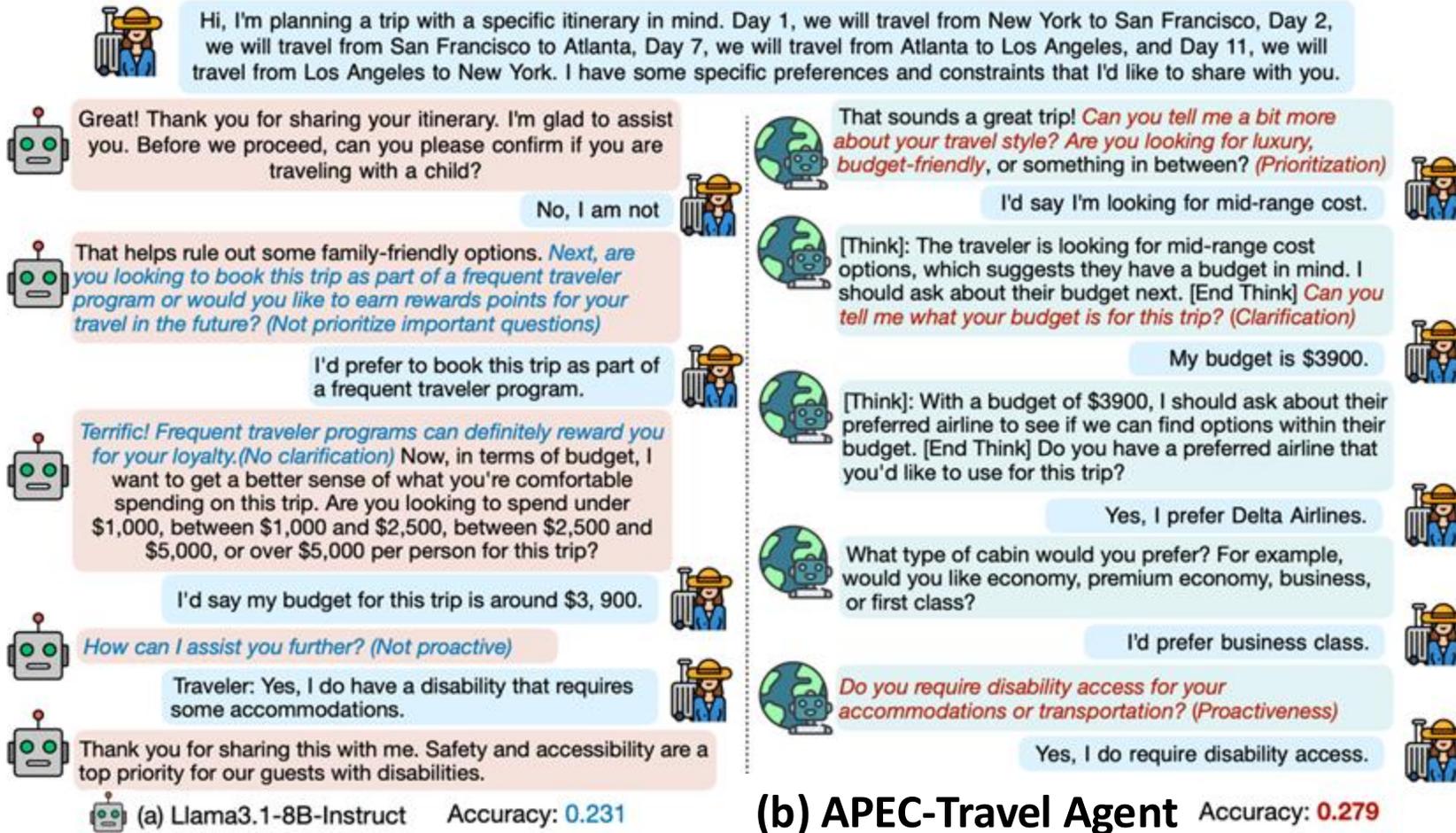
LLMs can not handle too many constraints? -> Combinatorial Solvers can!

Inference



- Realistic dataset: collect from the real world
- User instruction translator: Fine-tuned LLM to convert user request into symbolic description, augmented by flight/hotel information from database.
- Impose constraints and formalize the travel planning as Mixed Integer Linear Programming (MILP).
- Build a combinatorial solver to give optimal solution.

Multi-round Dialogs to Collect Information



User has hidden constraints, how to figure out?

→ Proactively ask!

APEC Agent Constitution

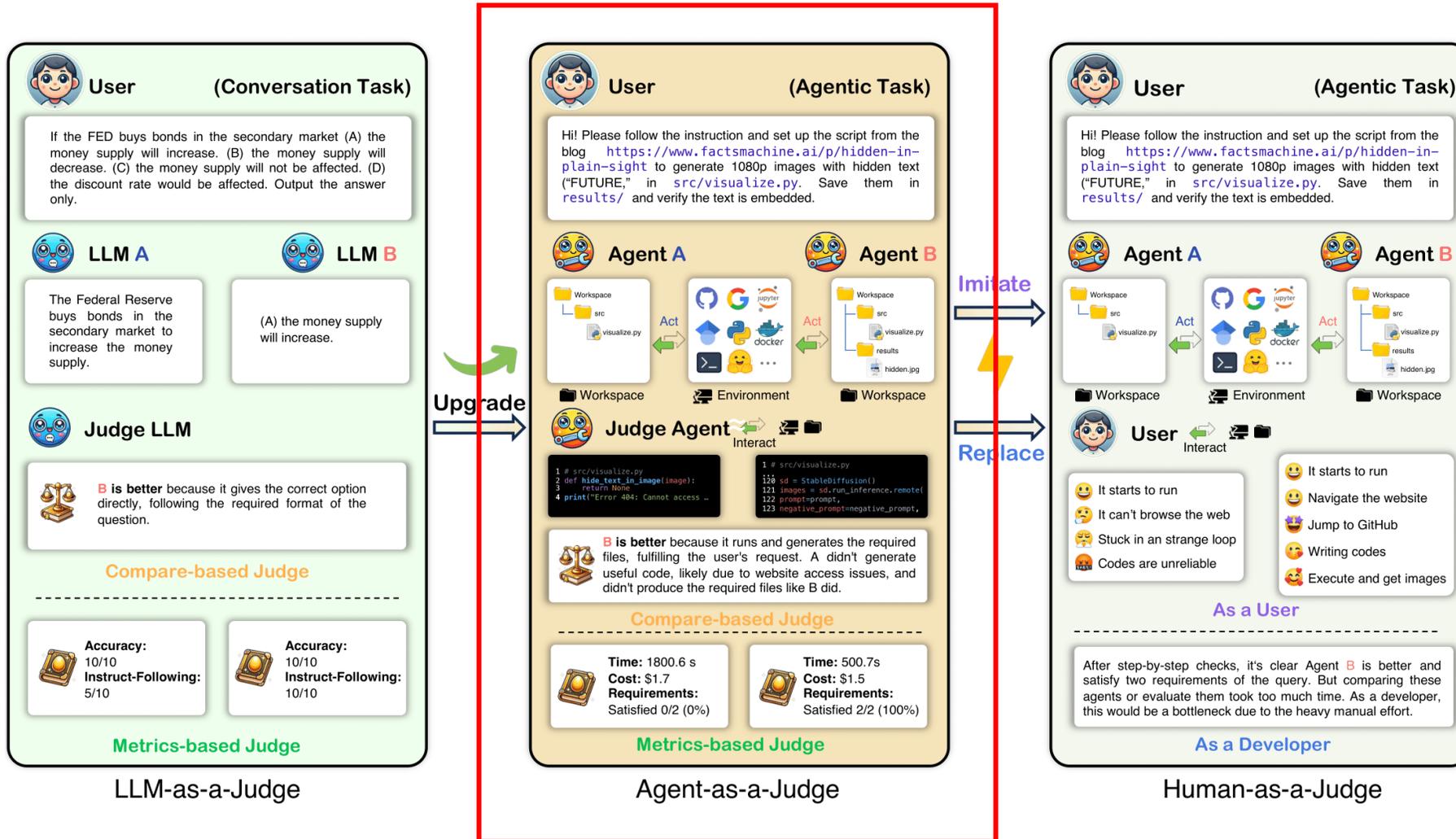
LLM agents should be evaluated and optimized not only based on final outcome, but also based on the **procedure** of how agents achieve the goal.

- **Accuracy**. The quality of the final solution that the agent provides (e.g., number of questions that are answered correctly).
- **Proactivity**. Whether the agent proactively collects useful information to solve the task. Such information may be public or private, vague or precise, explicitly provided or inferred from requests.
- **Efficiency**. Whether the agent can achieve its goal with a minimal number of interactions (e.g., number of questions asked, API calls and tool uses).
- **Credibility**. The reliability with which agents achieve positive outcomes (e.g., amount of hallucination and inconsistency).

Using Agent Constitution to fine-tune the models

Model	Average	Accuracy		Efficiency		Agentic Scores (Full score in each axis: 5)			
	#Rounds	Overall	Critical	Overall	Critical	Plan & Priority	Proactive	Clarification	Total
Llama-3.1-8B	15.49	0.231	0.301	0.015	0.019	3.88	4.07	3.90	11.86
Llama-3.1-8B-Reasoning	15.50	0.217	0.287	0.014	0.018	3.80	4.06	3.87	11.75
APEC-Travel-SFT	9.39	0.261	0.417	0.029	0.047	4.46	4.25	3.68	12.41
APEC-Travel-DPO									
Iteration 1	11.19	0.286	0.423	0.027	0.041	4.36	4.22	3.86	12.46
Iteration 2	9.77	0.279	0.425	0.031	0.047	4.48	4.32	4.13	12.95
Iteration 3	11.18	0.295	0.442	0.029	0.044	4.35	4.30	3.99	12.67
Iteration 2+3	11.36	0.296	0.448	0.028	0.043	4.44	4.28	3.79	12.52
<i>Other SoTA LLMs</i>									
Llama3.1-70B	15.49	0.243	0.308	0.016	0.020	3.95	4.19	3.84	12.00
Llama3.1-70B-Reasoning	15.48	0.229	0.310	0.015	0.020	3.93	4.31	4.02	12.28

Agent-as-a-Judge: Evaluate Agents with Agents



Option **Two**: Hybrid Systems

Deep Models



Tool uses

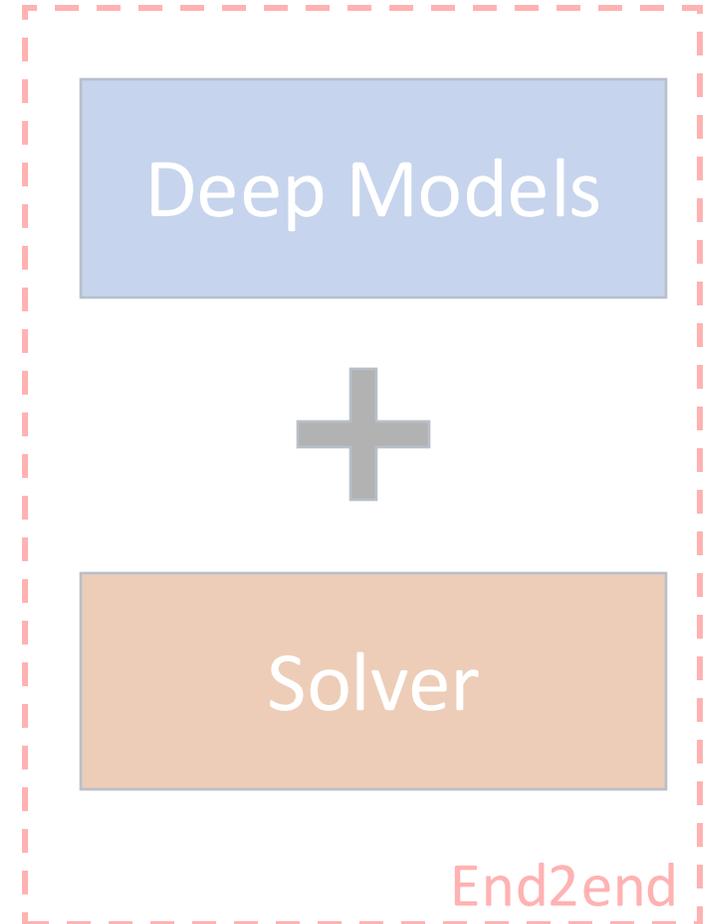
Solver

Deep Models



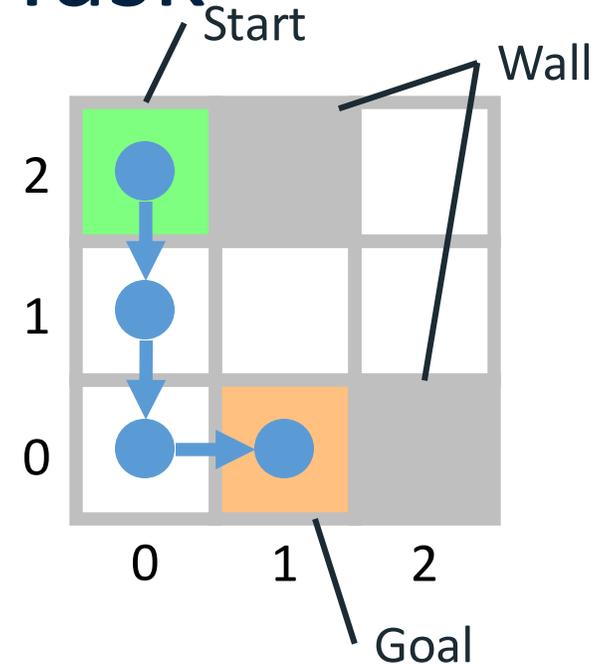
Provide data

Solver



Searchformer: A* Search as a Token Prediction

Task

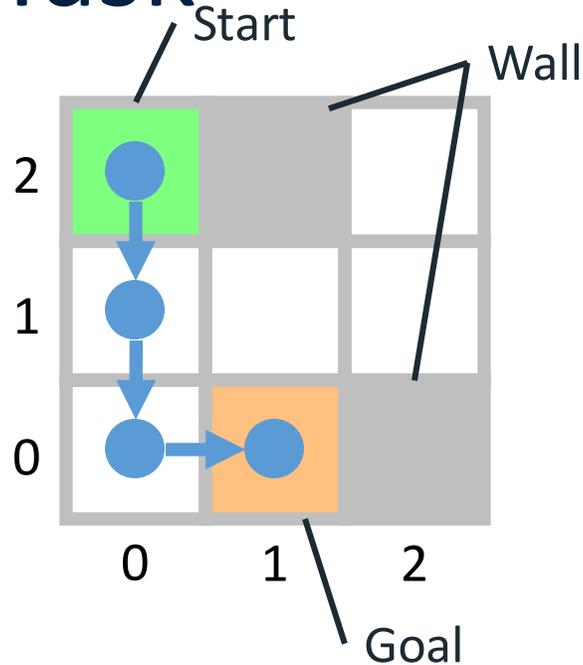


-  Plan step
-  Frontier state
-  Closed state



Searchformer: A* Search as a Token Prediction

Task



-  Plan step
-  Frontier state
-  Closed state

<prompt>

```

bos
start 0 2
goal 1 0
wall 1 2
wall 2 0
eos
    
```



<trace><plan>

```

bos
create 0 2 c0 c3
close 0 2 c0 c3
create 0 1 c1 c2
close 0 1 c1 c2
create 0 0 c2 c1
create 1 1 c2 c1
close 0 0 c2 c1
create 1 0 c3 c0
close 1 0 c3 c0
plan 0 2
plan 0 1
plan 0 0
plan 1 0
eos
    
```

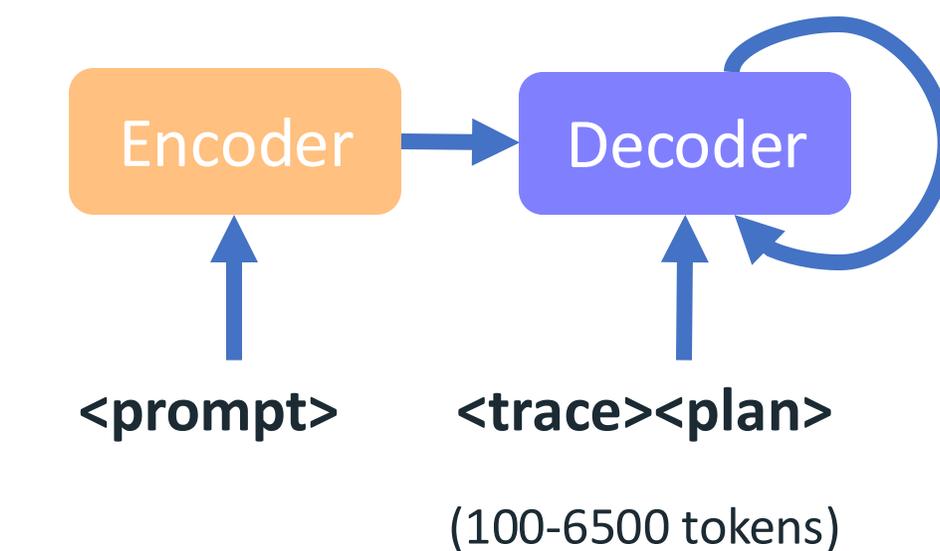
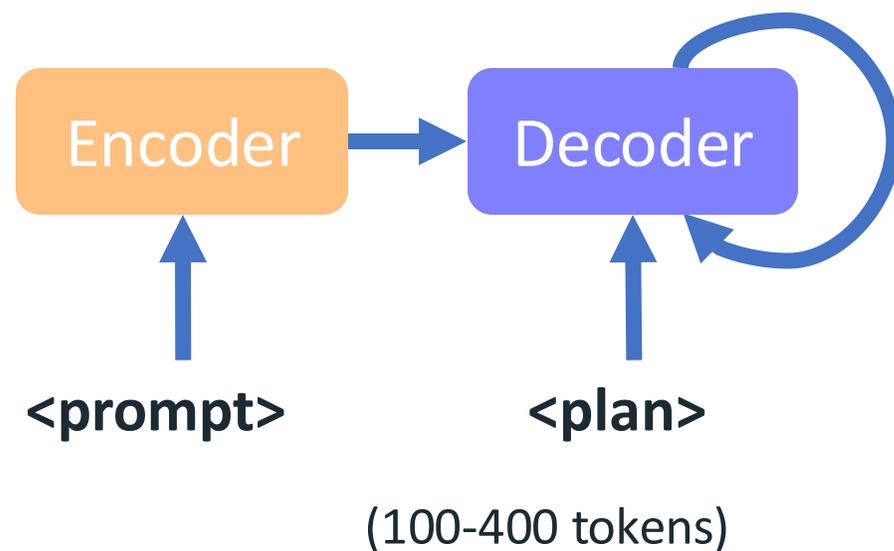
Training Method

Train a Transformer to predict the next token via teacher forcing.

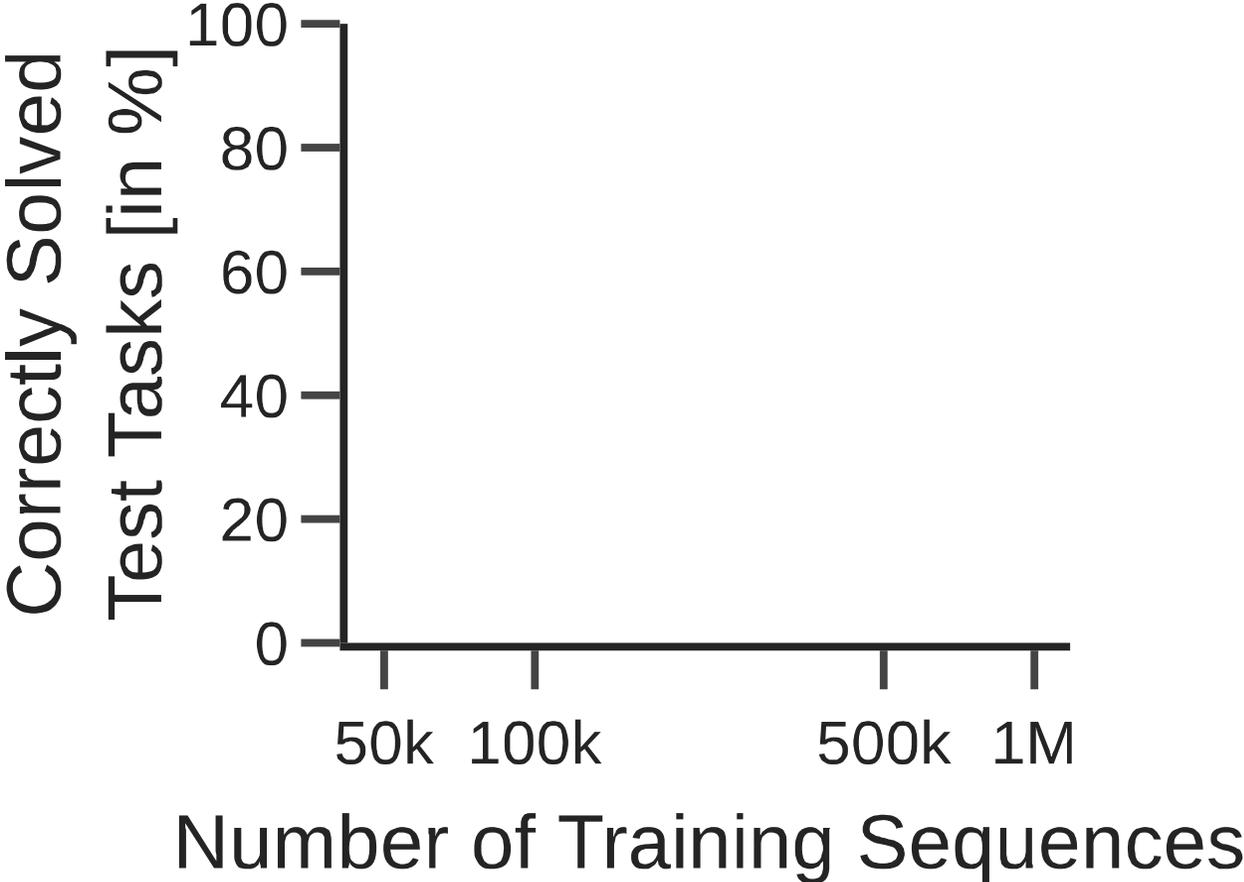
Model

Solution-Only Model

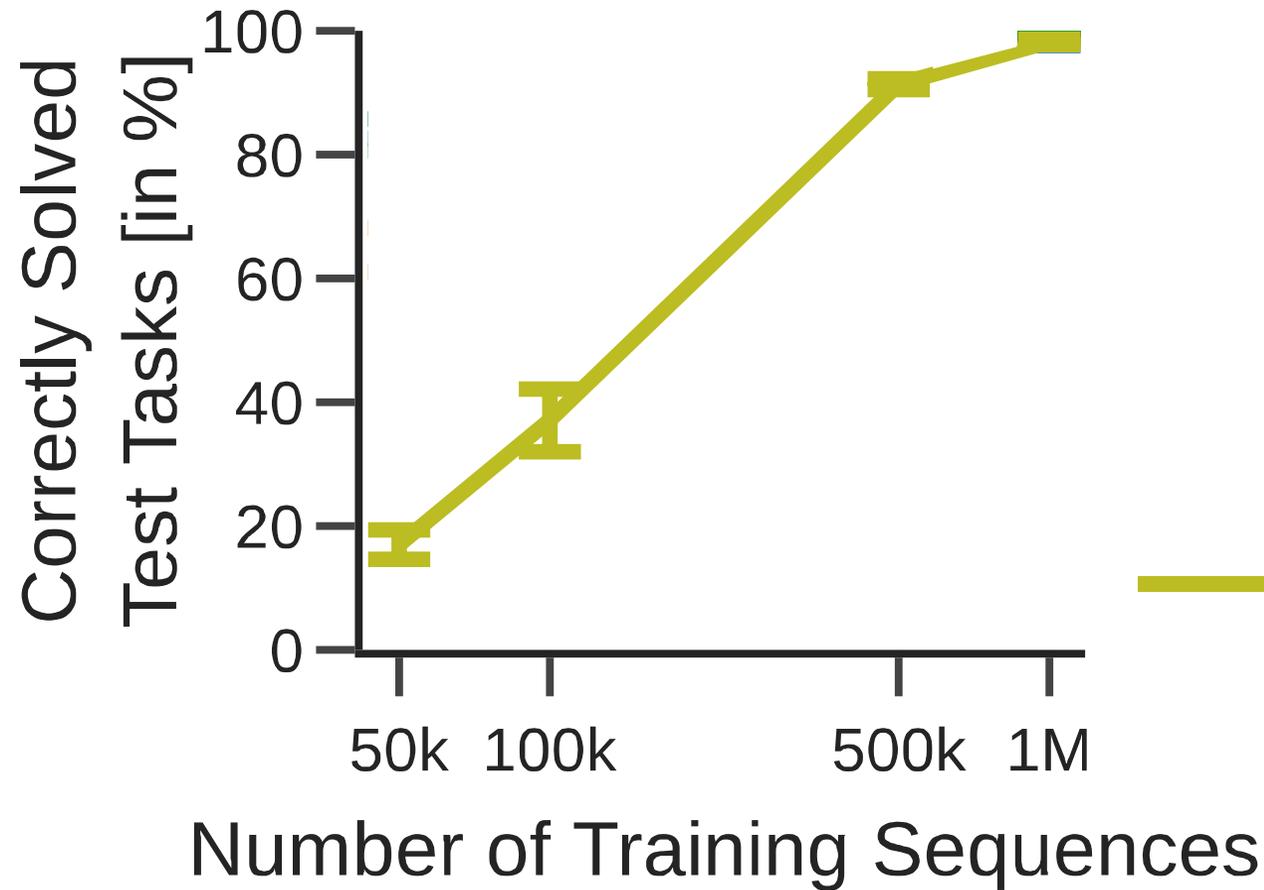
Search-Augmented Model



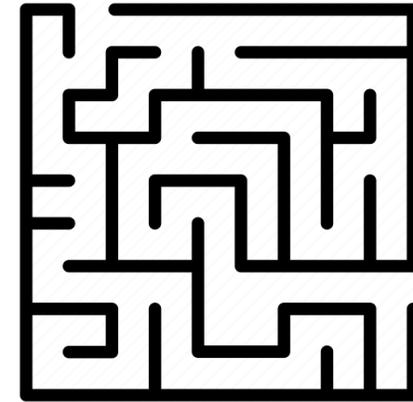
Search-Augmented vs. Solution-Only Models



Search-Augmented vs. Solution-Only Models

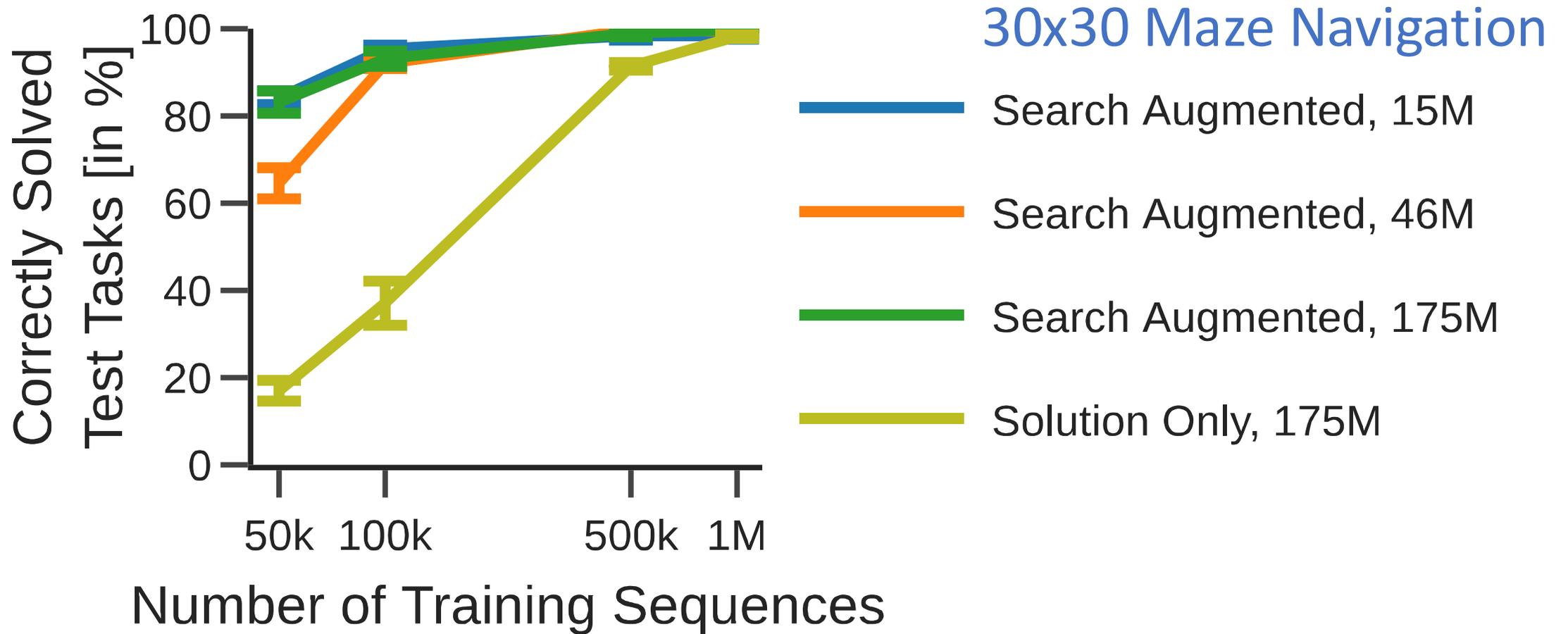


30x30 Maze Navigation

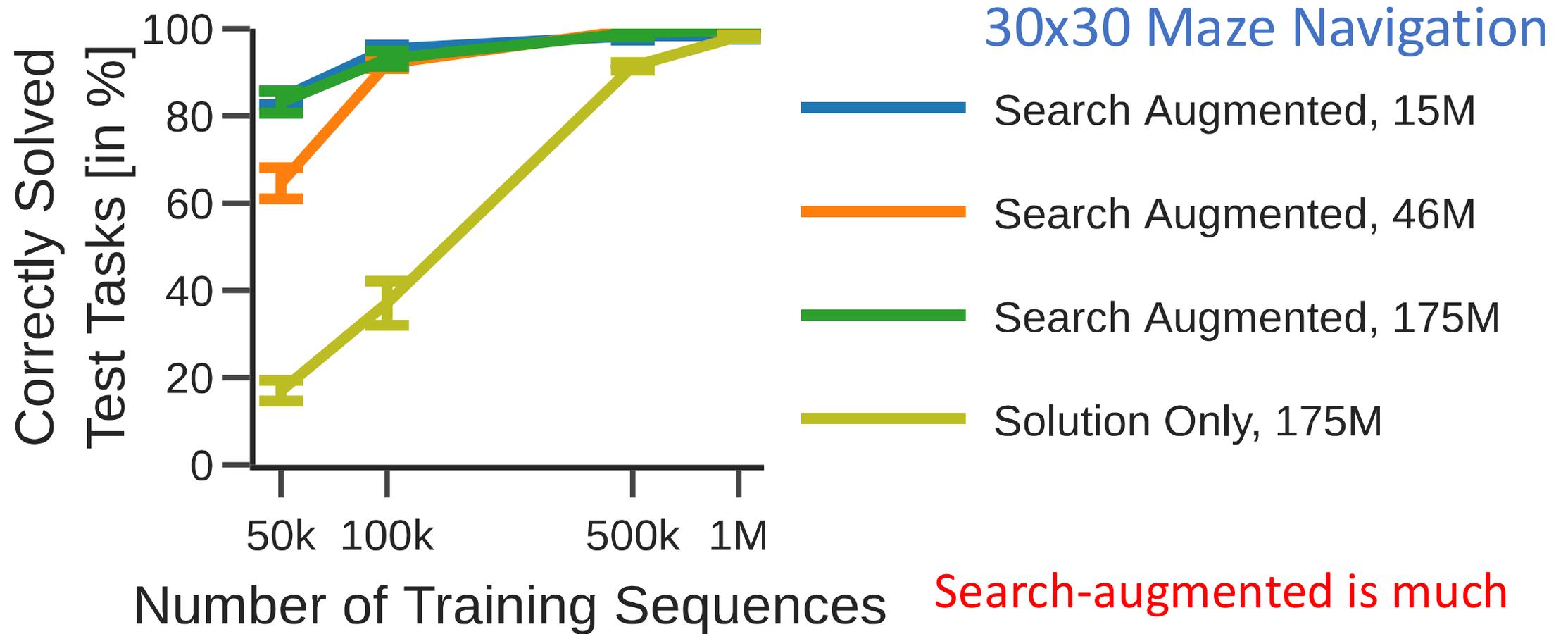


— Solution Only, 175M

Search-Augmented vs. Solution-Only Models

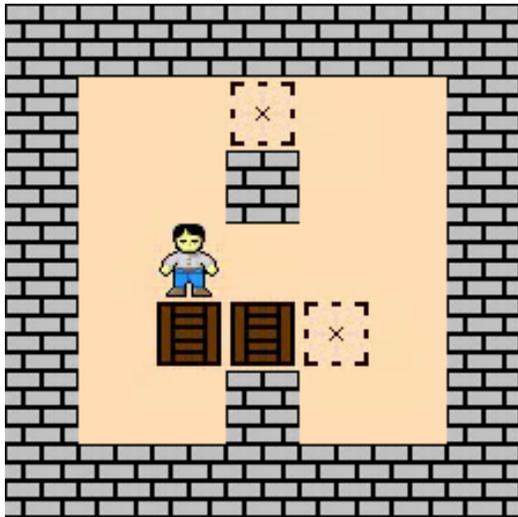


Search-Augmented vs. Solution-Only Models

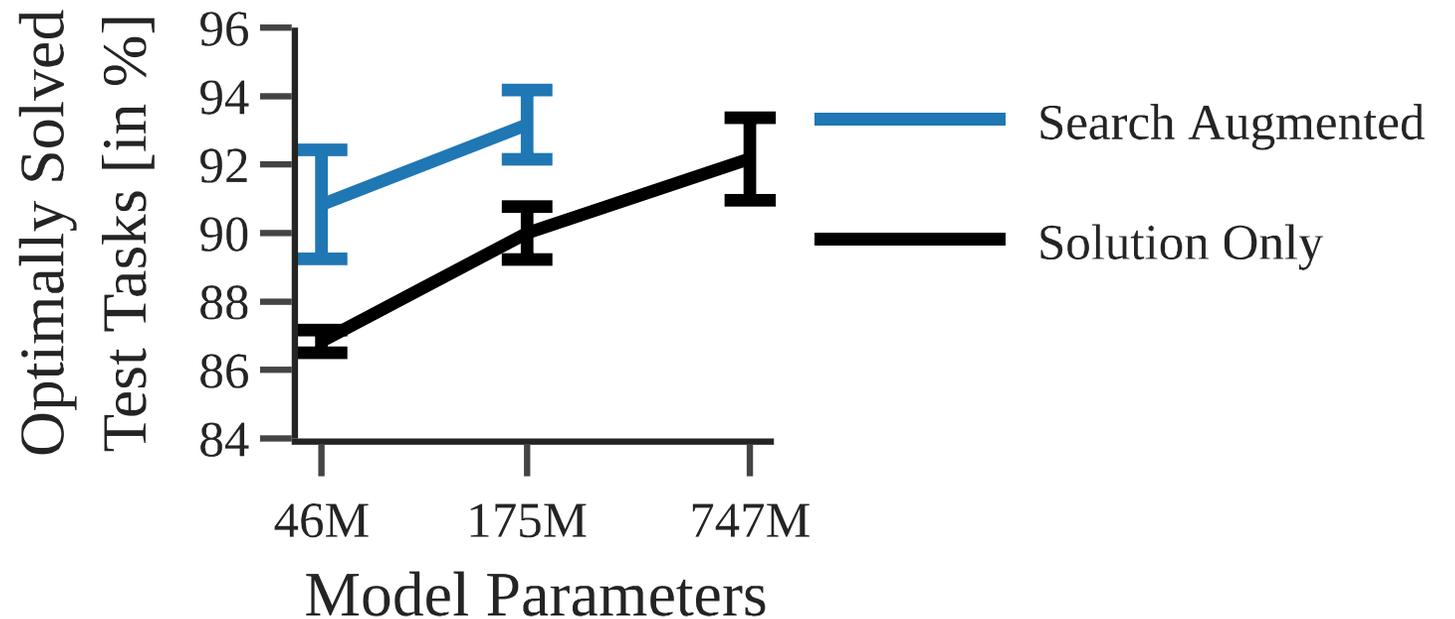


Search-augmented is much more parameter & data efficient!

Search-Augmented vs. Solution-Only Models



Sokoban



How to go beyond?

Imitation
Learning



Fine-tuning

Using solver's trace to train the
Transformer with teacher forcing

Fine-tune the model to achieve **shorter**
trace but still leads to **optimal** plan!
(Reinforcement Learning task)

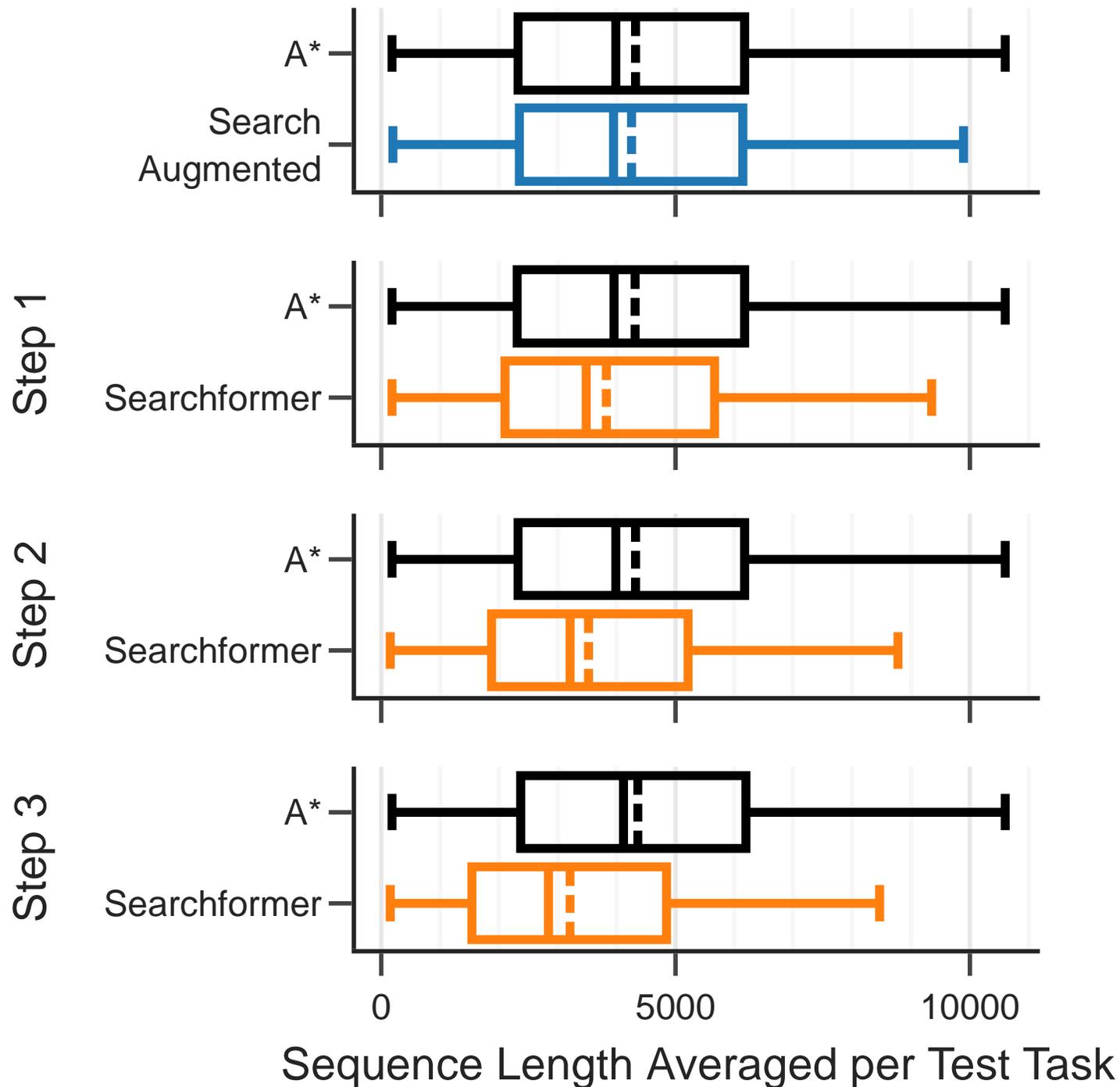
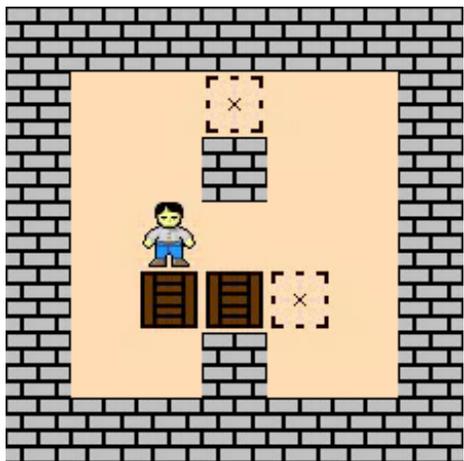


Search-augmented Models



Searchformer

Beyond A*: Improving search dynamics via bootstrapping



Improving search dynamics via bootstrapping

Params.	Model	ILR-on-solved	ILR-on-optimal
45M	Solution only	–	–
	Search augmented	0.908 ±0.020	0.919 ±0.019
	Searchformer, step 1	1.054 ±0.025	1.062 ±0.015
	Searchformer, step 2	1.158 ±0.025	1.181 ±0.012
	Searchformer, step 3	1.292 ±0.044	1.343 ±0.067
175M	Solution only	–	–
	Search augmented	0.925 ±0.010	0.933 ±0.011
757M	Solution only	–	–

Repeated bootstrapping increases the
Improved Length Ratio (ILR)



Improving search dynamics via bootstrapping

Params.	Model	Solved (%)	Optimal (%)
45M	Solution only	90.3 \pm 1.0	86.8 \pm 0.3
	Search augmented	92.5 \pm 1.0	90.8 \pm 1.6
	Searchformer, step 1	95.5 \pm 1.0	93.5 \pm 1.0
	Searchformer, step 2	96.0 \pm 0.5	93.4 \pm 0.6
	Searchformer, step 3	95.5 \pm 0.8	93.7 \pm 1.6
175M	Solution only	95.7 \pm 0.2	90.0 \pm 0.8
	Search augmented	95.2 \pm 0.9	93.2 \pm 1.0
757M	Solution only	96.5 \pm 0.1	92.2 \pm 1.2

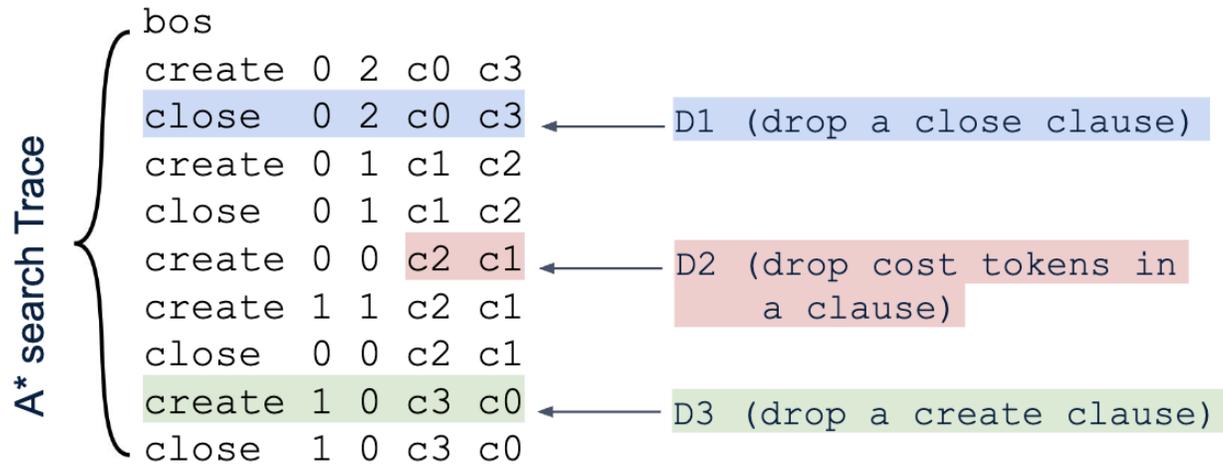
Fine-tuning improves performance initially.

Improving search dynamics via bootstrapping

Params.	Model	Solved (%)	Optimal (%)
45M	Solution only	90.3 \pm 1.0	86.8 \pm 0.3
	Search augmented	92.5 \pm 1.0	90.8 \pm 1.6
	Searchformer, step 1	95.5 \pm 1.0	93.5 \pm 1.0
	Searchformer, step 2	96.0 \pm 0.5	93.4 \pm 0.6
	Searchformer, step 3	95.5 \pm 0.8	93.7 \pm 1.6
175M	Solution only	95.7 \pm 0.2	90.0 \pm 0.8
	Search augmented	95.2 \pm 0.9	93.2 \pm 1.0
757M	Solution only	96.5 \pm 0.1	92.2 \pm 1.2

Searchformer
outperforms largest
solution-only model.

DualFormer (Searchformer v2)



Structured Trace Dropping Strategies

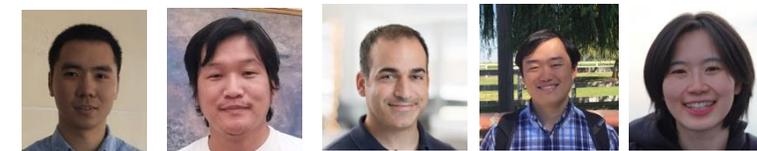
LvL 1 = D1 // drop all the close clauses

LvL 2 = D1 + D2 // drop all the close clauses + all the cost tokens

Lvl 3 = D1 + D2 + sampled D3 // Lvl 2 + drop some create clauses

Lvl 4 = drop the entire trace

DualFormer (Searchformer v2)



	Method	Avg Trace Length	1-Optimal-64 / 3-Optimal-64	1-Solved-64 / 3-Solved-64	SWC	Diversity
Maze 15 x 15	Dualformer (auto)	222	99.7 / 99.4	99.9 / 99.8	0.999	12.52
	Complete-Trace	495	94.6 / 90.1	96.7 / 93.0	0.964	7.60
	Solution-Only	-	72.0 / 68.9	82.7 / 80.1	0.610	1.52
Maze 20 x 20	Dualformer (auto)	351	99.5 / 98.6	99.9 / 99.3	0.997	20.28
	Complete-Trace	851	98.3 / 95.5	98.8 / 93.0	0.987	14.53
	Solution-Only	-	56.3 / 52.0	71.9 / 67.5	0.690	1.52
Maze 25 x 25	Dualformer (auto)	427	98.6 / 96.9	99.8 / 99.0	0.998	24.81
	Complete-Trace	1208	95.2 / 85.7	97.0 / 90.4	0.968	18.85
	Solution-Only	-	39.7 / 34.7	60.3 / 55.4	0.570	1.9
Maze 30 x 30	Dualformer (auto)	617	96.6 / 92.1	98.4 / 97.7	0.989	24.42
	Complete-Trace	1538	93.3 / 82.4	95.9 / 88.1	0.964	7.60
	Solution-Only	-	30.0 / 26.0	54.1 / 47.8	0.500	1.86
Sokoban	Dualformer (auto)	494	94.0 / 90.0	97.4 / 94.7	0.979	4.97
	Complete-Trace	3600	92.9 / 84.4	94.7 / 89.0	0.944	2.91
	Solution-Only	-	86.8 / 83.4	92.8 / 90.0	0.919	1.24

Dualformer **automatically** switches between fast mode (System 1) and slow mode (System 2) and works **better** for **dedicated** models on either modes.

Fast mode performance

	Method	1-Optimal-64 / 3-Optimal-64	1-Solved-64 / 3-Solved-64	SWC	Diversity
Maze 15x15	Dualformer (fast)	91.8 / 87.6	97.1 / 94.8	0.960	9.05
	Solution-Only	72.0 / 68.9	82.7 / 80.1	0.610	1.52
Maze 20x20	Dualformer (fast)	90.9 / 84.0	97.0 / 94.0	0.960	17.27
	Solution-Only	56.3 / 52.0	71.9 / 67.5	0.690	1.52
Maze 25x25	Dualformer (fast)	83.9 / 72.9	95.5 / 90.6	0.940	21.23
	Solution-Only	39.7 / 34.7	60.3 / 55.4	0.570	1.9
Maze 30x30	Dualformer (fast)	80.0 / 66.0	91.8 / 85.7	0.906	18.23
	Solution-Only	30.0 / 26.0	54.1 / 47.8	0.500	1.86
Sokoban	Dualformer (fast)	97.3 / 94.4	94.8 / 90.0	0.970	4.92
	Solution-Only	86.8 / 83.4	92.8 / 90.0	0.919	1.24

Slow mode performance

	Method	Avg Trace Length	1-Optimal-64 / 3-Optimal-64	1-Solved-64 / 3-Solved-64	SWC	Diversity
Maze 15 x 15	Dualformer (slow)	278	99.6 / 99.2	99.9 / 99.9	0.999	12.54
	Complete-Trace	495	94.6 / 90.1	96.7 / 93.0	0.964	7.60
Maze 20 x 20	Dualformer (slow)	439	98.9 / 97.8	99.9 / 99.7	0.998	18.86
	Complete-Trace	851	98.3 / 95.5	98.8 / 93.00	0.987	14.53
Maze 25 x 25	Dualformer (slow)	589	99.9 / 97.2	99.7 / 99.3	0.997	25.05
	Complete-Trace	1208	95.2 / 85.7	97.0 / 90.4	0.968	18.85
Maze 30 x 30	Dualformer (slow)	854	97.6 / 93.2	99.5 / 98.2	0.993	25.77
	Complete-Trace	1538	93.3 / 82.4	95.9 / 88.1	0.964	7.60
Sokoban	Dualformer (slow)	1482	94.5 / 87.6	97.4 / 94.1	0.970	4.66
	Complete-Trace	3600	92.9 / 84.4	94.7 / 89.0	0.944	2.91

Math Problems

Question 1

In Pascal's Triangle, the third row has four elements, and the sum of these elements is 8. What is the sum of the elements in the tenth row? (Note that we are counting the top row with a single 1 as the 0th row).

Llama-3-Aug (baseline) Here is a detailed step-by-step explanation of the reasoning:

- Step 1: Understand the problem and the given information. We are asked to find the sum of the elements in the tenth row of Pascal's Triangle, given that the third row has four elements and their sum is 8.
- Step 2: Recall the formula for the sum of the elements in a row of Pascal's Triangle. The sum of the elements in the n th row is given by the formula: $\binom{n}{0} + \binom{n}{1} + \binom{n}{2} + \dots + \binom{n}{n} = 2^n$.
- Step 3: Identify the relationship between the sum of the elements in a row and the sum of the elements in the previous row. Since the sum of the elements in the n th row is 2^n , the sum of the elements in the $(n-1)$ th row is 2^{n-1} .
- Step 4: Recognize that the sum of the elements in the third row is 8, which is equal to 2^3 . This is because the sum of the elements in the third row is $\binom{3}{0} + \binom{3}{1} + \binom{3}{2} = 1 + 3 + 3 = 7$, and the extra 1 comes from the top row, which is counted as the 0th row.

- Step 5: Use the relationship between the sums of the elements in consecutive rows to find the sum of the elements in the tenth row. Since the sum of the elements in the third row is 2^3 , and the sum of the elements in the $(n-1)$ th row is 2^{n-1} , we can set up the equation: $2^3 = 2^{10-1}$.
- Step 6: Solve the equation for n . Taking the logarithm of both sides, we get: $3 \log 2 = (10 - 1) \log 2$. Simplifying, we get: $3 \log 2 = 9 \log 2$, which implies that $\log 2 = 0$. This is a contradiction, since $\log 2$ is a positive number.
- Step 7: Conclude that the equation $2^3 = 2^{10-1}$ has no solution, and therefore, the sum of the elements in the tenth row is not equal to 2^{10-1} .
- Step 8: Recognize that the sum of the elements in the tenth row is still given by the formula: $\binom{10}{0} + \binom{10}{1} + \binom{10}{2} + \dots + \binom{10}{10} = 2^{10}$.

The answer is: 1024.

Llama-3-Aug (p=0.4, ours) Here is a detailed step-by-step explanation of the reasoning:

- Step 1: Understand the problem and the given information. We are asked to find the sum of the elements in the tenth row of Pascal's Triangle, given that the third row has four elements and their sum is 8.
- Step 2: Recall the properties of Pascal's Triangle. The elements in each row of Pascal's Triangle are the binomial coefficients, which represent the number of ways to choose k items from a set of n items. The sum of the elements in each row is equal to 2^n , where n is the row number.
- Step 3: Identify the relationship between the sum of the elements in the third row and the sum of the elements in the tenth row. Since the sum of the elements in each row is equal to 2^n , we can write the sum of the elements in the third row as $2^3 = 8$. Similarly, the sum of the elements in the tenth row is 2^{10} .
- Step 4: Calculate the sum of the elements in the tenth row. $2^{10} = 1024$.

The answer is: 1024.

Baseline

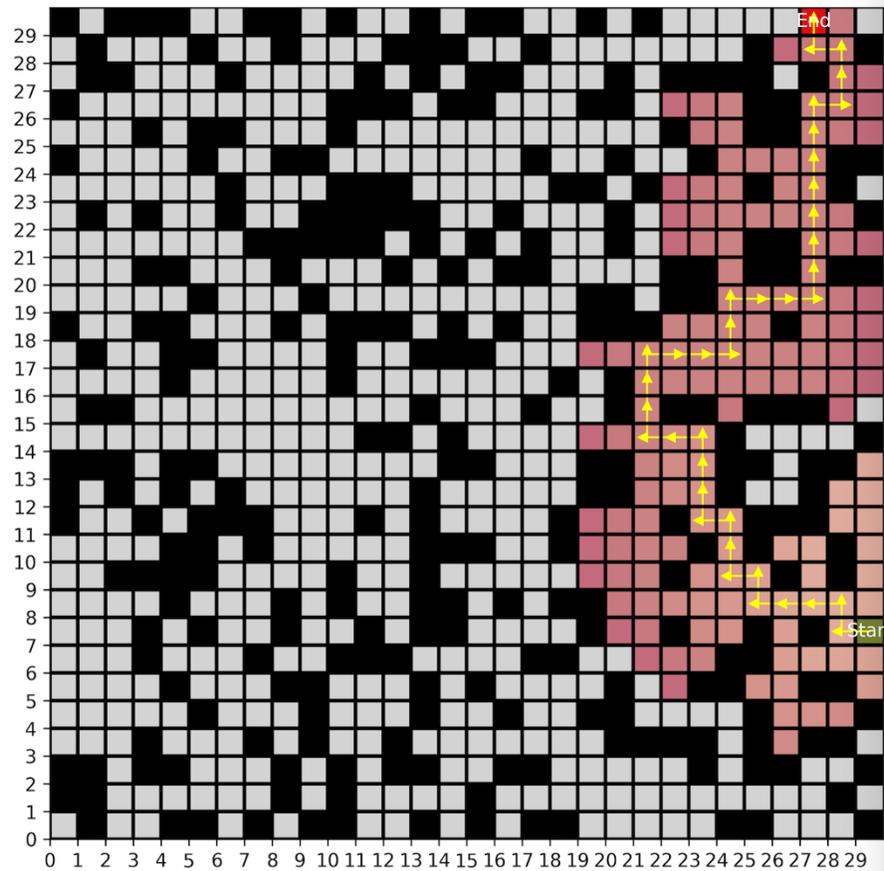
Dualformer

Math Problems

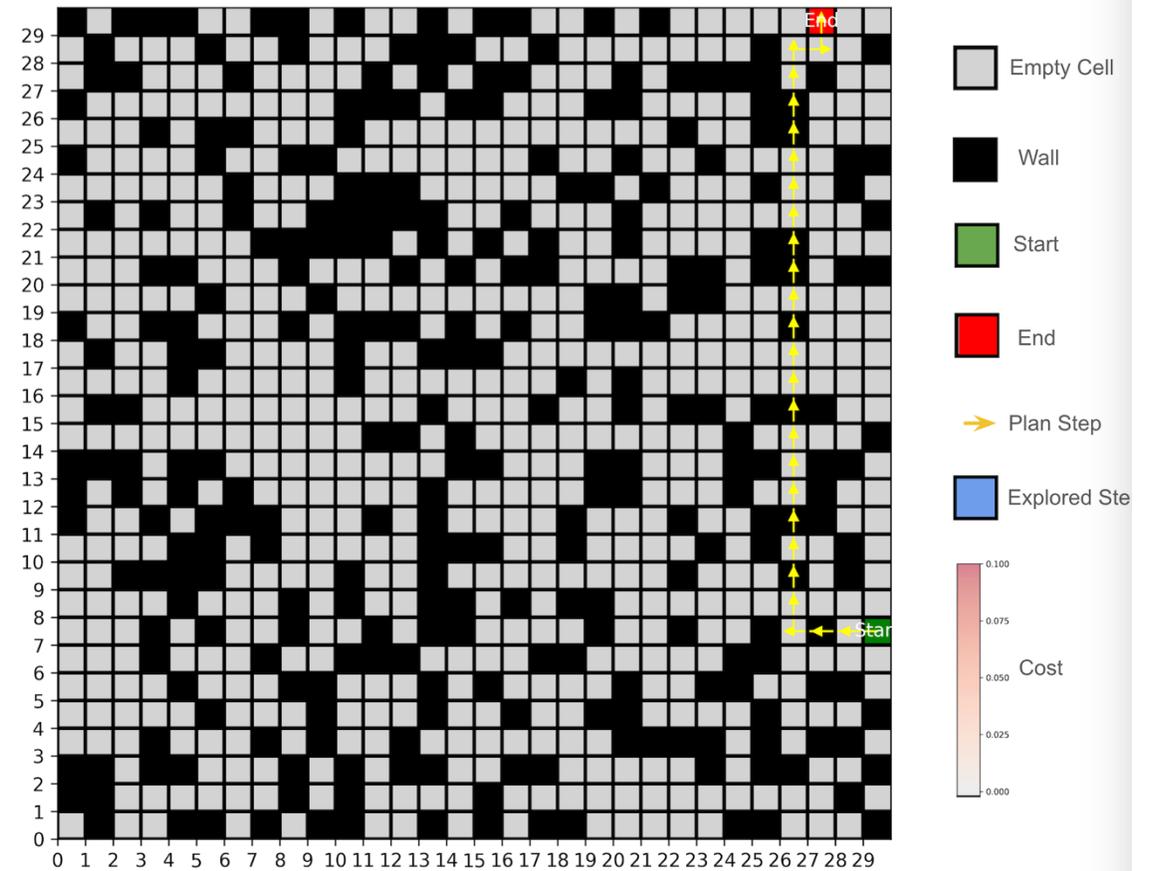
Model	Dataset & Dropping Prob	Greedy@1(%) (slow / fast)	Trace Length	Pass@20(%) (slow / fast)	Trace Length
Mistral-7B	Aug-MATH (baseline)	16.9 / 9.6	527 / -	59.6 / 29.8	521 / -
	Aug-MATH (p=0.1)	18.6 / 11.3	508 / -	61.6 / 32.0	479 / -
	Aug-MATH (p=0.2)	17.8 / 11.2	477 / -	61.4 / 31.9	470 / -
	Aug-MATH (p=0.3)	17.8 / 11.8	497 / -	61.9 / 31.7	466 / -
	Aug-MATH (p=0.4)	17.0 / 11.0	434 / -	56.4 / 28.9	397 / -
	MATH	13.1 / 8.5	290 / -	53.0 / 29.4	227 / -
Llama-3-8B	Aug-MATH (baseline)	19.7 / 13.1	548 / -	62.7 / 35.6	535 / -
	Aug-MATH (p=0.1)	20.1 / 13.3	544 / -	63.4 / 36.2	522 / -
	Aug-MATH (p=0.2)	20.5 / 13.8	525 / -	63.9 / 36.7	497 / -
	Aug-MATH (p=0.3)	20.5 / 13.5	515 / -	63.4 / 37.5	474 / -
	Aug-MATH (p=0.4)	20.4 / 13.5	490 / -	63.4 / 37.2	450 / -
	MATH	13.3 / 12.6	432 / -	52.8 / 35.5	332 / -

DualFormer

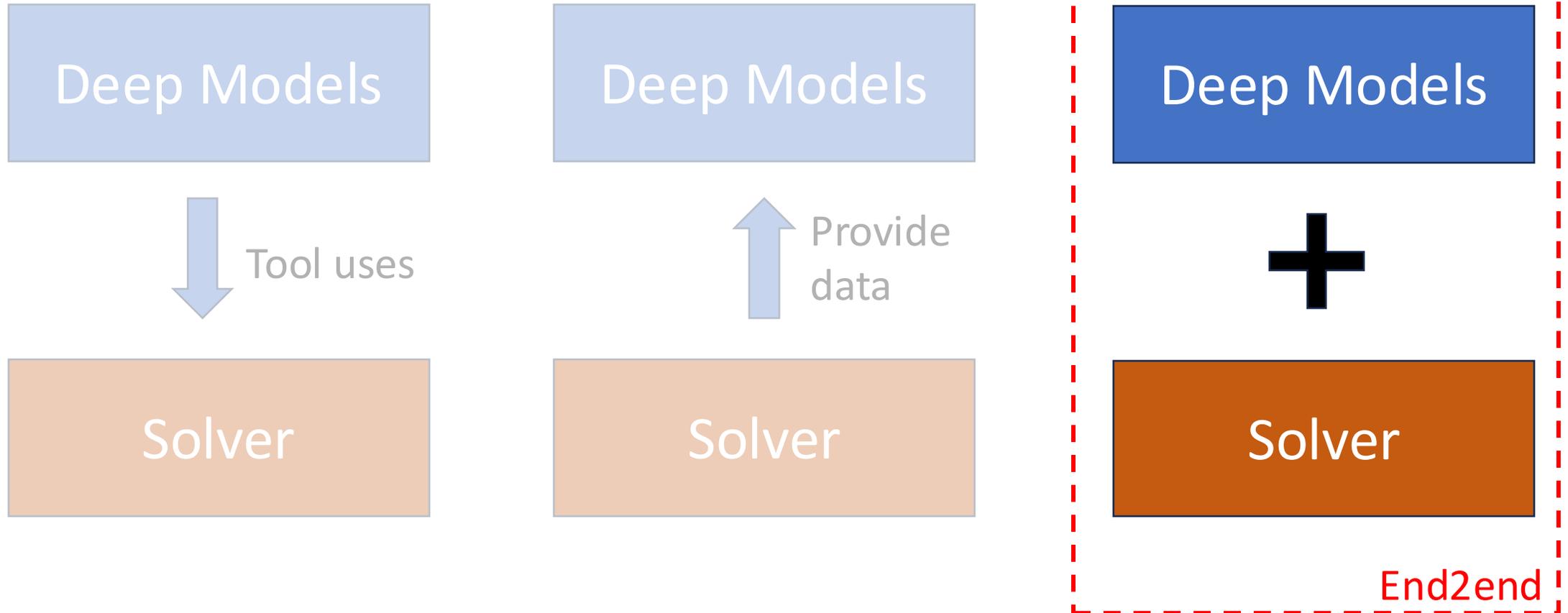
Dualformer



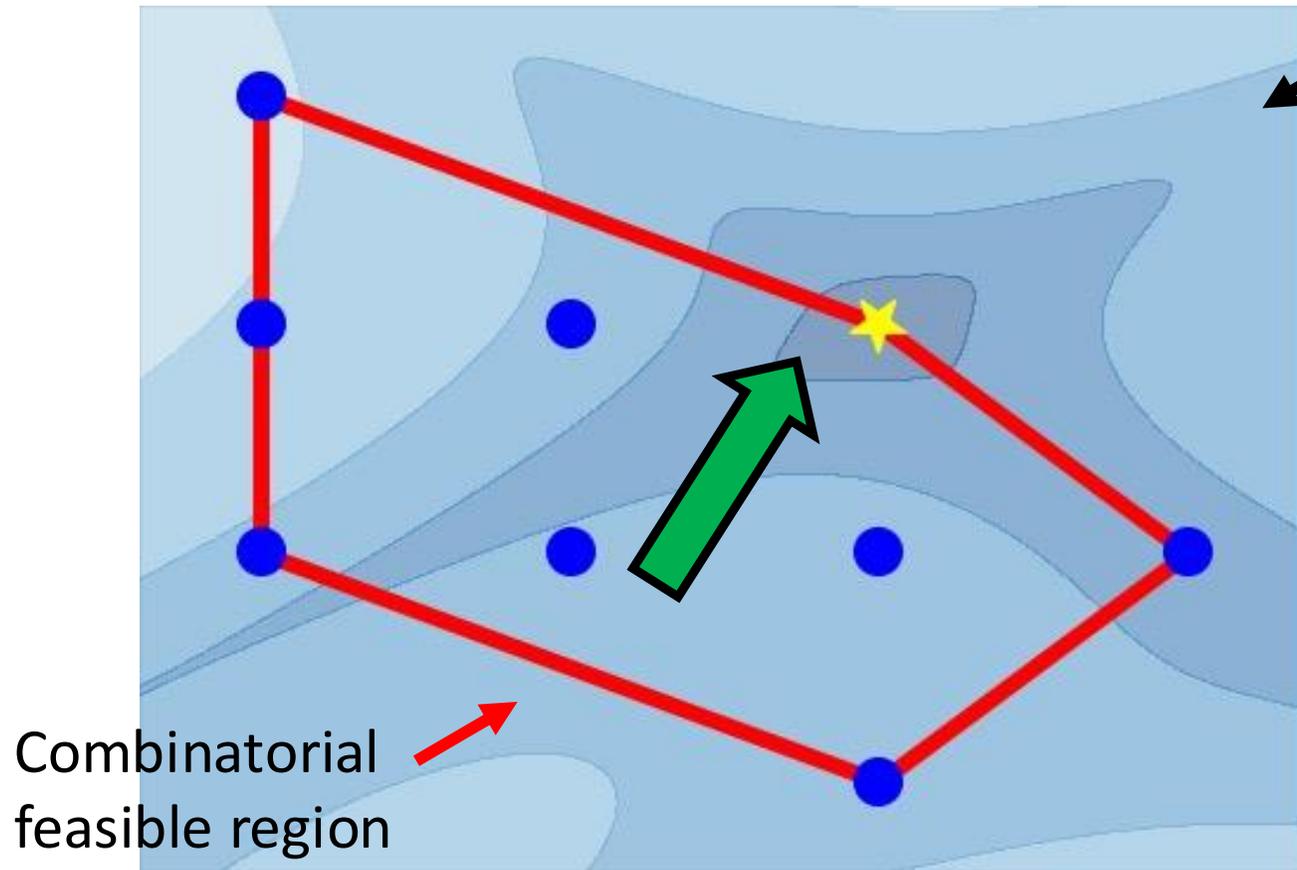
o1-preview (OpenAI)



Option **Two**: Hybrid Systems



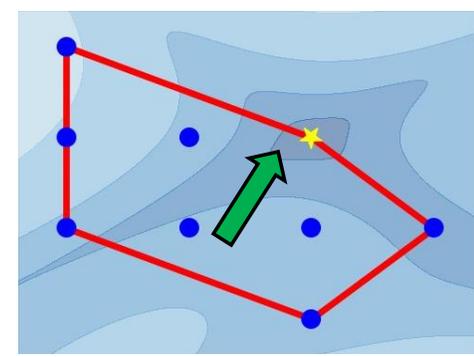
Nonlinear objective with combinatorial constraints



Nonlinear + differentiable objective $f(x)$

- Real-world domains:
 - Computer system planning
 - Designing photonic devices
 - Throughput optimization
 - Antenna design
 - Energy grid

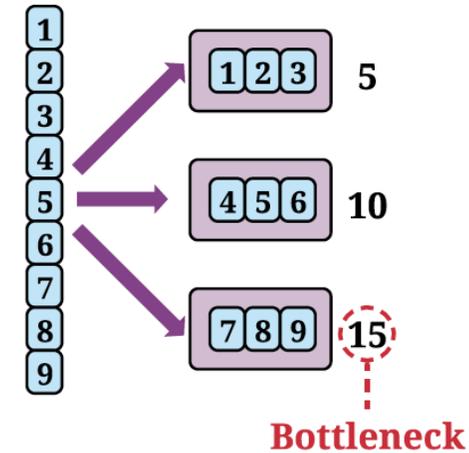
Example: Embedding Table Placement



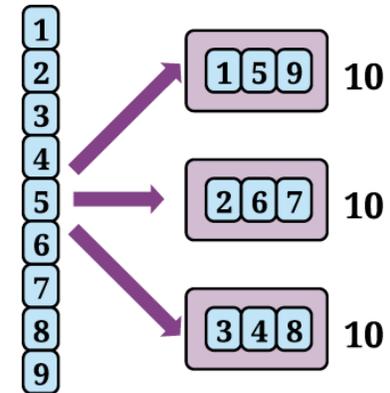
Given:

- k tables
- n identical devices
- Table i has memory requirement m_i
- Device j has memory capacity M_j

Naive Sharding



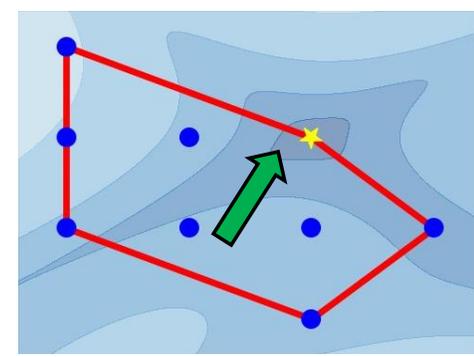
Balanced Sharding



Find

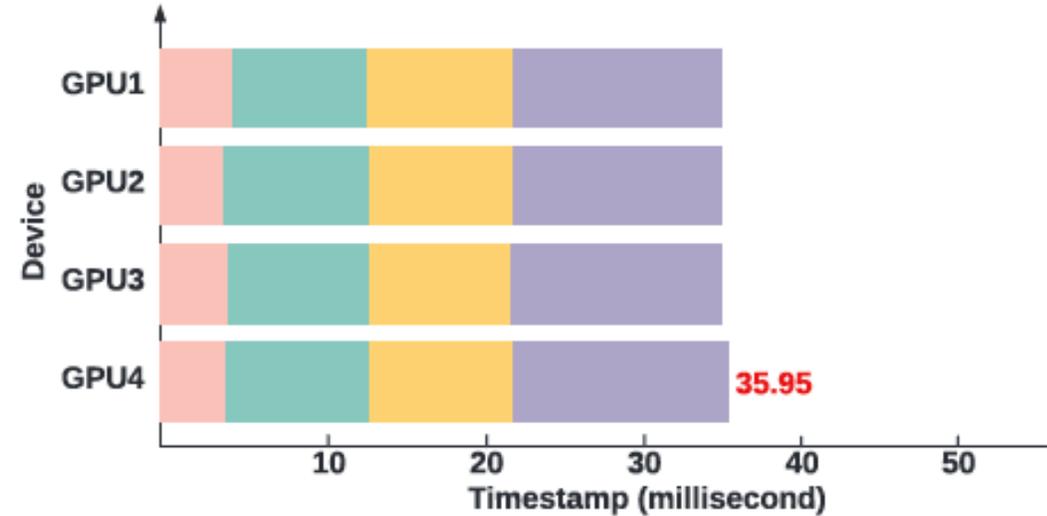
- Allocation of tables to devices observing device memory limits
- Minimize latency which is **estimated by a neural network** (capturing nonlinear interactions)

Example: Embedding Table Placement



Given:

- k tables
- n identical devices
- Table i has memory requirement m_i
- Device j has memory capacity M_j



Formulation

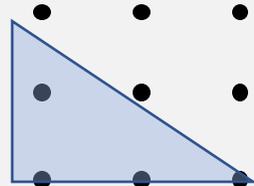
$$\text{Min}_x \mathbf{L}(\{x_{ij}\}) \quad \text{s.t.} \quad \sum_i x_{ij} m_i \leq M_j, \quad \sum_j x_{ij} = 1, \quad x_{ij} \in \{0,1\}$$

\mathbf{L} is nonlinear due to system issues (e.g., batching, communication, etc)

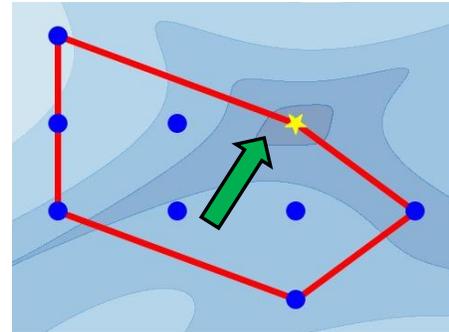
Solve the Combinatorial Problem in the Latent Space

Original Space

Nonlinear optimization with combinatorial constraints

$$\begin{aligned} \min_x & f(\mathbf{x}; \mathbf{y}) \\ \text{s.t. } & \mathbf{x} \in \Omega = \end{aligned}$$


combinatorial constraints



Latent Space

Surrogate optimization

$$\begin{aligned} \mathbf{x}^*(\mathbf{y}) &= \operatorname{argmin}_x \mathbf{c}(\mathbf{y})^T \mathbf{x} \\ \text{s.t. } & \mathbf{x} \in \Omega \end{aligned}$$

solved by existing combinatorial solvers

Predict surrogate cost $\mathbf{c} = \mathbf{c}(\mathbf{y})$

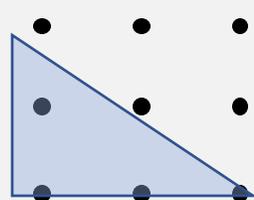


$\mathbf{x}^*(\mathbf{y})$ optimizes $f(\mathbf{x}; \mathbf{y})$ as much as possible

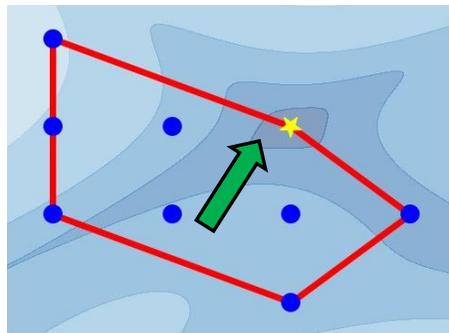
Solve the Combinatorial Problem in the Latent Space

Original Space

Nonlinear optimization with combinatorial constraints

$$\begin{aligned} \min_x f(\mathbf{x}; \mathbf{y}) \\ \text{s.t. } \mathbf{x} \in \Omega = \end{aligned}$$


combinatorial constraints



Latent Space

Surrogate optimization

$$\begin{aligned} \mathbf{x}^*(\mathbf{y}) = \operatorname{argmin}_x \mathbf{c}(\mathbf{y})^T \mathbf{x} \\ \text{s.t. } \mathbf{x} \in \Omega \end{aligned}$$

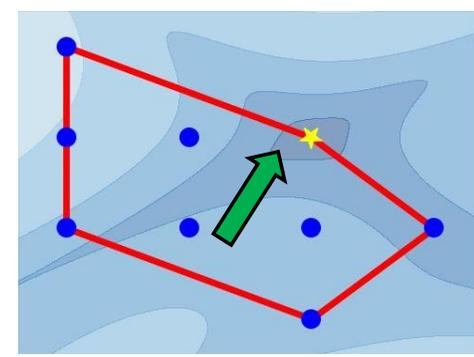
solved by existing combinatorial solvers

Predict surrogate cost $\mathbf{c} = \mathbf{c}(\mathbf{y})$

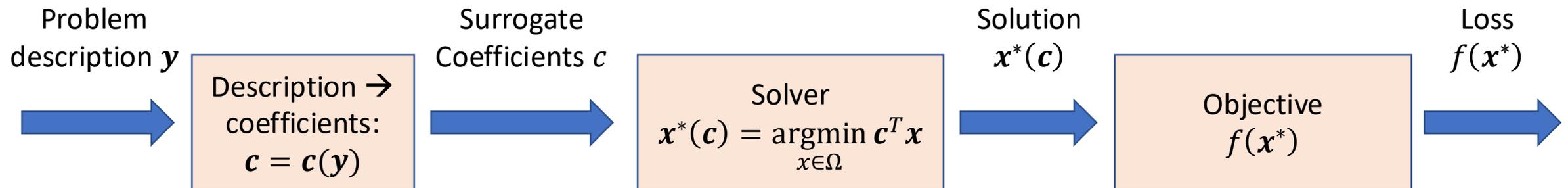


$\mathbf{x}^*(\mathbf{y})$ optimizes $f(\mathbf{x}; \mathbf{y})$ as much as possible

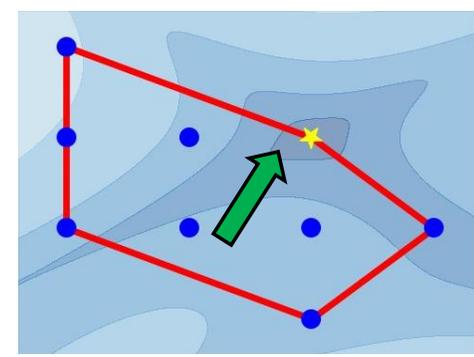
SurCo: Surrogate combinatorial opt



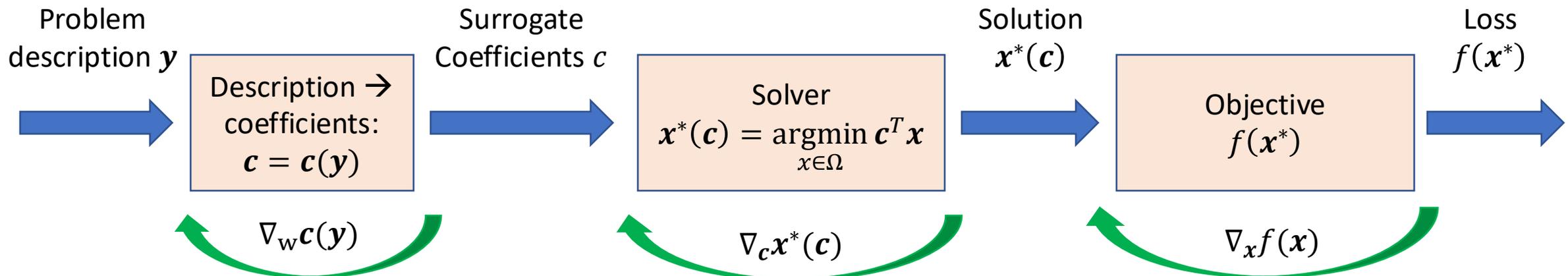
- Use surrogate MILP to solve original problem
- Find linear coefficients \mathbf{c} such that $\underset{x \in \Omega}{\operatorname{argmin}} f(x) = \underset{x \in \Omega}{\operatorname{argmin}} \mathbf{c}^T \mathbf{x}$



Gradient-based Optimization



- Use surrogate MILP to solve original problem
- Find linear coefficients \mathbf{c} such that $\operatorname{argmin}_{\mathbf{x} \in \Omega} f(\mathbf{x}) = \operatorname{argmin}_{\mathbf{x} \in \Omega} \mathbf{c}^T \mathbf{x}$



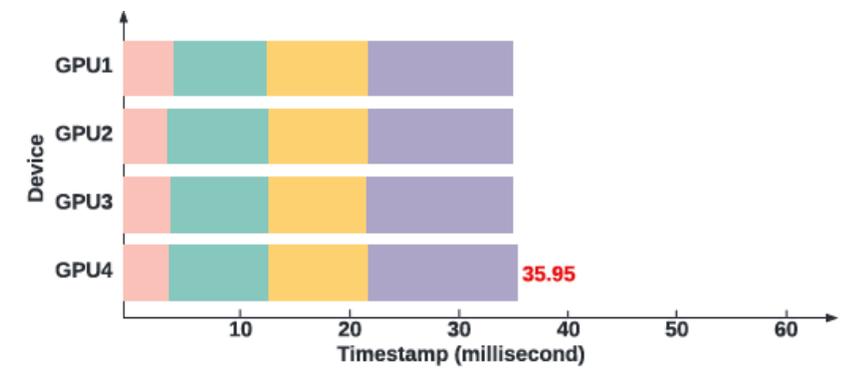
Assumed differentiable

Recent work on differentiable optimization

Differentiation of blackbox optimizers
CVXPYLayers
MIPaL
Etc.

Assumed differentiable

Embedding Table Sharding

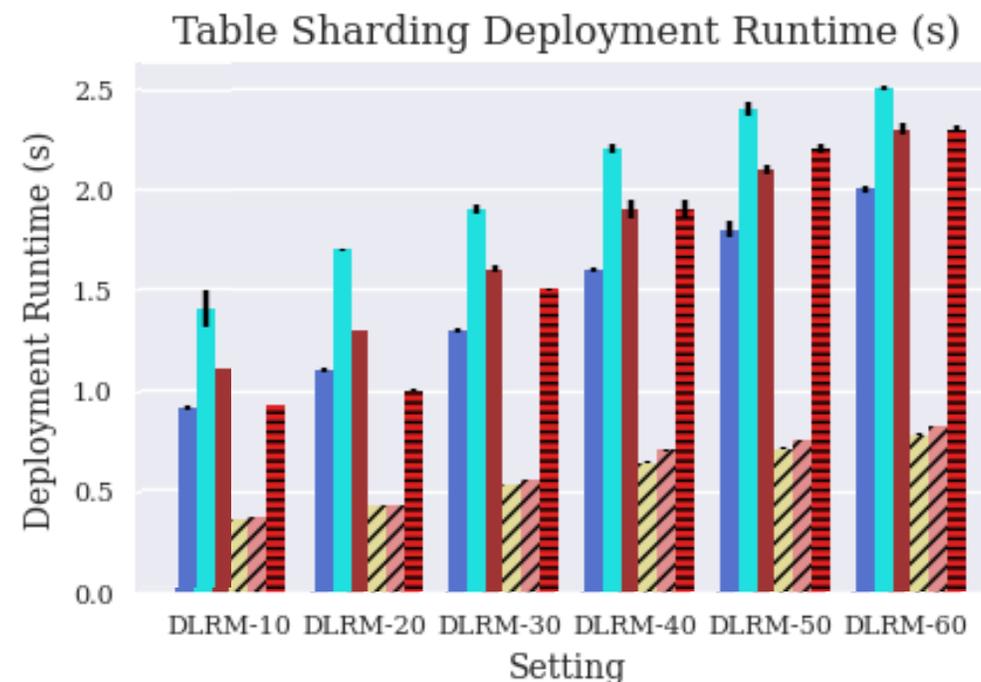
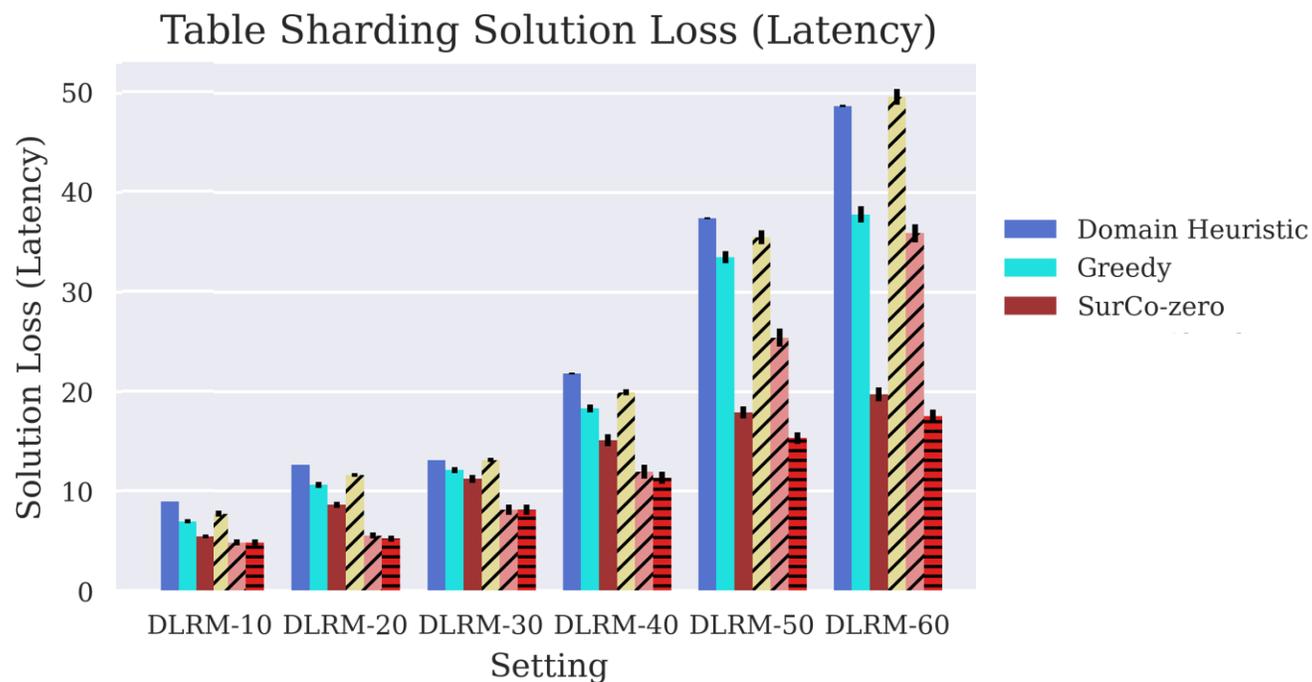


- Public **D**eep **L**earning **R**ecommendation **M**odel (DLRM dataset) placing between 10 to 60 tables on 4 GPUs
- Baseline: Greedy
- SoTA: RL approach Dreamshard¹
- SurCo: Surrogate NN model learned via CVXPYLayers (differentiable LP Solver)

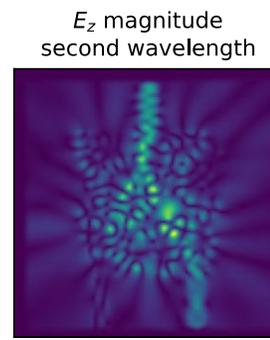
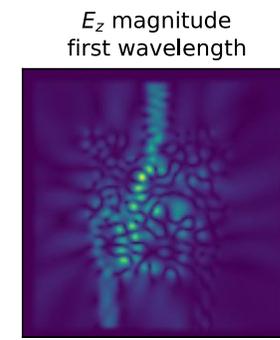
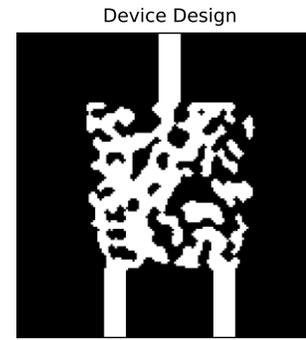
¹ Zha et al. NeurIPS 2022

Dataset: https://github.com/facebookresearch/dlrm_datasets

Results – Table Sharding



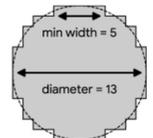
Inverse Photonic Design



- Design physically-viable devices that take light waves and routes different wavelengths to correct locations

$$\mathcal{L}(S) = \left(\left\| \text{softplus} \left(g \frac{|S|^2 - |S_{\text{cutoff}}|^2}{\min(w_{\text{valid}})} \right) \right\|_2 \right)^2$$

- Device design misspecification loss $f(\mathbf{x})$ computed by differentiable electromagnetic simulator
- Feasible solution: the design must be the union of brush pattern
 - $x = \text{binary_opening}(x, \text{brush})$
 - $x = \sim \text{binary_opening}(\sim x, \text{brush})$



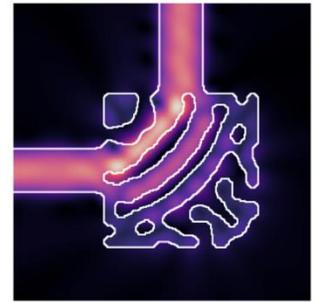
Inverse Photonic Design

- Dataset: Ceviche Challenges¹
- Most baselines don't work here due to combinatorial constraints
- SoTA: Brush-based algorithm ¹
- SurCo: Surrogate learned via blackbox differentiation² of brush solver

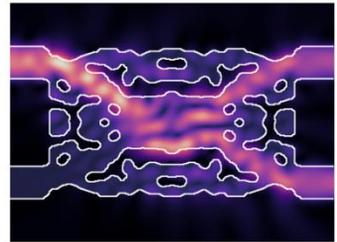
¹Schubert et al. ACS Photonics 2022

²Vlastelica et al. ICLR 2019

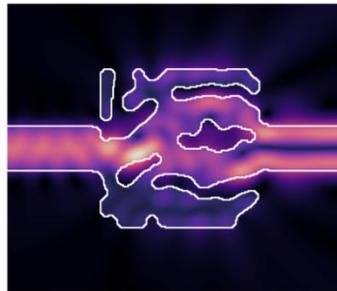
Dataset: <https://github.com/google/ceviche-challenges>



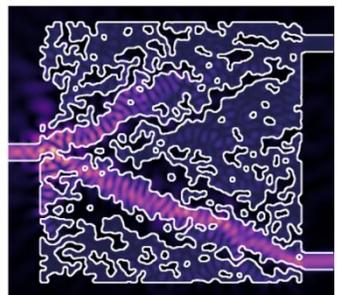
Waveguide bend



Beam splitter

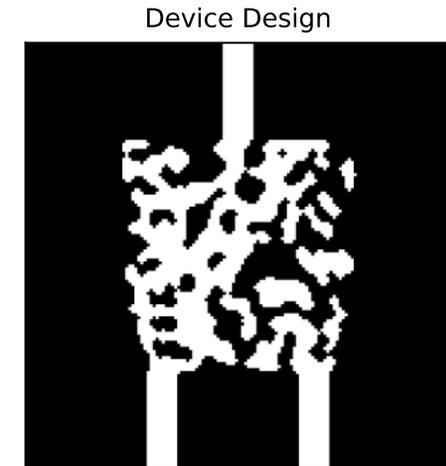
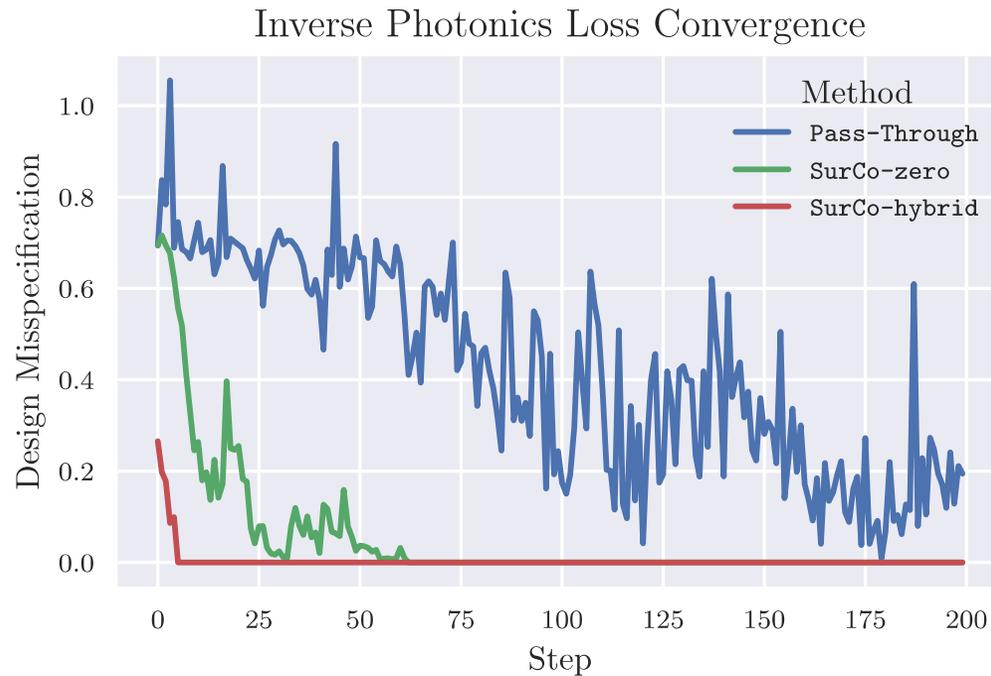


Mode converter

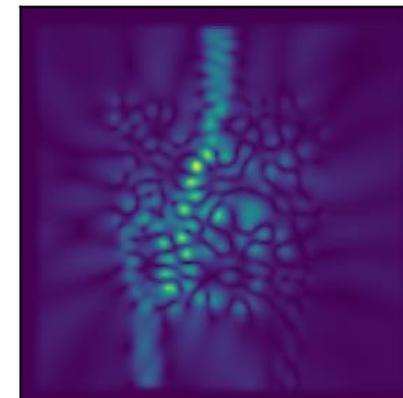


Wavelength division multiplexer

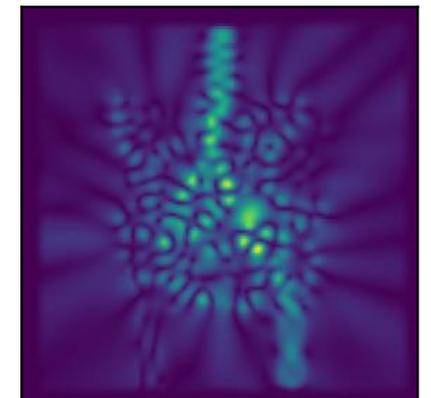
Inverse photonics Convergence comparison + Solution example



E_z magnitude
first wavelength



E_z magnitude
second wavelength



Wavelength division multiplexer

Takeaways:

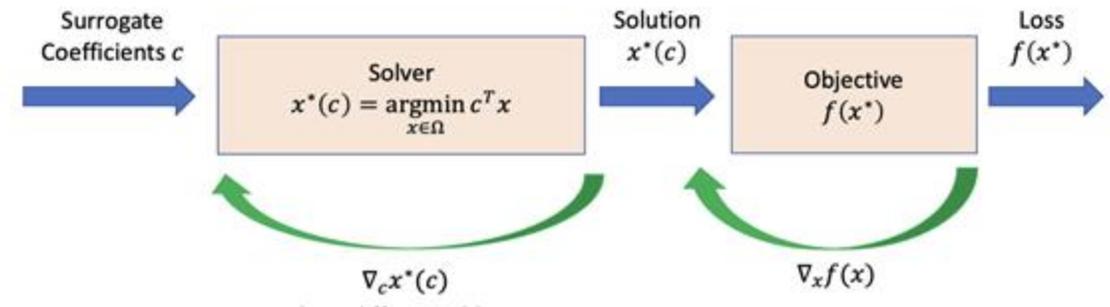
- SurCo-Zero finds loss-0 solutions quickly
- SurCo-Hybrid uses offline training data to get a head start

Limitation of SurCo

Recall **SurCo**: Update linear coefficients \mathbf{c} such that $x^*(\mathbf{c})$ improves objective $f(x^*(\mathbf{c}))$

$$\min_{\theta} \mathcal{L}(Y, Z) := \sum_{i=1}^N f(\mathbf{g}_{\theta}(\mathbf{y}_i); \mathbf{z}_i)$$

$$\mathbf{g}_{\theta}(\mathbf{y}) = \arg \min_{\mathbf{x} \in \Omega} \mathbf{x}^{\top} \mathbf{c}_{\theta}(\mathbf{y})$$



- Requires $\nabla_x f(x)$ → Does not apply to nondifferentiable functions
- Requires $\nabla_c \mathbf{g}_{\theta}(c)$ → Solver is backpropagatable

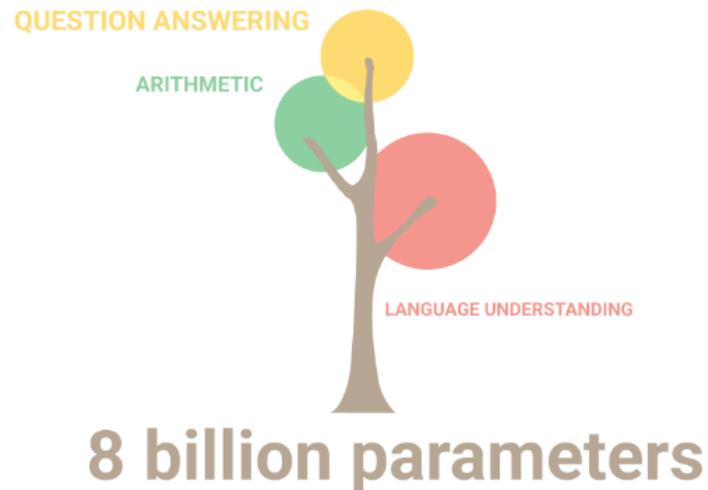
Option Three: Does Deep Model Actually Converge to Anything Symbolic?



Emerging Symbolic
Structure

Deep Models

Debate: Is LLM doing retrieval or true reasoning?



LLM shows emergent behaviors!!

Debate: Is LLM doing retrieval or true reasoning?



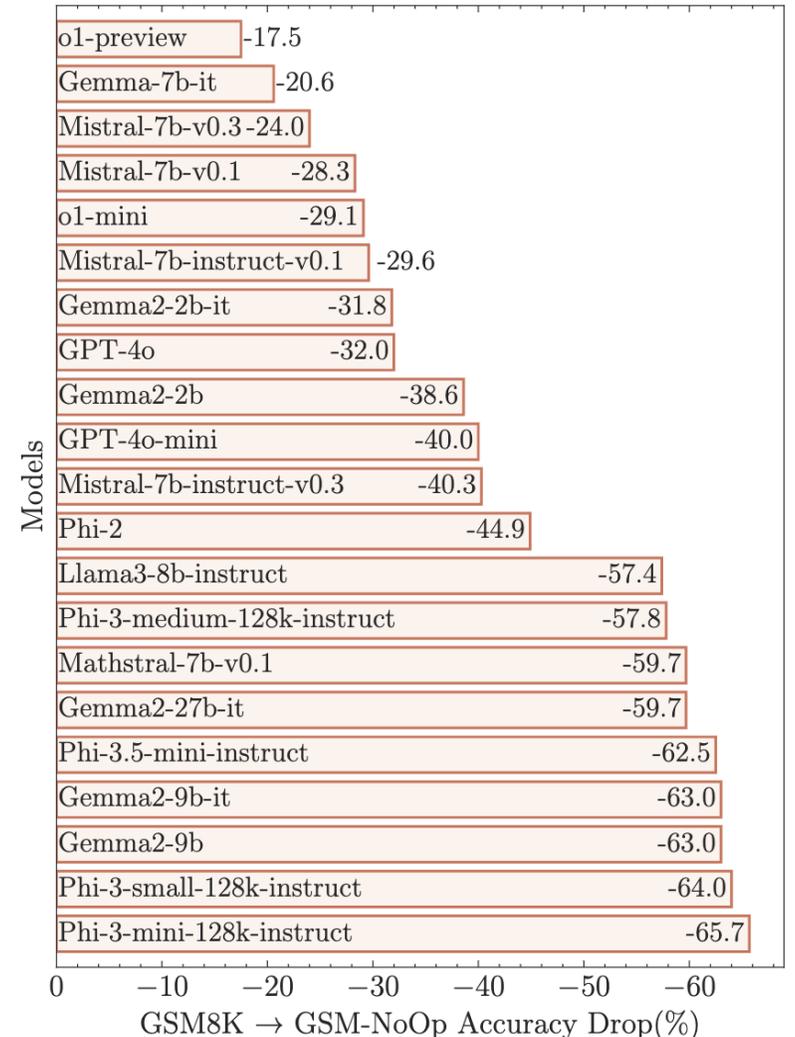
Do LLMs perform reasoning or approximate retrieval?
There is a continuum between the two, and Auto-Regressive LLMs are largely on the retrieval side.



Emergent Abilities (noun): The preferred euphemism for what your LLM does, when saying "approximate retrieval" sounds too unsexy.

[#AIAphorisms](#)

LLM is just doing retrievals!!



Concrete Example: Modular Addition

$$a + b = c \pmod{d}$$

Does neural network have an *implicit table* to do retrieval?

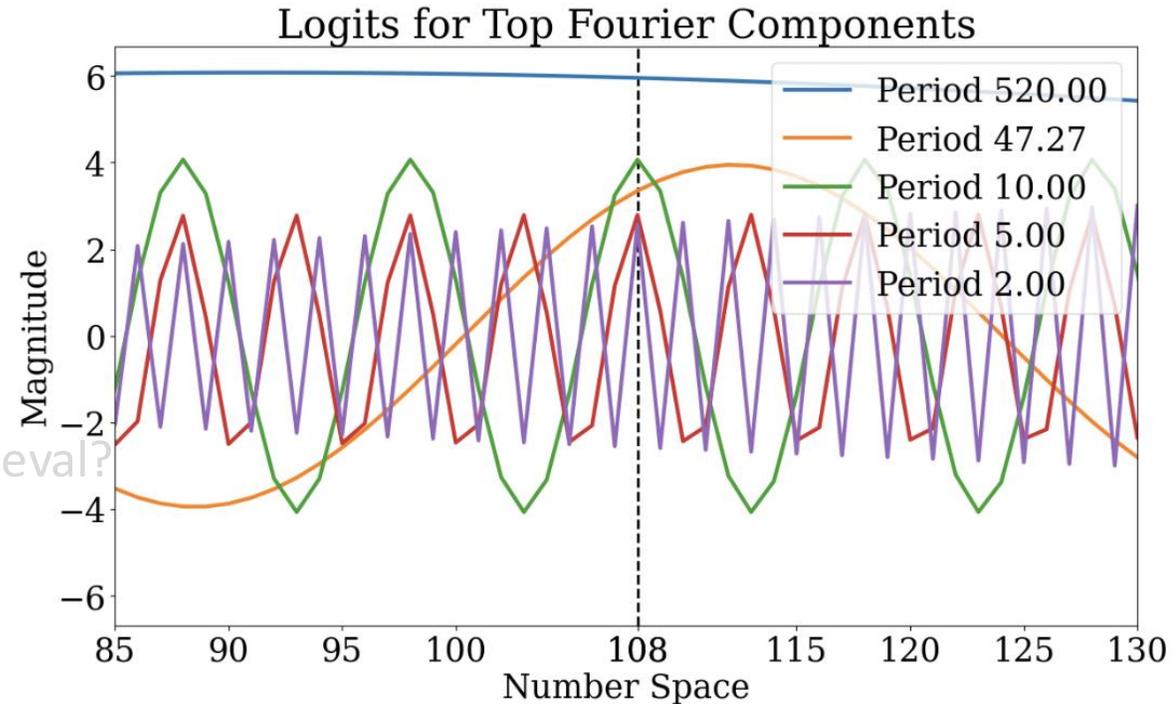
Concrete Example: Modular Addition

$$a + b = c \pmod d$$

Does neural network have an *implicit table* to do retrieval?

Learned representation = Fourier basis 🤖

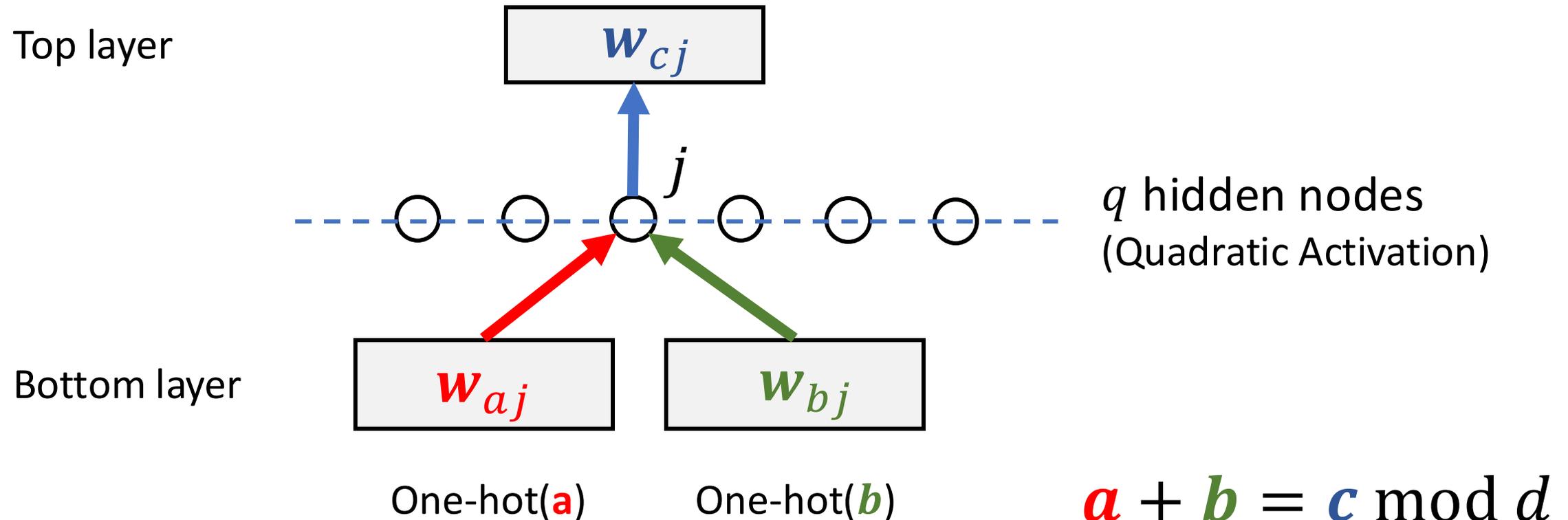
Why? 🤔



(a) Final logits for top Fourier components

Problem Setup

MSE Loss: $\text{Min } \|\text{Output} - \text{one-hot}(\mathbf{c})\|_2$



(Scaled) Fourier Transform

$$Z_{akj} = \sum_{m=0}^{d-1} W_{amj} e^{imk/d}$$

$$Z_{bkj} = \sum_{m=0}^{d-1} W_{bmj} e^{imk/d}$$

$$Z_{ckj} = \sum_{m=0}^{d-1} W_{cmj} e^{imk/d}$$

k : frequency

$\{W_a, W_b, W_c\}$ are real



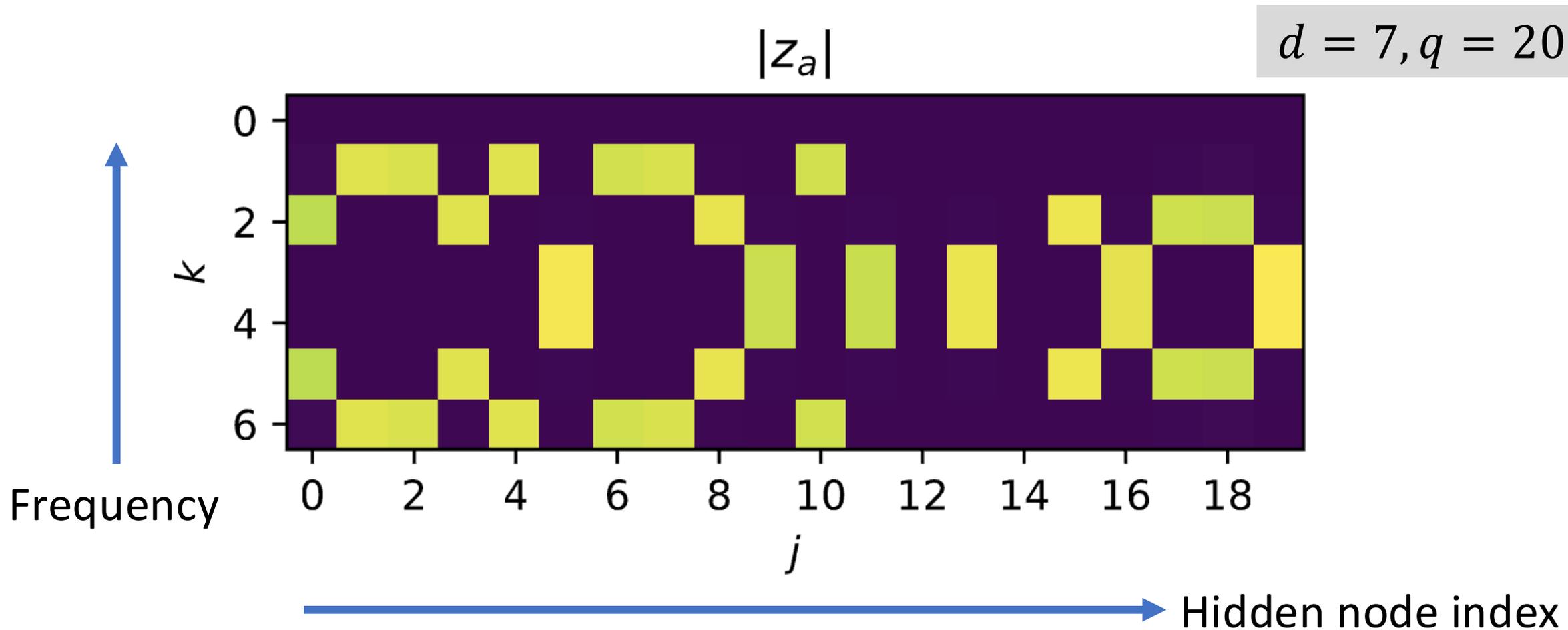
Hermitian condition holds

$$Z_{akj} = \overline{Z_{a,-k,j}}$$

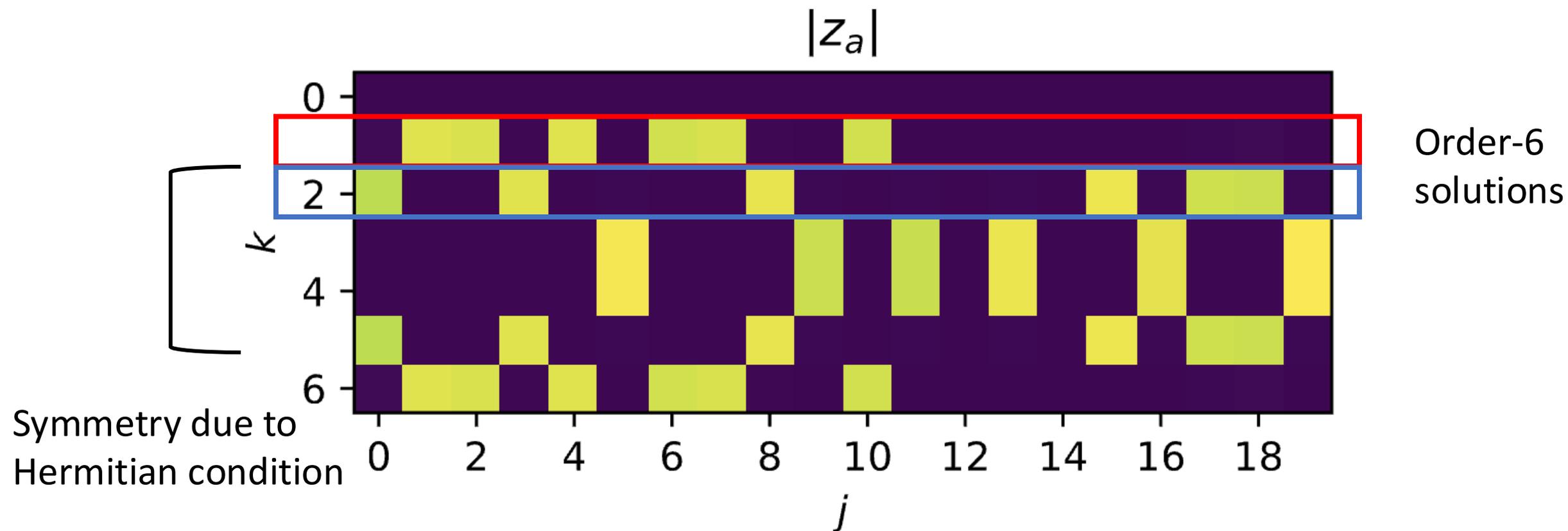
$$Z_{bkj} = \overline{Z_{b,-k,j}}$$

$$Z_{ckj} = \overline{Z_{c,-k,j}}$$

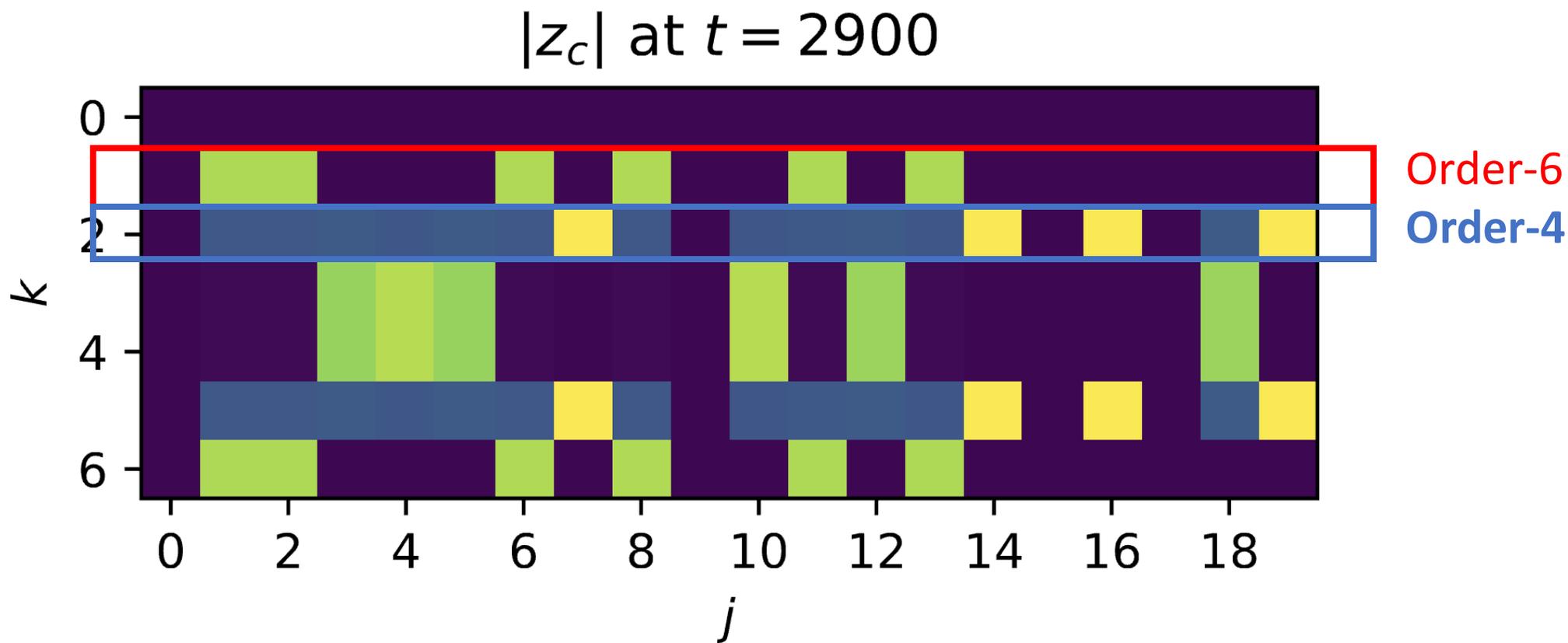
What a Gradient Descent Solution look like?



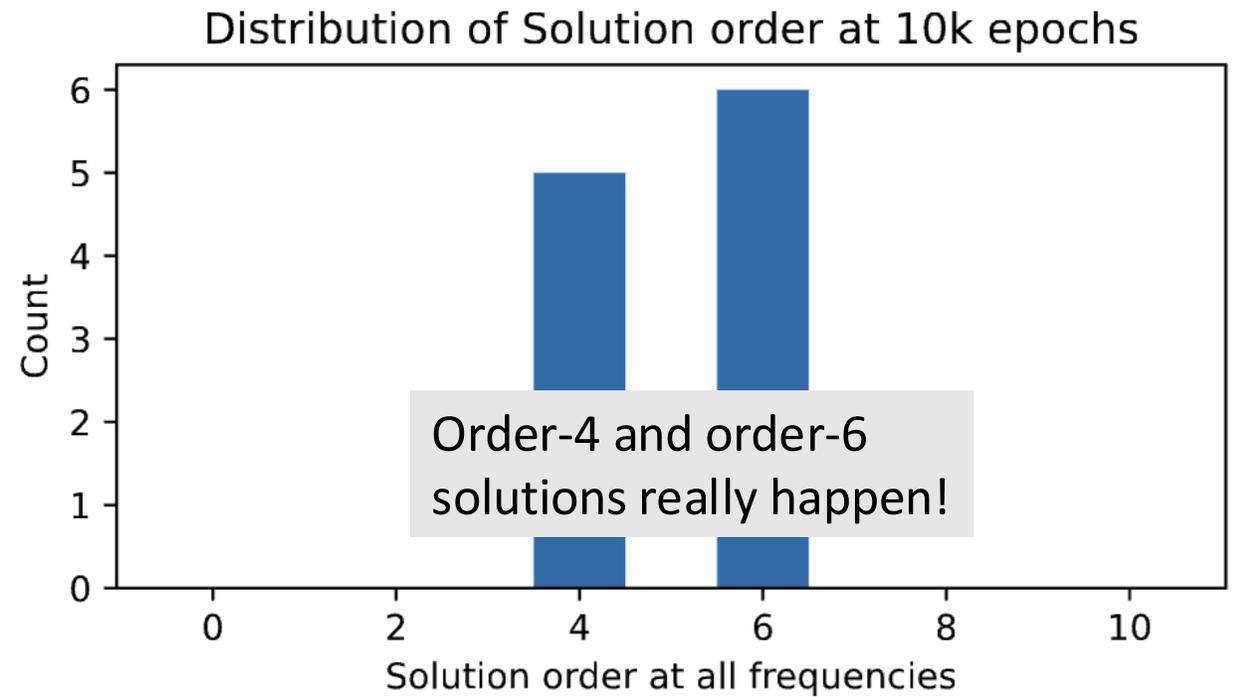
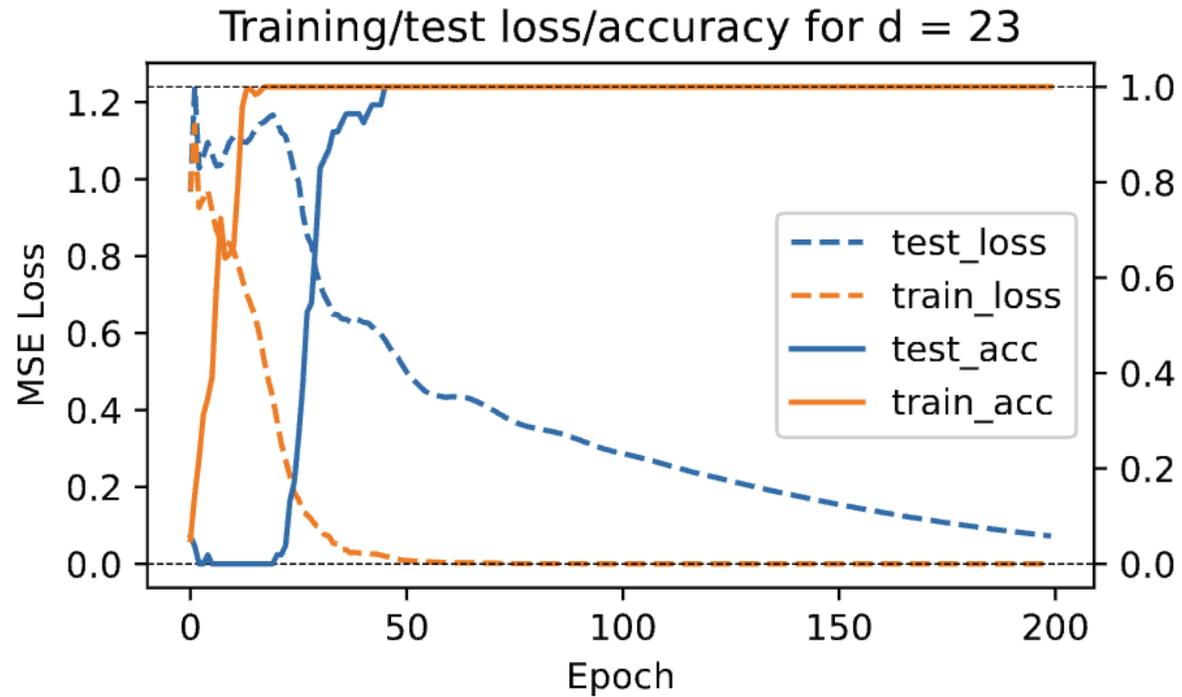
What a Gradient Descent Solution look like?



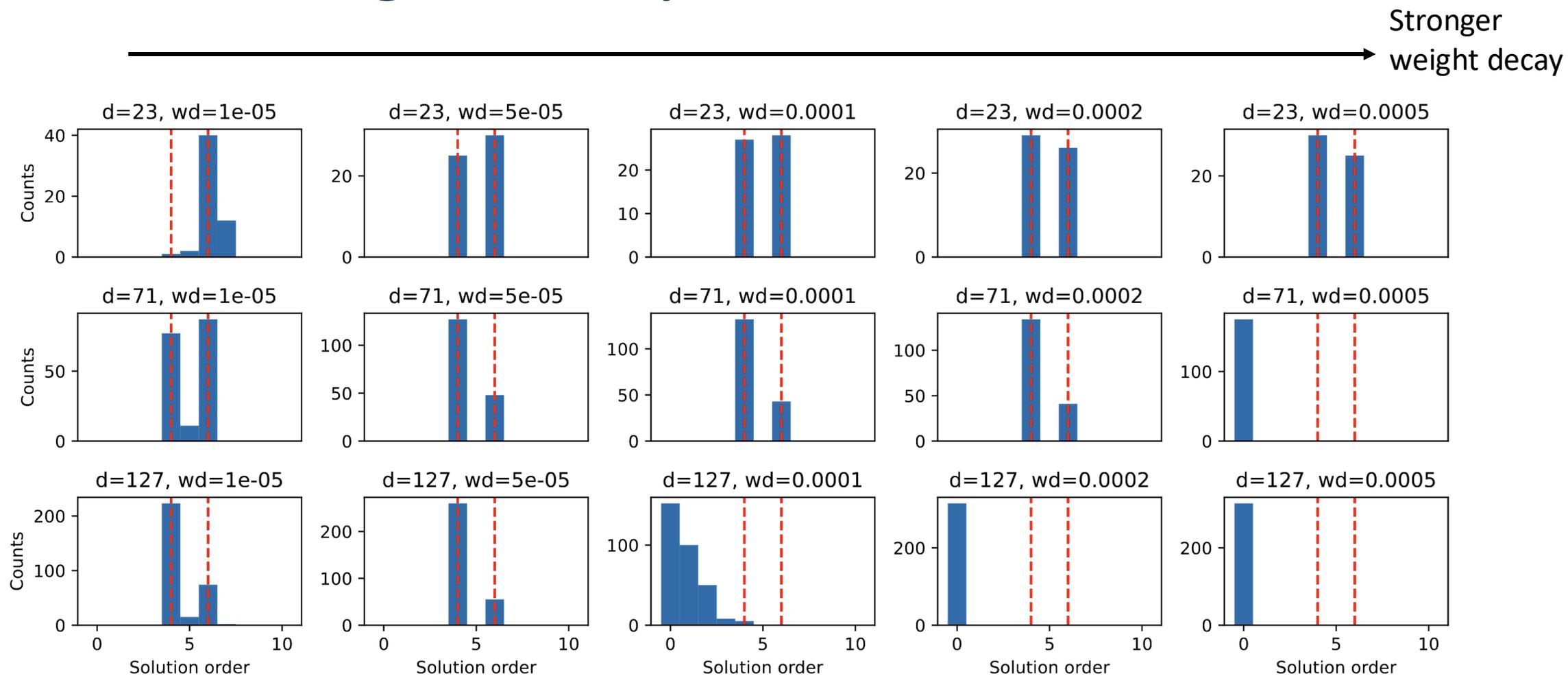
What a Gradient Descent Solution look like?



More Statistics on Gradient Descent Solutions



Effect of Weight Decay



Why? 🤔

Structure of Loss Functions

$$\text{MSE loss } \ell(\mathbf{z}) = d^{-1} \sum_{k \neq 0} \ell_k(\mathbf{z}) + 1 - 1/d$$

$$\ell_k(\mathbf{z}) = -2r_{kkk} + \sum_{k_1 k_2} |r_{k_1 k_2 k}|^2 + \frac{1}{4} \left| \sum_{p \in \{a, b\}} \sum_{k'} r_{p, k', -k', k} \right|^2 + \frac{1}{4} \sum_{m \neq 0} \sum_{p \in \{a, b\}} \left| \sum_{k'} r_{p, k', m - k', k} \right|^2$$

Term $r_{k_1 k_2 k}(\mathbf{z}) := \sum_j z_{a k_1 j} z_{b k_2 j} z_{c k j}$ and $r_{p k_1 k_2 k}(\mathbf{z}) := \sum_j z_{p k_1 j} z_{p k_2 j} z_{c k j}$

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Sufficient conditions of Global Optimizers:

R_g	R_c	R_n	R_*
$r_{kkk} = 1$	$r_{k_1 k_2 k} = 0$	$r_{p k', -k', k} = 0$	$r_{p k', m - k', k} = 0$

How to Optimize?

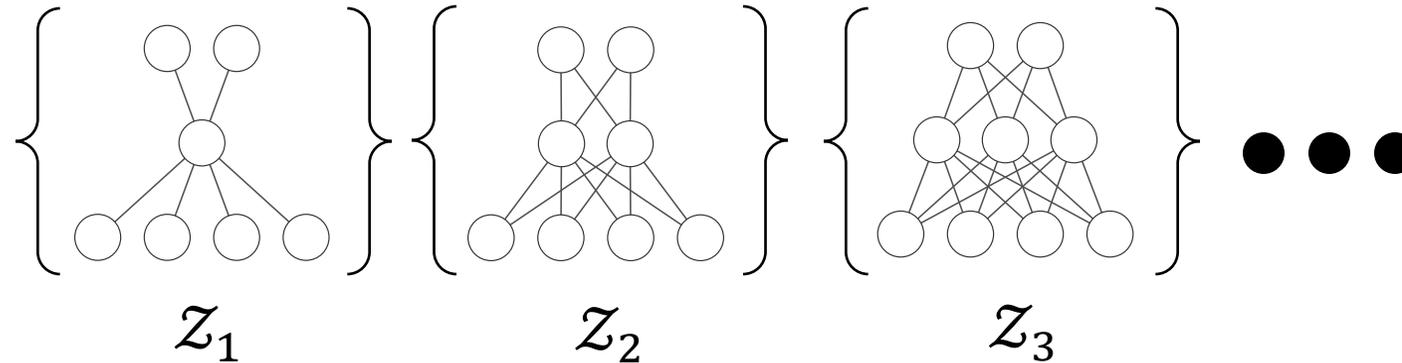
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However, nice *algebraic structures* exist!

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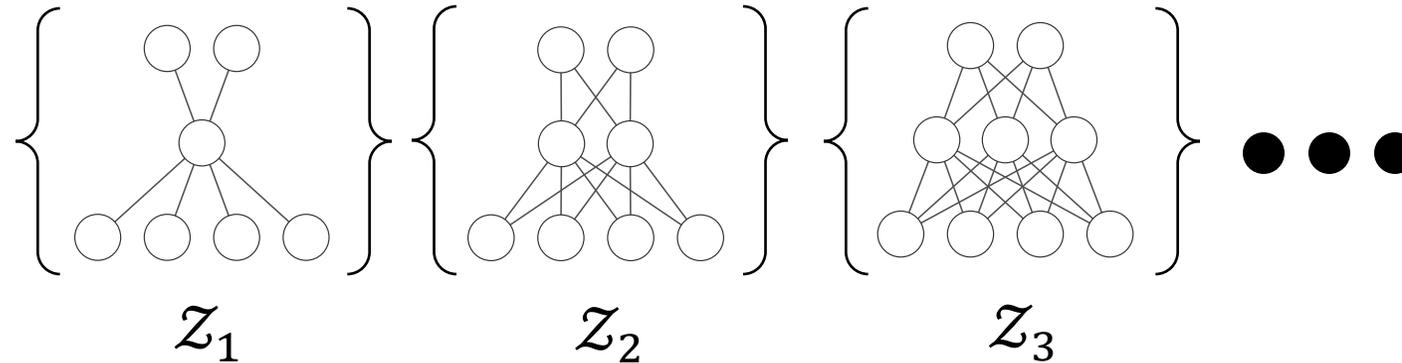


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How to Optimize?

The objective is highly nonlinear !!

However, nice *algebraic structures* exist!



$\mathcal{Z} = \bigcup_{q \geq 0} \mathcal{Z}_q$: All 2-layer networks with different number of hidden nodes

Ring addition $+$: Concatenate hidden nodes

Ring multiplication $*$: Kronecker production along the hidden dimensions

$\langle \mathcal{Z}, +, * \rangle$ is a *semi-ring*

Ring Homomorphism

A function $r(\mathbf{z}): \mathcal{Z} \mapsto \mathbb{C}$ is a *ring homomorphism*, if

- $r(\mathbf{1}) = 1$
- $r(\mathbf{z}_1 + \mathbf{z}_2) = r(\mathbf{z}_1) + r(\mathbf{z}_2)$
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 $r_{k_1 k_2 k}(\mathbf{z})$ and $r_{pk_1 k_2 k}(\mathbf{z})$ are **ring homomorphisms!**

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Partial solution \mathbf{z}_1 satisfies $r_{k_1 k_2 k}(\mathbf{z}_1) = 0$

Partial solution \mathbf{z}_2 satisfies $r_{p k', -k', k}(\mathbf{z}_2) = 0$

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Partial solution \mathbf{z}_1 satisfies $r_{k_1 k_2 k}(\mathbf{z}_1) = 0$

Partial solution \mathbf{z}_2 satisfies $r_{pk', -k', k}(\mathbf{z}_2) = 0$

} $\mathbf{z} = \mathbf{z}_1 * \mathbf{z}_2$ satisfies both $r_{k_1 k_2 k}(\mathbf{z}) = r_{pk', -k', k}(\mathbf{z}) = 0$

Composing Global Optimizers from Partial Ones

Partial solution #1

$$\mathbf{z}_{\text{syn}}^{(k)} \in R_c \cap R_n \text{ but } \mathbf{z}_{\text{syn}}^{(k)} \notin R_*$$

Partial solution #2

$$\mathbf{z}_v^{(k)} \in R_*$$

Composing Global Optimizers from Partial Ones

Composing
solutions using
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$$\mathbf{z}_{\text{syn}}^{(k)} * \mathbf{z}_v^{(k)} \in R_c \cap R_n \cap R_*$$

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Composing solutions using **ring multiplication** *

Composing solutions using **ring addition** +

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Global Optimizer to MSE loss $\ell(\mathbf{z})$!

$$\mathbf{z}_{F6} = \frac{1}{\sqrt[3]{6}} \sum_k \mathbf{z}_{\text{syn}}^{(k)} * \mathbf{z}_v^{(k)}$$

Exemplar constructed global optimizers

Order-6 \mathbf{z}_{F6} (2*3)

$$\mathbf{z}_{F6} = \frac{1}{\sqrt[3]{6}} \sum_{k=1}^{(d-1)/2} \mathbf{z}_{\text{syn}}^{(k)} * \mathbf{z}_{\nu}^{(k)} * \mathbf{y}_k$$

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Order-4 $\mathbf{z}_{F4/6}$ (2*2)
(mixed with order-6)

$$\mathbf{z}_{F4/6} = \frac{1}{\sqrt[3]{6}} \hat{\mathbf{z}}_{F6}^{(k_0)} + \frac{1}{\sqrt[3]{4}} \sum_{k=1, k \neq k_0}^{(d-1)/2} \mathbf{z}_{F4}^{(k)}$$

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Perfect memorization
(order-d per frequency)

$$\mathbf{z}_a = \sum_{j=0}^{d-1} \mathbf{u}_a^j, \quad \mathbf{z}_b = \sum_{j=0}^{d-1} \mathbf{u}_b^j$$

$$\mathbf{z}_M = d^{-2/3} \mathbf{z}_a * \mathbf{z}_b$$

Gradient Descent solutions matches with construction

d	%not	%non-factorable		error ($\times 10^{-2}$)		solution distribution (%) in factorable ones			
	order-4/6	order-4	order-6	order-4	order-6	$z_{\nu=i}^{(k)} * z_{\xi}^{(k)}$	$z_{\nu=i}^{(k)} * z_{\text{syn},\alpha\beta}^{(k)}$	$z_{\nu}^{(k)} * z_{\text{syn}}^{(k)}$	others
23	0.0 \pm 0.0	0.00 \pm 0.00	5.71 \pm 5.71	0.05 \pm 0.01	4.80 \pm 0.96	47.07 \pm 1.88	11.31 \pm 1.76	39.80 \pm 2.11	1.82 \pm 1.82
71	0.0 \pm 0.0	0.00 \pm 0.00	0.00 \pm 0.00	0.03 \pm 0.00	5.02 \pm 0.25	72.57 \pm 0.70	4.00 \pm 1.14	21.14 \pm 2.14	2.29 \pm 1.07
127	0.0 \pm 0.0	1.50 \pm 0.92	0.00 \pm 0.00	0.26 \pm 0.14	0.93 \pm 0.18	82.96 \pm 0.39	2.25 \pm 0.64	14.13 \pm 0.87	0.66 \pm 0.66

$q = 512, wd = 5 \cdot 10^{-5}$

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100% of the per-freq solutions are order-4/6

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95% of the solutions are factorizable into “2*3” or “2*2”

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Factorization error is very small

Gradient Descent solutions matches with construction

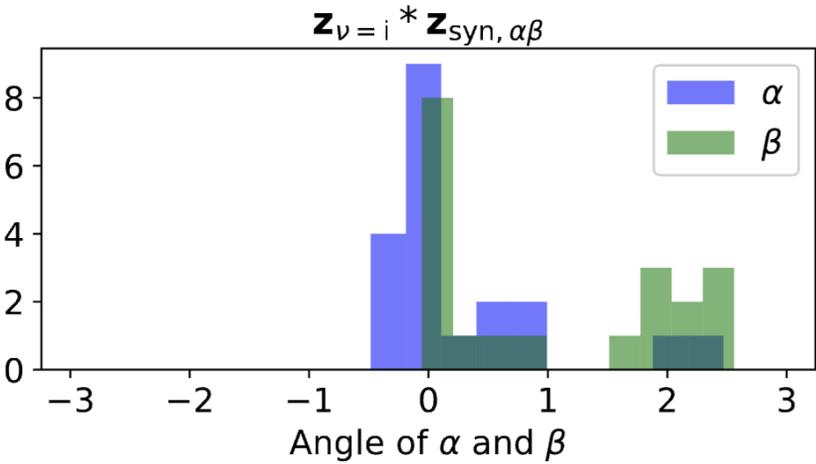
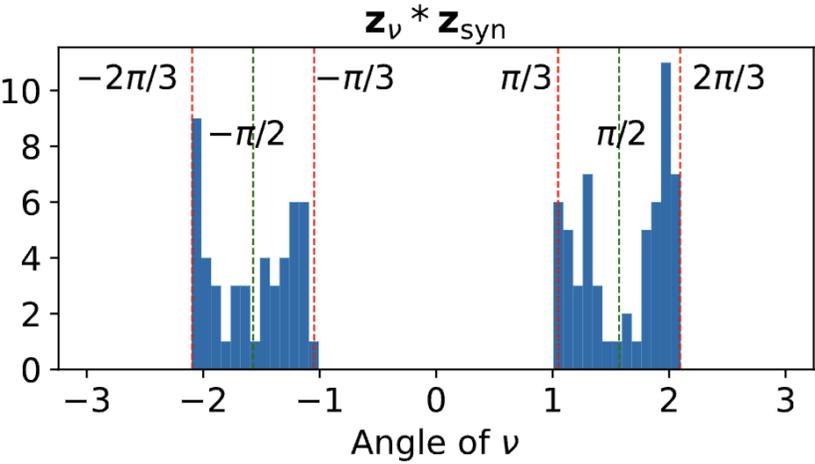
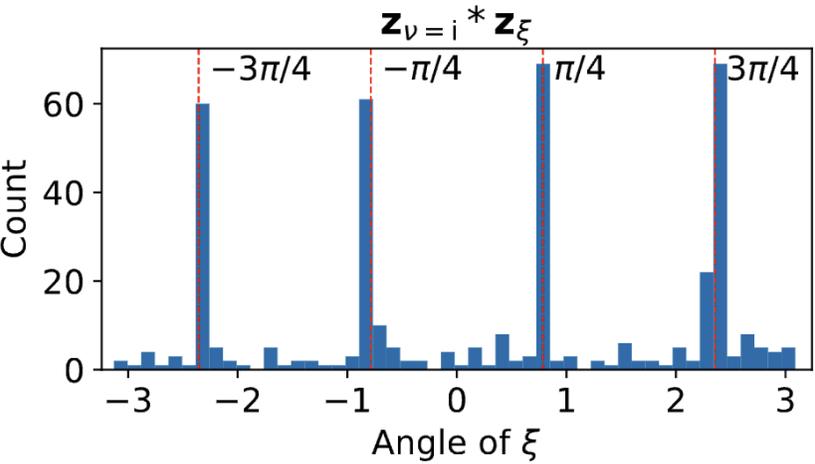
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98% of the solutions can be factorizable into the constructed forms

Gradient Descent solutions matches with construction

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						8	82.96 ± 0.39	2.25 ± 0.64	14.13 ± 0.87	0.66 ± 0.66

Distribution of the parameters in the solutions

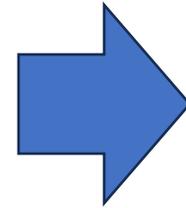


Possible Implications

Do neural networks end up learning more efficient symbolic representations that we don't know?

Does gradient descent lead to a solution that can be reached by advanced algebraic operations?

Will gradient descent become obsolete, eventually?



Thanks!