

Adventures with Agentic AI (in particle physics)

BNL Seminar

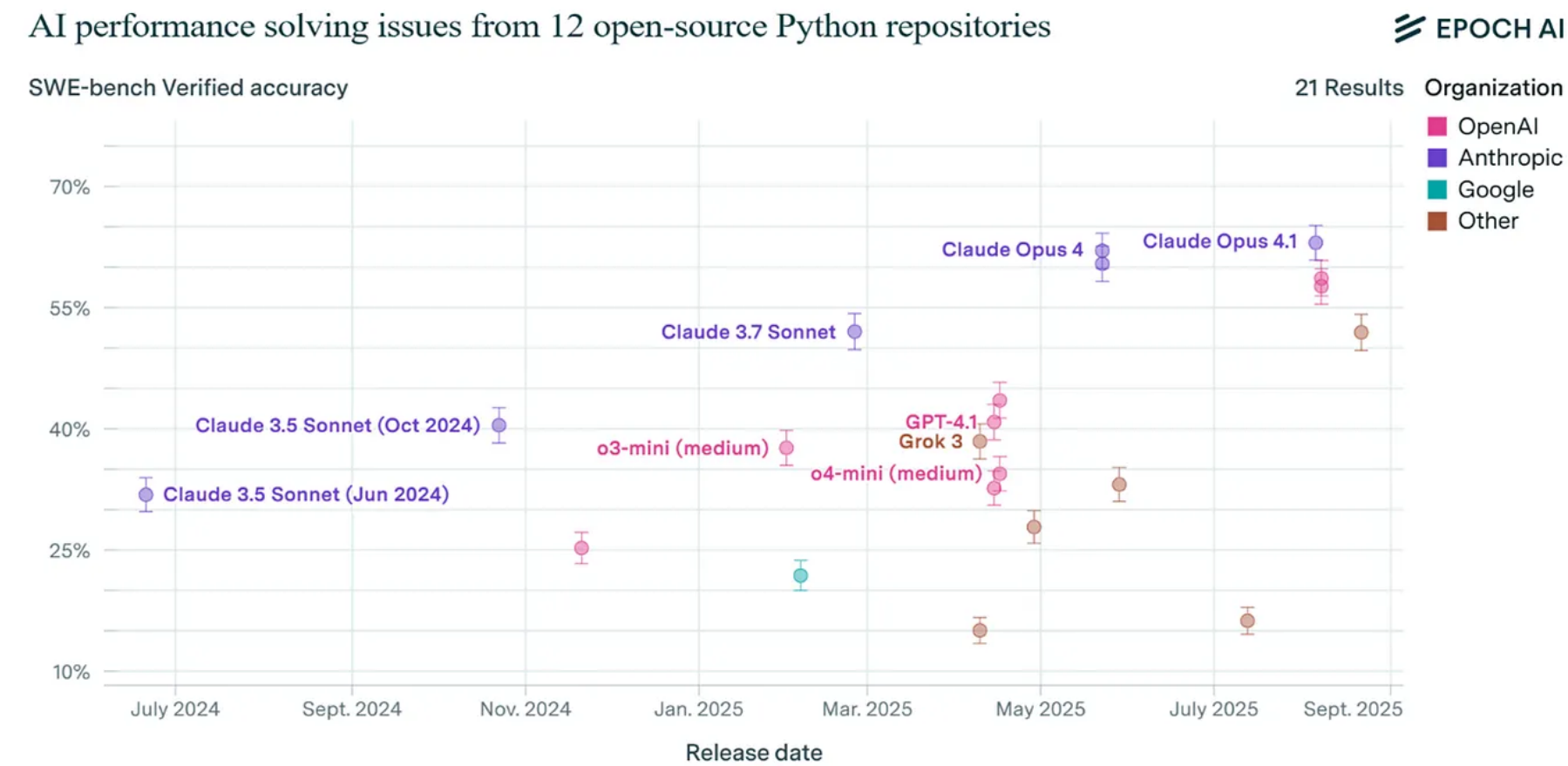
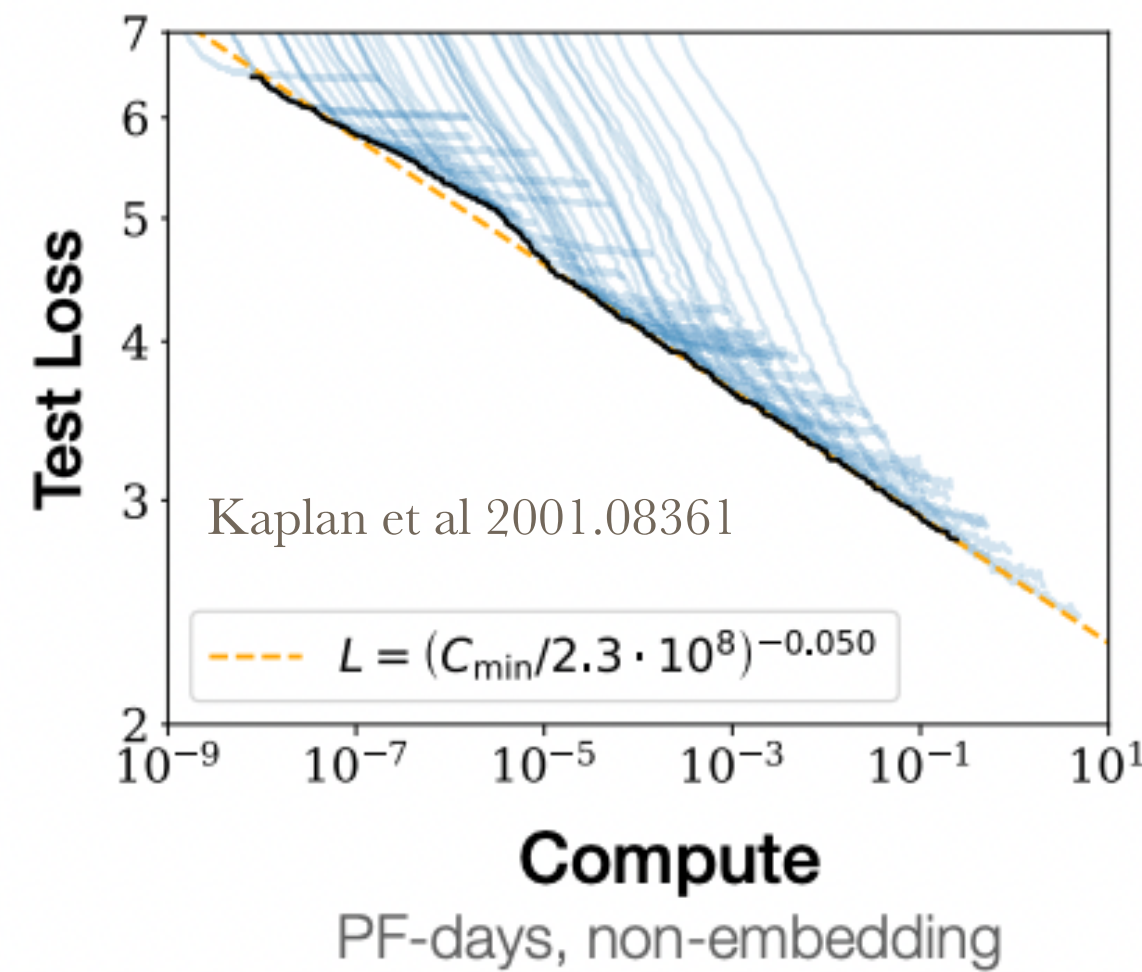
David Shih
June 12, 2026



RUTGERS
THE STATE UNIVERSITY
OF NEW JERSEY

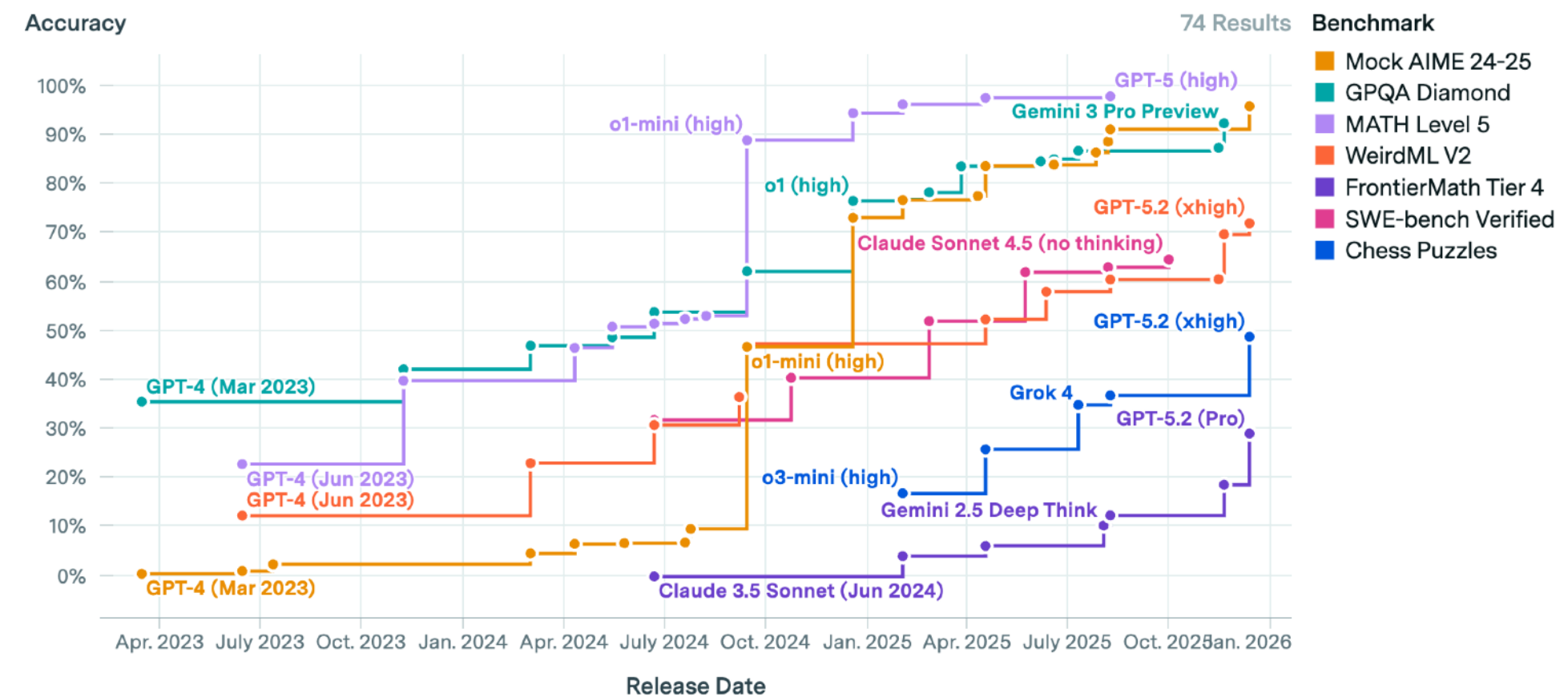
AI Revolution

We are witnessing a historic moment of technological advancement

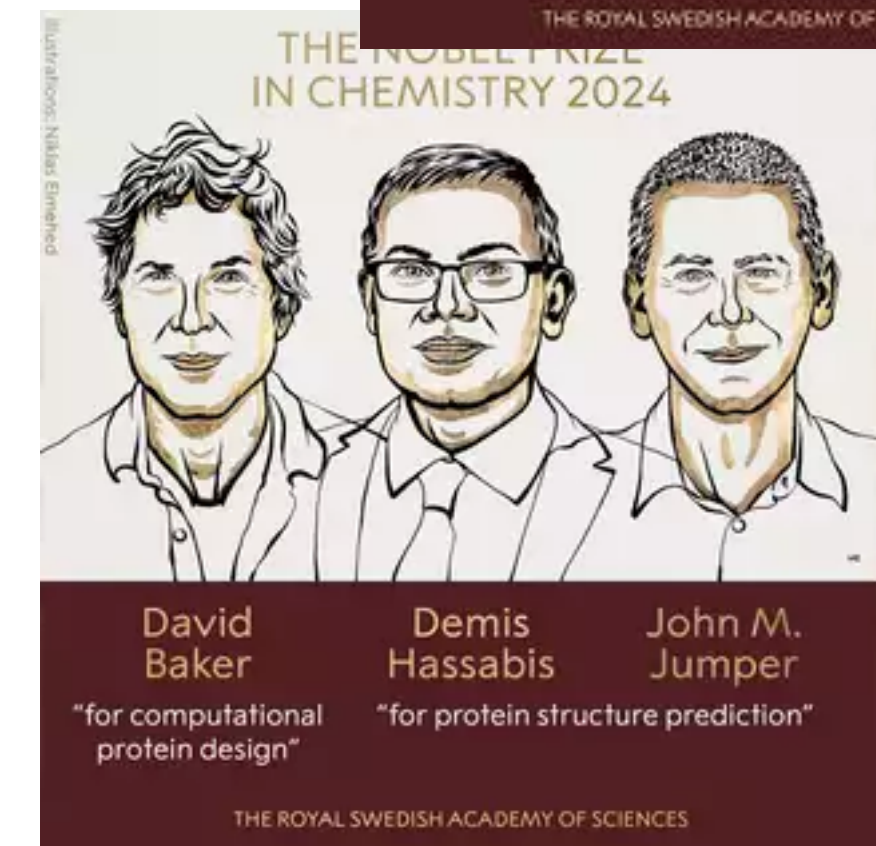
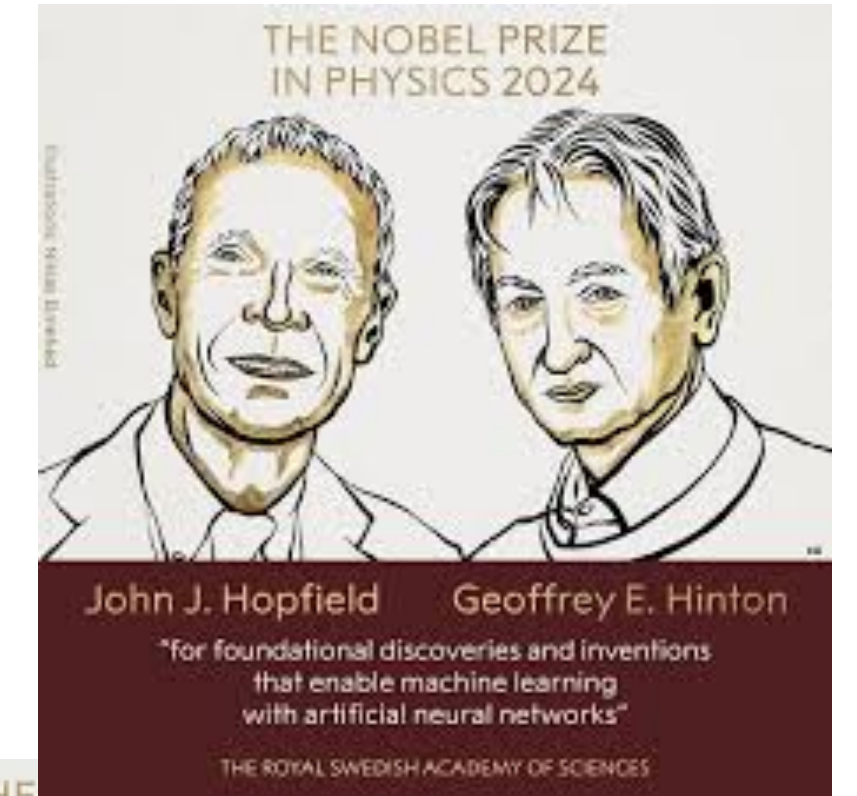


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Frontier performance across benchmarks



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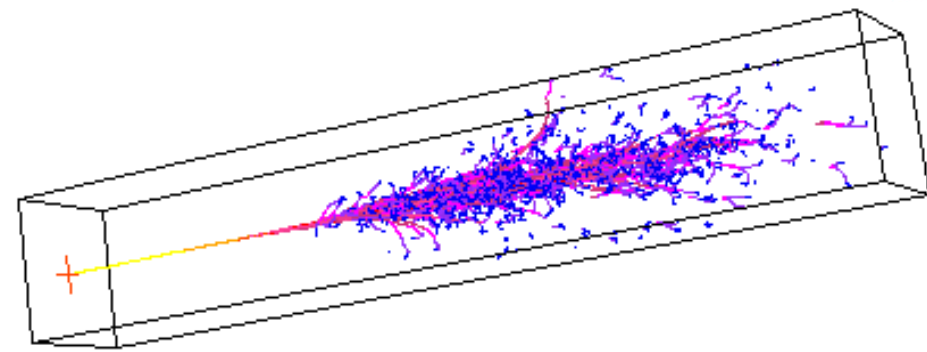


Google A.I. System Wins Gold Medal in International Math Olympiad

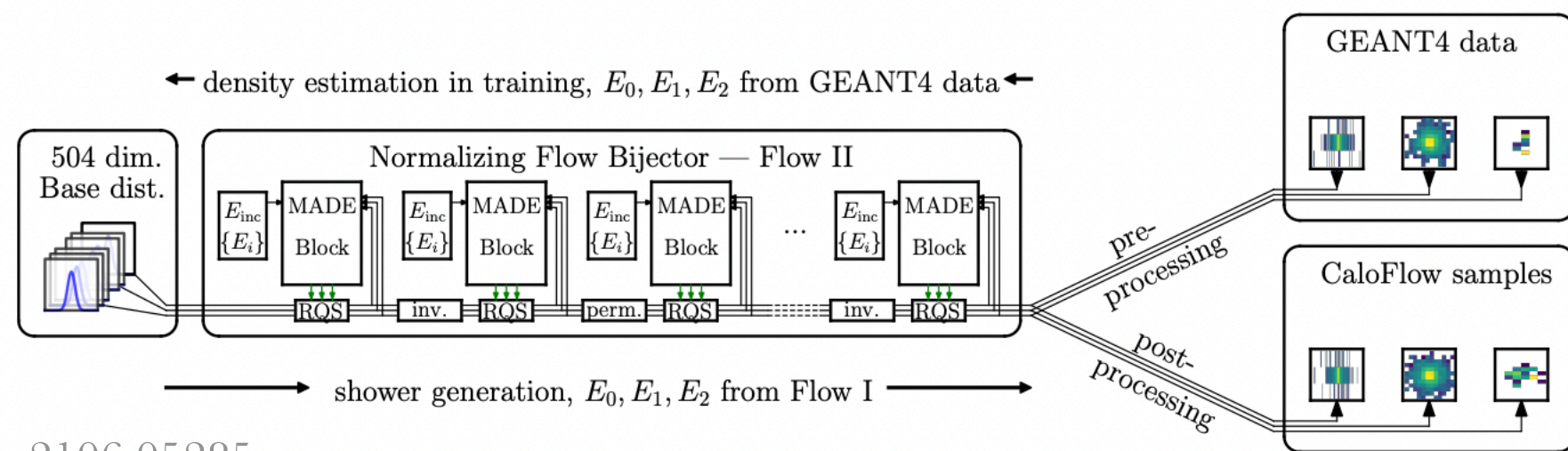
OpenAI said it, too, had built a system that achieved similar results.

Fast simulation

CaloChallenge 2022: A Community Challenge for Fast Calorimeter Simulation
2410.21611

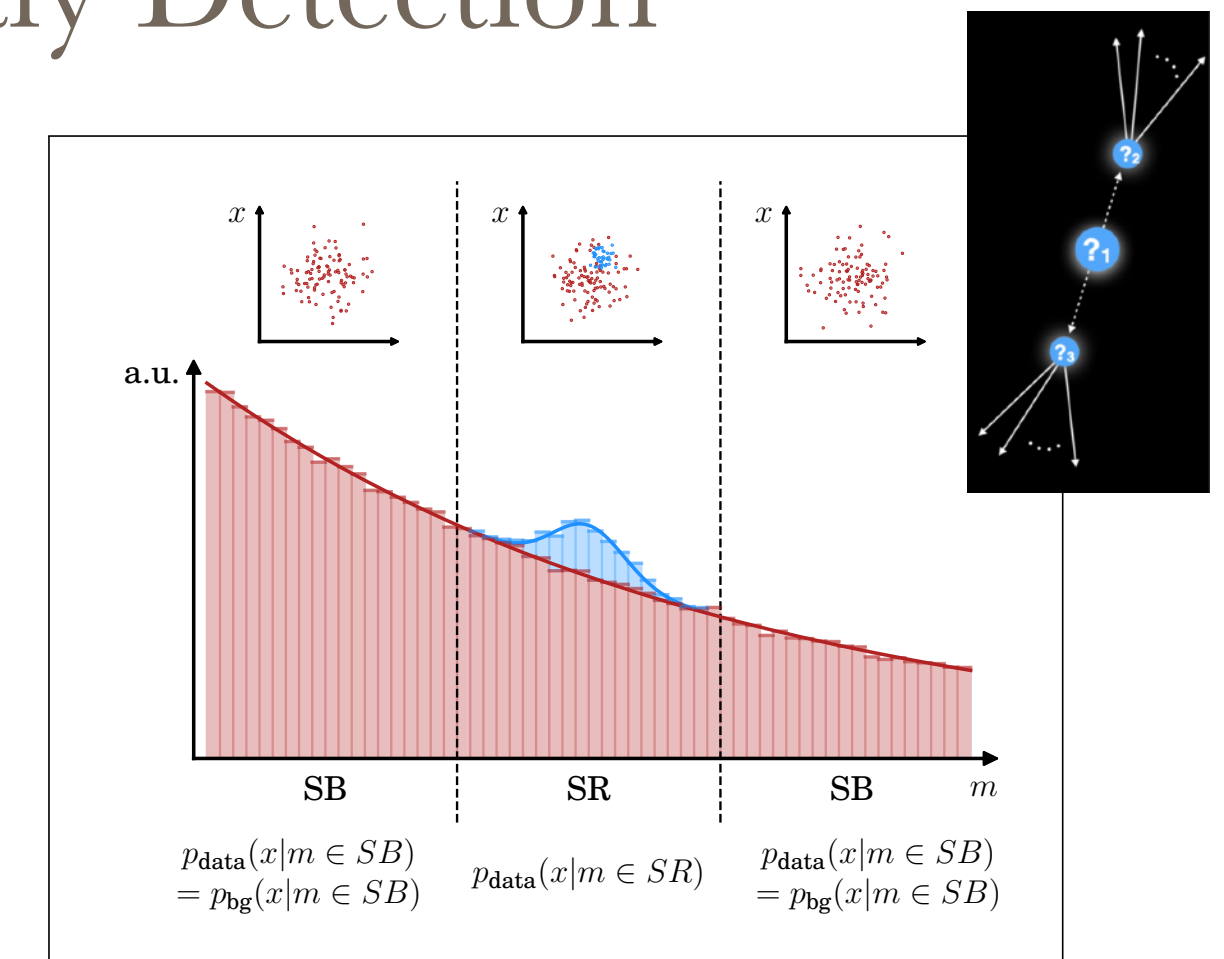
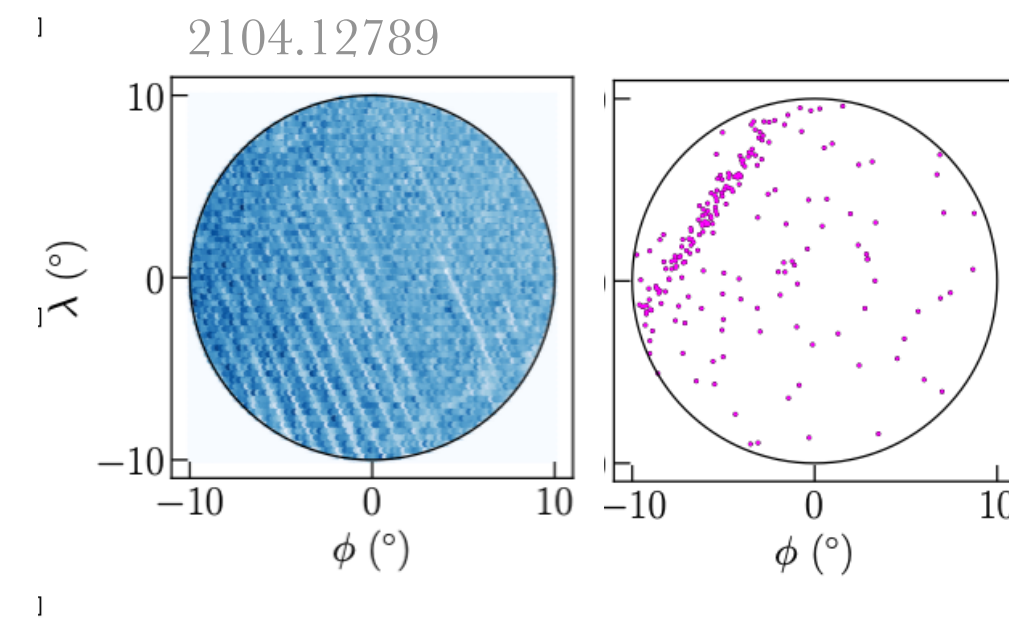


"Calorimeter Simulation", generated via midjourney, 2022

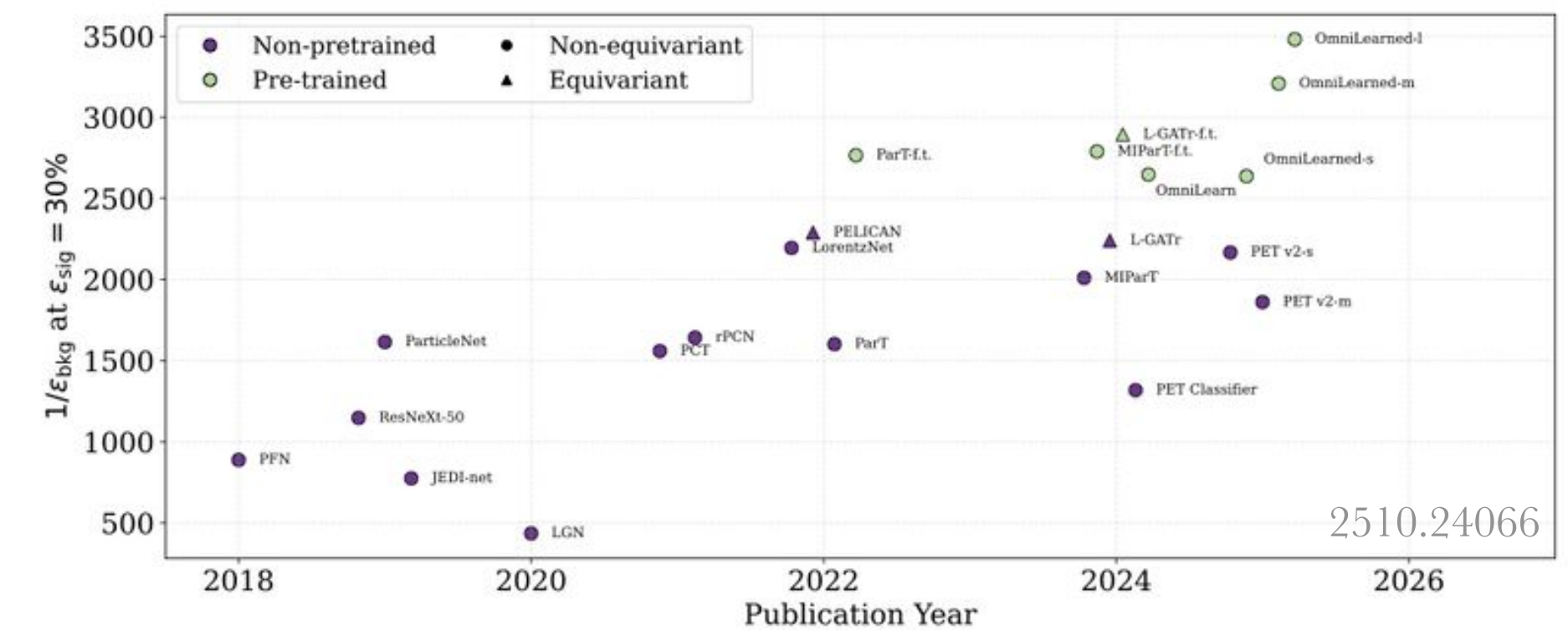


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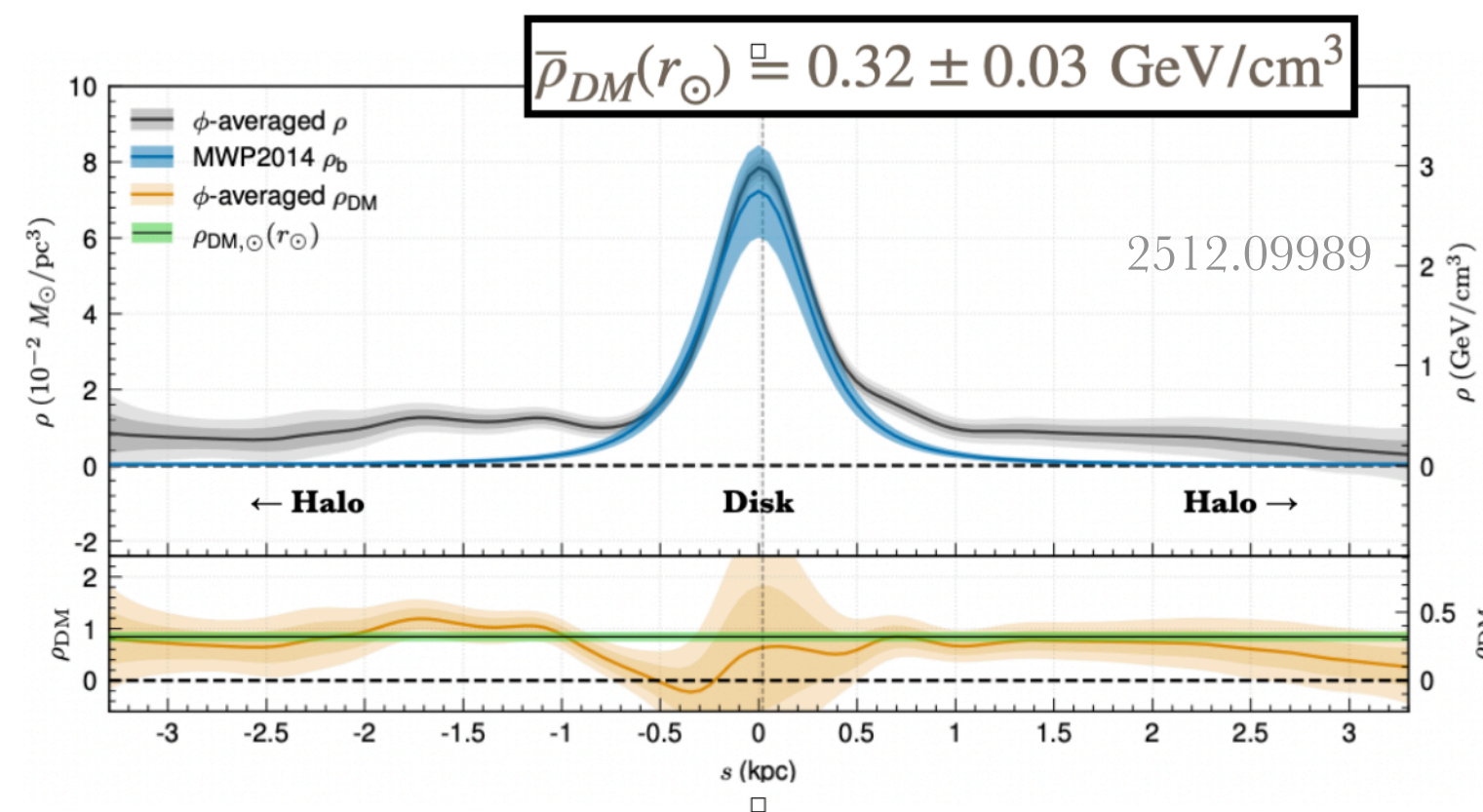
Anomaly Detection



Jet tagging



Novel measurements



And much, much more...

Agentic AI — a watershed moment

Claude Code, Codex — early 2025

Giving agency to LLMs — from question answering to reading/writing/executing code



Home News Sport Business Technology Health Culture Arts Travel Earth Audio Video Live

'Vibe coding' named word of the year by Collins Dictionary

☰ **The New York Times** 👤

Artificial Intelligence > Apple Settlement Job Losses Meta Sued Vetting A.I. Models A.I. Spending Rec

SHOP TALK

With 'Vibecoding,' A.I. Can Help Anyone Build an App

Bringing on artificial intelligence as a collaborator can make coding feel more accessible to those with little training in it, but there are trade-offs.

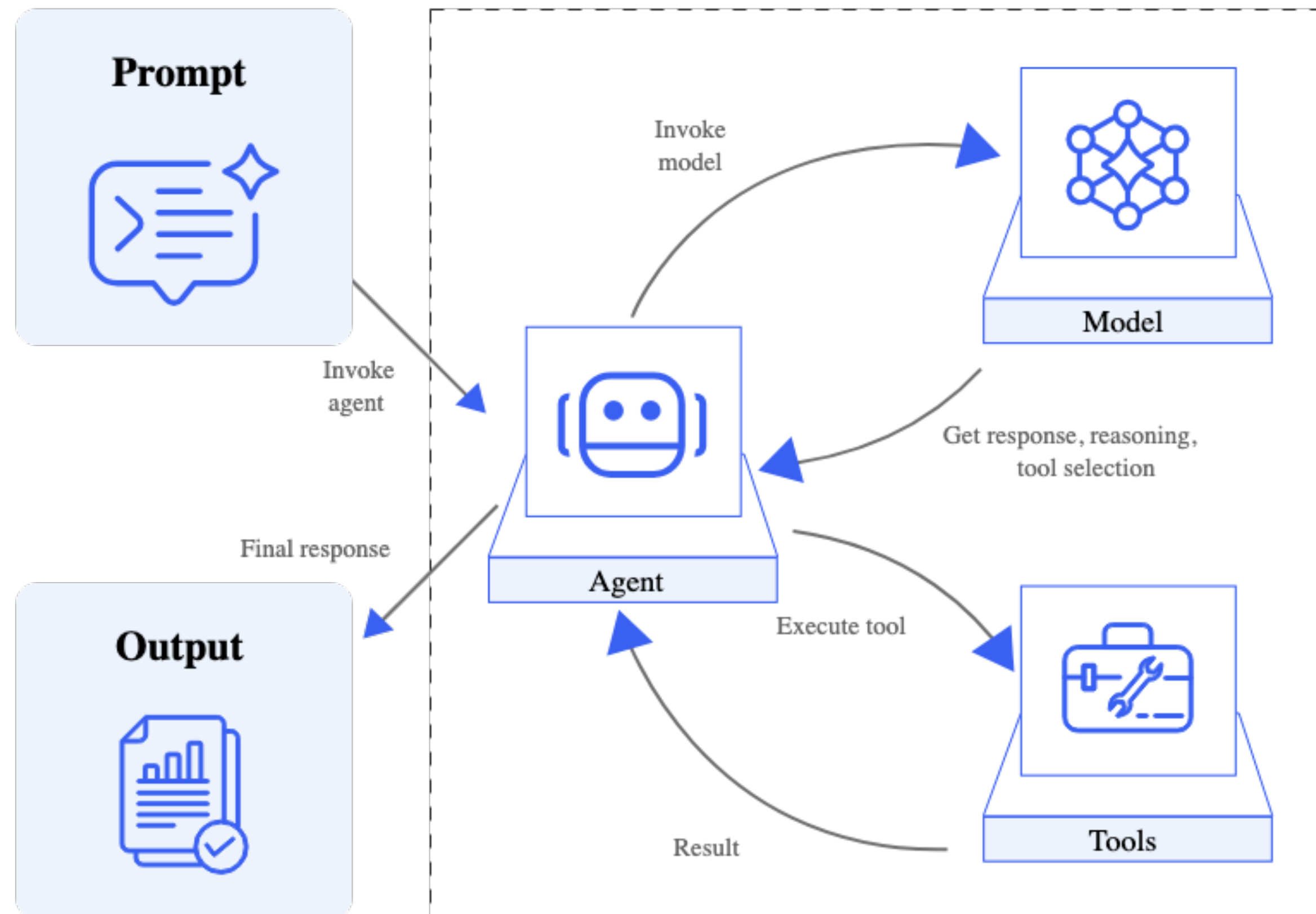
tom's **HARDWARE** [Follow](#)

Claude-powered AI coding agent deletes entire company database in 9 seconds — backups zapped, after Cursor tool powered by Anthropic's Claude goes rogue

TECH

20,000 job cuts at Meta, Microsoft raise concern that AI-driven labor crisis is here

Agentic AI explained



ZBrain

- Agentic AI consists of
 - LLM backend (Claude, GPT, Gemini ...)
 - a set of ***tools*** (bash, python, grep, text editor, ...)
 - a ***harness/scaffold*** (traditional code infrastructure managing model responses and tool use)
- Examples include Claude Code, Codex, Antigravity, ...

How are people using agentic AI?

- Particle physicists are exploring building custom harnesses for automating
 - anomaly detection
 - pheno tasks [ArgoLOOM, HEPTAPOD, MadAgents, CoLLM, FERMIACC, ColliderAgent/Magnus...]
 - experimental data analysis

Agents of Discovery

Sascha Diefenbacher¹, Anna Hallin²,
Gregor Kasieczka², Michael Krämer³, Anne Lauscher⁴, Tim Lukas²,

The FERMIACC: Agents for Particle Theory

AI Agents Can Already Autonomously Perform Experimental High Energy Physics

Eric A. Moreno^{*†1,2}, Samuel Bright-Thonney^{*†1,2}, Andrzej Novak^{*§1,2}, Dolores Garcia^{#3},
and Philip Harris^{‡1,2}

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Increasing interest in rigorous benchmarking

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- experimental data

See: **ColliderBench** [2605.13950]
Faroughy, Palacios Schweitzer, Pang, Mishra-Sharma & DS

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A new benchmark for agentic AI systems based on reinterpreting LHC searches (“recasting”)

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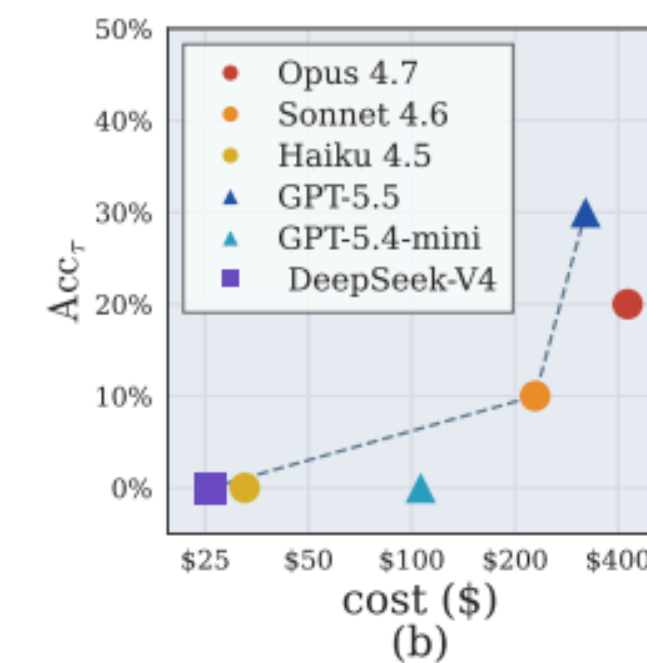
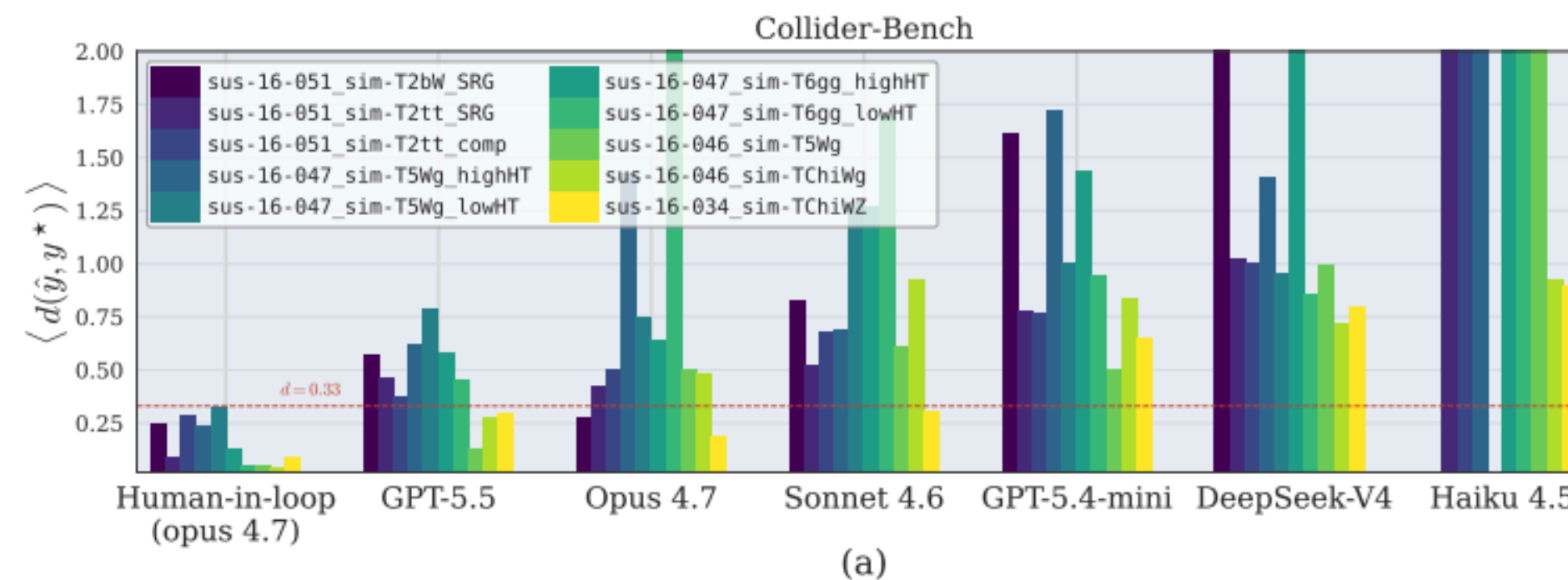
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Questions:

- Frontier LLM model
- Which frontier model
- Automation vs quality



om harness add?

e-loop is needed?

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As research assistants (~graduate student) — “vibe physics”

arXiv > hep-th > arXiv:2603.11164 Search...
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High Energy Physics – Theory

[Submitted on 11 Mar 2026 (v1), last revised 11 Apr 2026 (this version, v2)]

Learning to Unscramble: Simplifying Symbolic Expressions via Self-Supervised Oracle Trajectories

David Shih

We present a new self-supervised machine learning approach for symbolic simplification of complex mathematical expressions. Training data is generated by scrambling simple expressions and recording the inverse operations, creating oracle trajectories that provide both goal states and explicit paths to reach them. A permutation-equivariant, transformer-based policy network is then trained on this data step-wise to predict the oracle action given the input expression. We demonstrate this approach on two problems in high-energy physics: dilogarithm reduction and spinor-helicity scattering amplitude simplification. In both cases, our trained policy network achieves near perfect solve rates across a wide range of difficulty levels, substantially outperforming prior approaches based on reinforcement learning and end-to-end regression. When combined with contrastive grouping and beam search, our model achieves a 100% full simplification rate on a representative selection of 5-point gluon tree-level amplitudes in Yang-Mills theory, including expressions with over 200 initial terms.

Comments: 14 pages, 6 figures, 2 tables; work done in collaboration with Claude Code; v2: refs added

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High Energy Physics – Phenomenology

[Submitted on 6 Apr 2026]

Learning to Unscramble Feynman Loop Integrals with SAILIR

David Shih

Integration-by-parts (IBP) reduction of Feynman integrals to master integrals is a key computational bottleneck in precision calculations in high-energy physics. Traditional approaches based on the Laporta algorithm require solving large systems of equations, leading to memory consumption that grows rapidly with integral complexity. We present SAILIR (Self-supervised AI for Loop Integral Reduction), a new machine learning approach in which a transformer-based classifier guides the reduction of integrals one step at a time in a fully online fashion. The classifier is trained in an entirely self-supervised manner on synthetic data generated by a scramble/unscramble procedure: known reduction identities are applied in reverse to build expressions of increasing complexity, and the classifier learns to undo these steps. When combined with beam search and a highly parallelized, asynchronous, single-episode reduction strategy, SAILIR can reduce integrals of arbitrarily high weight with bounded memory. We benchmark SAILIR on the two-loop triangle-box topology, comparing against the state-of-the-art IBP reduction code Kira across 16 integrals of varying complexity. While SAILIR is slower in wall-clock time, its per-worker memory consumption remains approximately flat regardless of integral complexity, in contrast to Kira whose memory grows rapidly with complexity. For the most complex integrals considered here, SAILIR uses only 40% of the memory of Kira while achieving comparable reduction times. This demonstrates a fundamentally new paradigm for IBP reduction in which the memory bottleneck of Laporta-based approaches could be entirely overcome, potentially opening the door to precision calculations that are currently intractable.

Comments: 16 pages, 3 figures, 5 tables, work done in collaboration with Claude Code

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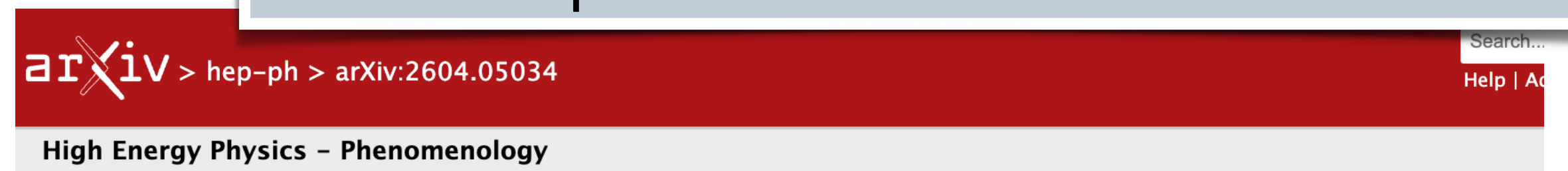
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Risky projects
— branching out into new subfields

Approx 2 months of work
— compared to 6-12 months for a student



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see also Schwartz 2601.02484, Guevara et al 2602.12176, Zhang 2604.27050

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Outline

- Learning to unscramble: general framework
- **Application 1:** Dilog identities
- **Application 2:** Tree-level YM scattering amplitudes
- **Application 3:** IBP reduction of Feynman loop integrals
- Lessons learned

Learning to Unscramble: general framework

- Goal: ML methods for mathematical (symbolic) simplification

$$E_{\text{complicated}} = X_1 + X_2 + X_3 + X_4 + \dots$$



mathematical identities

$$E_{\text{simple}} = Y_1$$

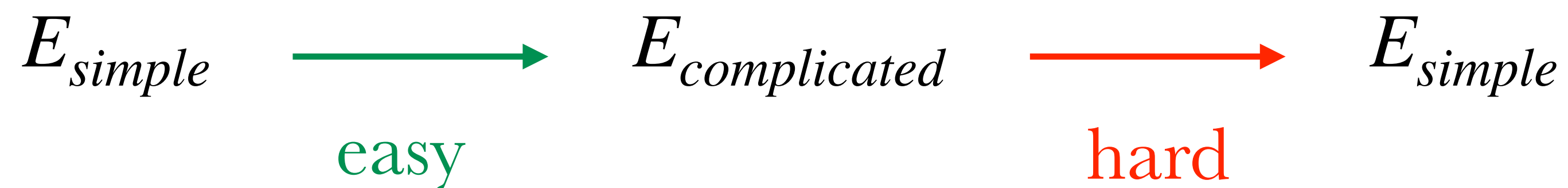
- Test beds: dilog sums, tree-level YM scattering amplitudes

(Dersy, Schwartz, Zhang [2206.04115](#); Cheung, Dersy, Schwartz [2408.04720](#))

Training data



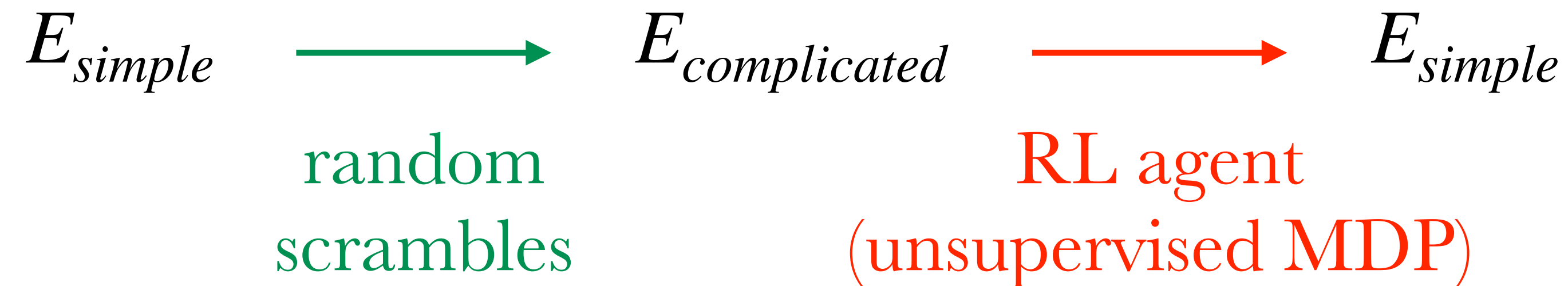
- ML methods need training data
- **Key insight:** can think of complicated expressions as *scrambles* of simple ones by mathematical identities.
- Process of simplification is then *unscrambling*. Dersy, Schwartz, Zhang [2206.04115](#)
- *Strong analogy with Rubik's cubes!*
- Can cheaply create training data by applying random identities to simple expressions



Prior approaches: RL

Dersy, Schwartz, Zhang [2206.04115](#)

MDP: Markov Decision Process
action classifier $\pi(a | s)$,
depends only on previous state



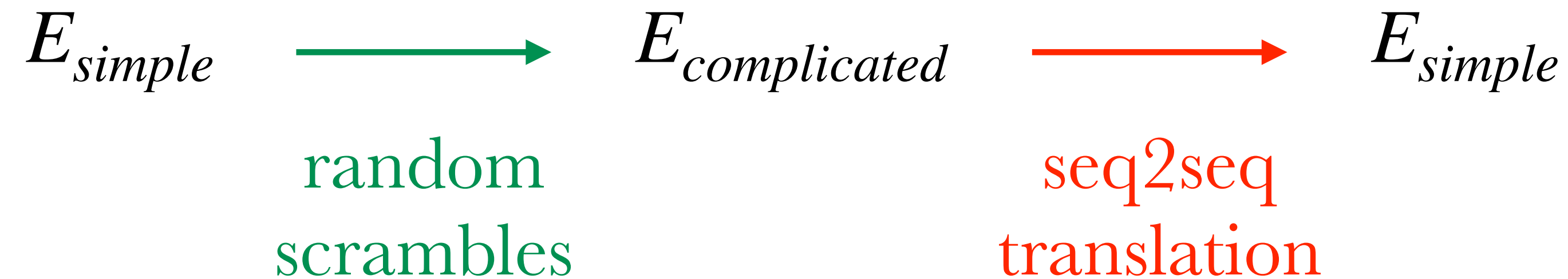
RL (PPO, TRPO) could not beat classical algorithm on even very simple simplification tasks (small dlog sums simplifying to zero).

Challenges: very sparse reward signal, non-monotonic reduction paths

Successful RL is very compute intensive and requires a lot of fine tuning.

Prior approaches: end-to-end regression

Cheung, Dersy, Schwartz [2408.04720](#)



End-to-end regression with a seq2seq transformer achieved decent performance (80-90%) for dilog sums and scattering amplitudes

Drawback: mathematical correctness not guaranteed, transformer can hallucinate simpler but incorrect expressions!

Our approach: “Learning to Unscramble”

DS 2603.11164

Key insight: random scrambles can be reversed, step-by-step.

—> A wealth of simplification training data!!!

$$-\frac{\langle 13 \rangle [14] [23]}{\langle 12 \rangle \langle 14 \rangle [12]^2}$$

$$\Downarrow \text{mom}^2: \langle 13 \rangle [31] + \langle 14 \rangle [41] + \langle 34 \rangle [43] = 0$$

$$\frac{\langle 14 \rangle [14]^2 [23] + \langle 34 \rangle [14] [23] [34]}{\langle 12 \rangle \langle 14 \rangle [12]^2 [13]}$$

$$\Downarrow \text{mom}^2: \langle 12 \rangle [21] - \langle 34 \rangle [43] = 0$$

Idea from *ML for Rubik’s cube literature*:
Takano 2106.03157

$$\frac{-\langle 12 \rangle [12] [14] [23] + \langle 14 \rangle [14]^2 [23] + 2\langle 34 \rangle [14] [23] [34]}{\langle 12 \rangle \langle 14 \rangle [12]^2 [13]}$$

$$\Downarrow \text{Schouten: } [24] [13] + [21] [34] + [23] [41] = 0$$



$$\frac{1}{\langle 12 \rangle \langle 14 \rangle [12]^2 [13] [23]} \left(\langle 14 \rangle [12]^2 [34]^2 + \langle 14 \rangle [13]^2 [24]^2 + \langle 12 \rangle [12]^2 [23] [34] \right. \\ \left. - 2\langle 34 \rangle [12] [23] [34]^2 - \langle 12 \rangle [12] [13] [23] [24] - 2\langle 14 \rangle [12] [13] [24] [34] + 2\langle 34 \rangle [13] [23] [24] [34] \right)$$

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$$\Downarrow \text{mom}^2: \langle 12 \rangle [21] - \langle 34 \rangle [43] = 0$$

Idea from *ML for Rubik’s cube literature*:
Takano 2106.03157

$$\frac{-\langle 12 \rangle [12][14][23] + \langle 14 \rangle [14]^2 [23] + 2\langle 34 \rangle [14][23][34]}{\langle 12 \rangle \langle 14 \rangle [12]^2 [13]}$$

$$\Downarrow \text{Schouten: } [24][13] + [21][34] + [23][41] = 0$$



$$\frac{1}{\langle 12 \rangle \langle 14 \rangle [12]^2 [13][23]} \left(\langle 14 \rangle [12]^2 [34]^2 + \langle 14 \rangle [13]^2 [24]^2 + \langle 12 \rangle [12]^2 [23][34] \right. \\ \left. - 2\langle 34 \rangle [12][23][34]^2 - \langle 12 \rangle [12][13][23][24] - 2\langle 14 \rangle [12][13][24][34] + 2\langle 34 \rangle [13][23][24][34] \right)$$

Our approach: “Learning to Unscramble”

DS 2603.11164

Key insight: random scrambles can be reversed, step-by-step.

—> A wealth of simplification training data!!!

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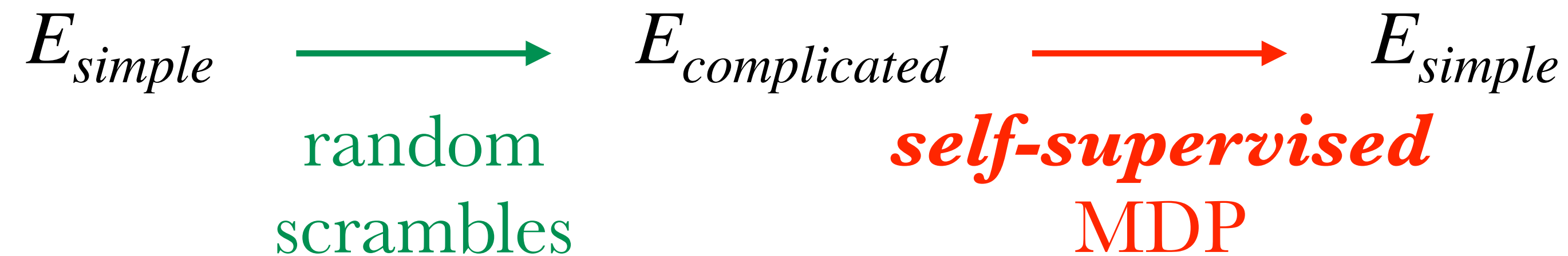
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Our approach: “Learning to Unscramble”

DS 2603.11164



Instead of unsupervised MDP of RL, train a **self-supervised MDP** on **reversed random scramble sequences**

Learns to predict the best action from unscrambling steps

**Addresses limitations of both previous approaches:
highly dense reward signal and no hallucinations!**

Application 1: Dilog sums

[DS 2603.11164]

$$\text{Li}_2(x) = - \int_0^x dz \frac{\log(1-z)}{z}$$

$$(inversion) \quad \text{Li}_2(x) = -\text{Li}_2\left(\frac{1}{x}\right) - \frac{\pi^2}{6} - \frac{\ln^2(-x)}{2}$$

$$(reflection) \quad \text{Li}_2(x) = -\text{Li}_2(1-x) + \frac{\pi^2}{6} - \ln(x) \ln(1-x)$$

$$(duplication) \quad \text{Li}_2(x) = -\text{Li}_2(-x) + \frac{1}{2}\text{Li}_2(x^2)$$

- Toy version of Feynman loop integral simplification
- Class of expressions that Mathematica struggles to simplify

$$-4 \text{Li}_2\left(\frac{4}{x^2-8x+16}\right) + 8 \text{Li}_2\left(\frac{2}{x-4}\right) - 8 \text{Li}_2\left(\frac{2}{x-2}\right)$$

$$-6 \text{Li}_2\left(\frac{1}{x^2+2x}\right) - 6 \text{Li}_2(x^2+2x) + \frac{7}{2} \text{Li}_2\left(\frac{4}{x^2-4x+4}\right)$$

$$-7 \text{Li}_2\left(\frac{x}{2}\right) - 7 \text{Li}_2\left(\frac{2}{x-2}\right)$$

$$-8 \text{Li}_2\left(\frac{x^2}{2x-2}\right) - 8 \text{Li}_2\left(-\frac{x^2}{2x-2}\right) - \frac{7}{2} \text{Li}_2\left(\frac{4}{x^2+2x+1}\right)$$

$$+4 \text{Li}_2(x^2+4x+4) + 4 \text{Li}_2\left(\frac{x^4}{4x^2-8x+4}\right) - 7 \text{Li}_2\left(-\frac{x}{2} - \frac{1}{2}\right)$$

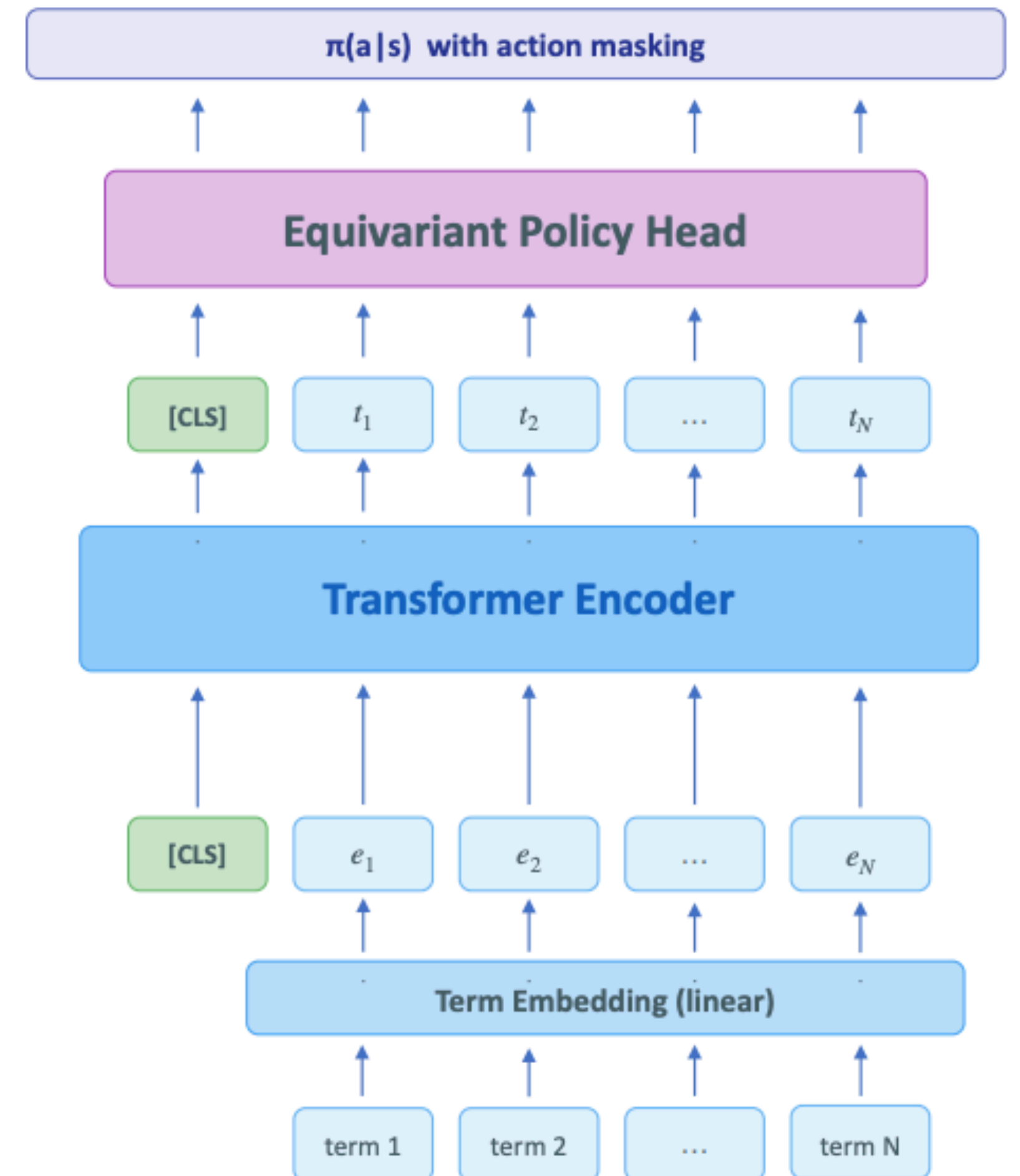
$$-2 \text{Li}_2\left(\frac{1}{x+2}\right) + 8 \text{Li}_2\left(-\frac{1}{x+2}\right) - 10 \text{Li}_2(x+2)$$

examples from Dersy,
Schwartz, Zhang

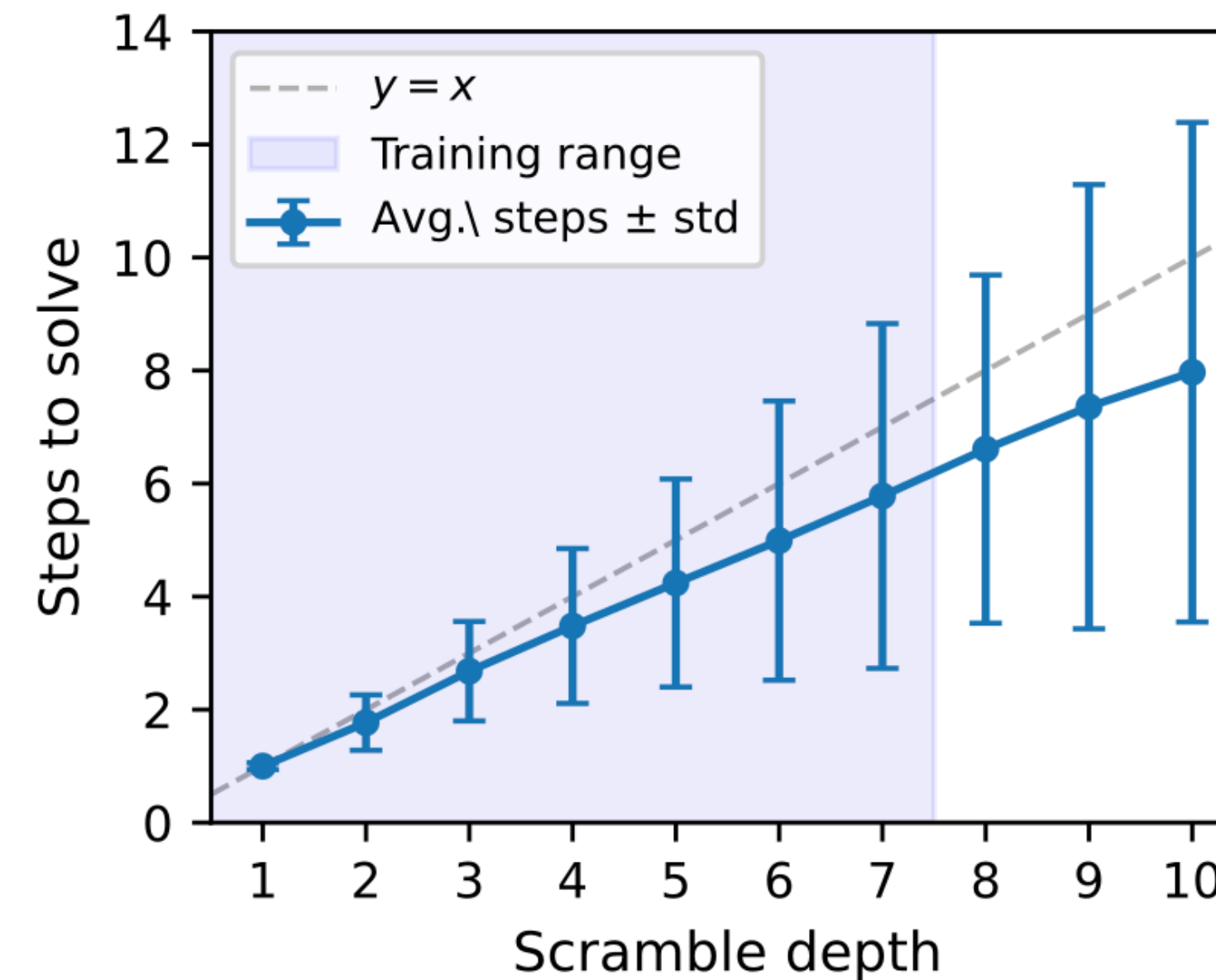
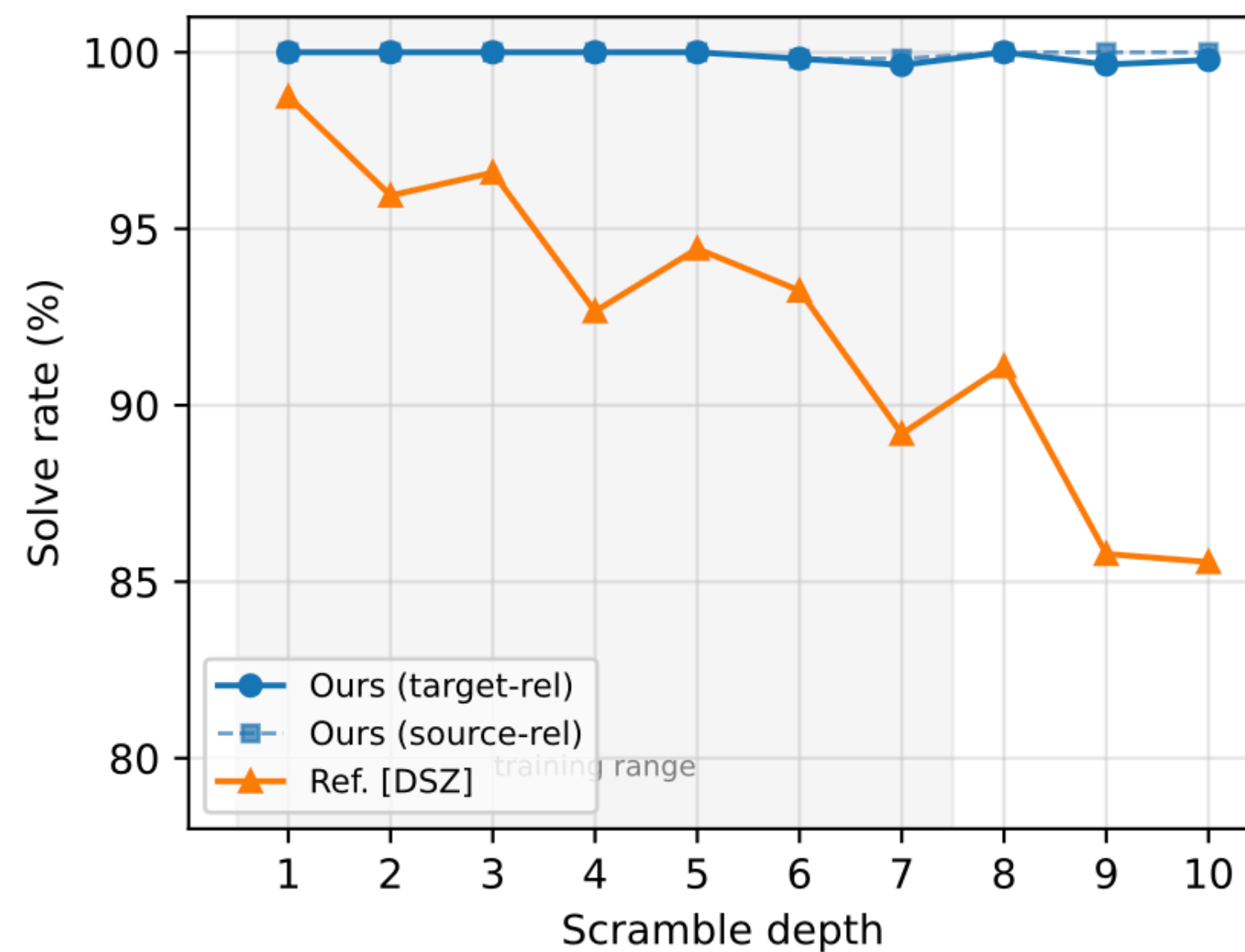
Learning to unscramble dialogs: setup

- Action space: (3 actions) x (up to 15 terms)
- Permutation-equivariant action classifier: 45 dimensional softmax (irrelevant actions masked)
- **Training data:** 100k samples scrambled from simple expressions -> 500k individual unscramble steps
- **Test data:** 5k expressions from DSZ

Policy Network Architecture



Learning to unscramble dialogs



- Nearly 100% simplification rate! Much better than end-to-end transformer (DSZ)
- Only 6 failures out of 5k test set. (Only 2 if we demand some simplification)
- Excellent performance generalizes beyond training set!
- Finds *shorter* simplification paths than training data on average

Application 2: scattering amplitudes

[DS 2603.11164]

Application 2: scattering amplitudes

[DS 2603.11164]

- Example of 5pt YM tree amplitude computed with Feynman diagrams (from Cheung, Dersy, Schwartz)
- Known to simplify to **Parke-Taylor amplitude**
- through repeated application of identities:

Schouten identity :
$$\begin{cases} \langle ij \rangle \langle kl \rangle = \langle il \rangle \langle kj \rangle + \langle ik \rangle \langle jl \rangle \\ [ij][kl] = [il][kj] + [ik][jl] \end{cases}$$

momentum squared :
$$\sum_{\substack{i < j \\ (i,j) \in S_1^n}} \langle ij \rangle [ji] = \sum_{\substack{k < l \\ (k,l) \in S_2^n}} \langle kl \rangle [lk]$$

momentum conservation :
$$\sum_{j=1}^n \langle ij \rangle [jk] = 0 \quad \forall i, k$$

$$A_5 = \frac{\langle 12 \rangle^3}{\langle 13 \rangle \langle 23 \rangle \langle 45 \rangle^2} - \frac{\langle 12 \rangle^2 \langle 23 \rangle}{\langle 13 \rangle \langle 45 \rangle^2 [12]} - \frac{\langle 12 \rangle^3 \langle 15 \rangle [14]}{\langle 13 \rangle \langle 23 \rangle \langle 25 \rangle \langle 45 \rangle^2 [24]} - \frac{\langle 12 \rangle^2 \langle 15 \rangle [14] [23]}{\langle 13 \rangle \langle 25 \rangle \langle 45 \rangle^2 [12] [24]} - \frac{\langle 12 \rangle^2 [34]}{\langle 13 \rangle \langle 45 \rangle^2 [14]} - \frac{\langle 12 \rangle^2 \langle 23 \rangle [34]}{\langle 13 \rangle \langle 25 \rangle \langle 34 \rangle \langle 45 \rangle [14]} - \frac{\langle 12 \rangle^3 \langle 35 \rangle [34]}{\langle 13 \rangle \langle 15 \rangle \langle 25 \rangle \langle 34 \rangle \langle 45 \rangle [14]} - \frac{\langle 12 \rangle \langle 15 \rangle \langle 23 \rangle [15] [34]}{\langle 13 \rangle \langle 25 \rangle \langle 34 \rangle \langle 45 \rangle [12] [14]} - \frac{\langle 12 \rangle^3 [12] [34]}{\langle 13 \rangle \langle 25 \rangle \langle 34 \rangle \langle 45 \rangle [12] [14]} - \frac{\langle 13 \rangle \langle 25 \rangle \langle 34 \rangle \langle 45 \rangle [12] [14]}{\langle 13 \rangle \langle 23 \rangle \langle 25 \rangle \langle 45 \rangle^2 [23] [24]} - \frac{\langle 12 \rangle^3 \langle 15 \rangle [12] [34]}{\langle 13 \rangle \langle 23 \rangle \langle 25 \rangle \langle 45 \rangle^2 [23] [24]} - \frac{\langle 12 \rangle^2 \langle 35 \rangle [23] [34]}{\langle 13 \rangle \langle 25 \rangle \langle 45 \rangle^2 [12] [24]} + \frac{\langle 14 \rangle \langle 23 \rangle [34]}{\langle 13 \rangle \langle 45 \rangle^2 [12] [14]} + \frac{\langle 12 \rangle \langle 34 \rangle [34]}{\langle 13 \rangle \langle 45 \rangle^2 [12] [14]} + \frac{\langle 12 \rangle \langle 14 \rangle [34]}{\langle 13 \rangle \langle 45 \rangle^2 [14] [23]} + \frac{\langle 12 \rangle^2 \langle 34 \rangle [34]^2}{\langle 13 \rangle \langle 23 \rangle \langle 45 \rangle^2 [14] [23]} + \frac{\langle 15 \rangle \langle 23 \rangle \langle 45 \rangle [14] [23]}{\langle 12 \rangle^2 [34]^2} - \frac{\langle 12 \rangle^3 \langle 35 \rangle [34]^2}{\langle 13 \rangle \langle 15 \rangle \langle 23 \rangle \langle 25 \rangle \langle 45 \rangle [14] [23]} + \frac{\langle 14 \rangle [34]^2}{\langle 45 \rangle^2 [12] [24]} + \frac{\langle 12 \rangle [34]^2}{\langle 45 \rangle^2 [14] [24]} - \frac{\langle 12 \rangle^2 \langle 35 \rangle [34]^2}{\langle 13 \rangle \langle 25 \rangle \langle 45 \rangle^2 [14] [24]} - \frac{\langle 12 \rangle \langle 23 \rangle [34]^2}{\langle 12 \rangle^3 \langle 35 \rangle [12] [34]^2} - \frac{\langle 12 \rangle \langle 15 \rangle [15] [34]^2}{\langle 25 \rangle \langle 34 \rangle \langle 45 \rangle [14] [24]} + \frac{\langle 14 \rangle [34]^3}{\langle 45 \rangle^2 [14] [23] [24]} + \frac{\langle 12 \rangle \langle 34 \rangle [34]^3}{\langle 23 \rangle \langle 45 \rangle^2 [14] [23] [24]} - \frac{\langle 12 \rangle [34]^3}{\langle 25 \rangle \langle 45 \rangle [14] [23] [24]} + \frac{\langle 13 \rangle \langle 25 \rangle \langle 34 \rangle \langle 45 \rangle [12] [14]}{\langle 13 \rangle \langle 25 \rangle \langle 34 \rangle \langle 45 \rangle [12] [14]} + \frac{\langle 13 \rangle \langle 25 \rangle \langle 34 \rangle \langle 45 \rangle [12] [14]}{\langle 13 \rangle \langle 25 \rangle \langle 34 \rangle \langle 45 \rangle [12] [14]} + \frac{\langle 12 \rangle \langle 23 \rangle^2 [34] [35]}{\langle 13 \rangle \langle 25 \rangle \langle 34 \rangle \langle 45 \rangle [14] [15]} + \frac{\langle 12 \rangle^2 \langle 23 \rangle \langle 35 \rangle [34] [35]}{\langle 13 \rangle \langle 15 \rangle \langle 25 \rangle \langle 34 \rangle \langle 45 \rangle [14] [15]} + \frac{\langle 15 \rangle \langle 23 \rangle [34] [35]}{\langle 25 \rangle \langle 34 \rangle \langle 45 \rangle [12] [24]} + \frac{\langle 12 \rangle \langle 35 \rangle [34] [35]}{\langle 25 \rangle \langle 34 \rangle \langle 45 \rangle [12] [24]} + \frac{\langle 12 \rangle \langle 23 \rangle [34]^2 [35]}{\langle 13 \rangle \langle 25 \rangle \langle 45 \rangle [14] [15] [23]} + \frac{\langle 12 \rangle \langle 23 \rangle [34] [35]}{\langle 13 \rangle \langle 25 \rangle \langle 45 \rangle [14] [15] [23]} + \frac{\langle 23 \rangle^2 [34]^2 [35]}{\langle 25 \rangle \langle 34 \rangle \langle 45 \rangle [14] [15] [24]} + \frac{\langle 12 \rangle \langle 34 \rangle [34]^2 [35]}{\langle 15 \rangle \langle 25 \rangle \langle 34 \rangle \langle 45 \rangle [14] [15] [24]} + \frac{\langle 23 \rangle [34]^3 [35]}{\langle 25 \rangle \langle 45 \rangle [14] [15] [23] [24]} + \frac{\langle 12 \rangle \langle 35 \rangle [34]^3 [35]}{\langle 12 \rangle \langle 15 \rangle \langle 23 \rangle [15] [34]^2} - 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$$\frac{\langle 12 \rangle^3}{\langle 12 \rangle \langle 23 \rangle \langle 34 \rangle \langle 45 \rangle \langle 51 \rangle} \frac{5}{[45]} \frac{1}{[45]}$$

Scattering amplitudes: setup

- Start from 1-3 terms (shared denominator, same mass dimension and little-group scaling)
- Scramble with identities; also multiplication by unity and addition by zero
 - Total action space: ~1.4k for 4 pts, ~4k for 5 pts and ~30k for 6 pts

$$\overline{\mathcal{M}} \rightarrow \overline{\mathcal{M}} \frac{\langle 12 \rangle}{\langle 12 \rangle} \rightarrow \overline{\mathcal{M}} \frac{\langle 13 \rangle \langle 25 \rangle - \langle 15 \rangle \langle 23 \rangle}{\langle 12 \rangle \langle 35 \rangle}$$

$$\overline{\mathcal{M}} + \frac{[34] - [34]_{\mathcal{F}}}{\mathcal{D}} \rightarrow \overline{\mathcal{M}} + \frac{[14][35] - [13][45] - [15][34]_{\mathcal{F}}}{\mathcal{D}[15]}$$

Training data

500k scramble trajectories.
—> ~1M single steps
(per n-pt).

Test data

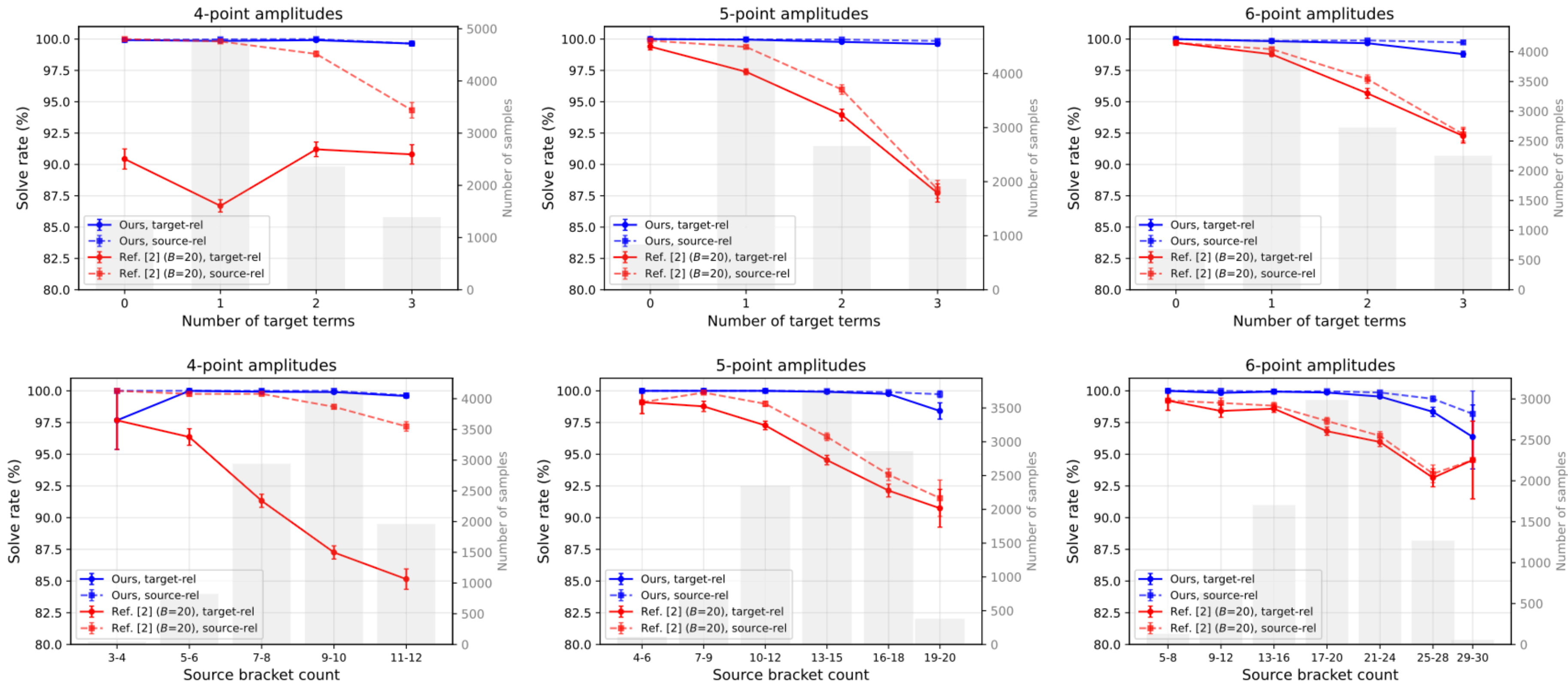
10k test expressions from
CDS enabling head-to-head
comparison.

Additional test data

100 actual 5pt YM
amplitudes
(all simplifying down
to PT form)

Scattering amplitudes: results

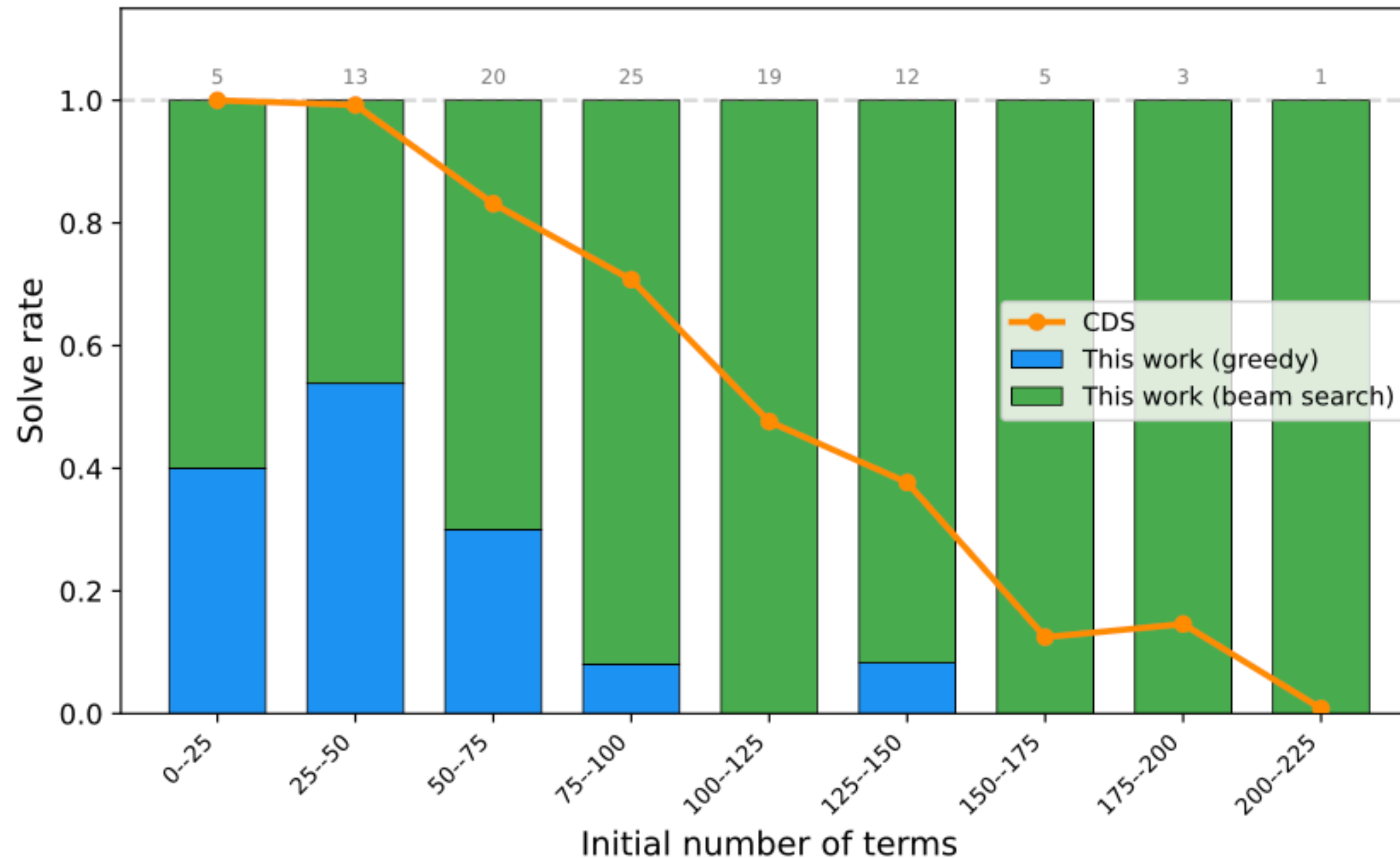
Target relative: simplifies completely to target
Source relative: simplifies source any amount



- We achieve nearly perfect simplification rate across all target and source complexities
- Again, big improvement vs the end-to-end transformer of CDS

Scattering amplitudes: results

- We also achieved 100% simplification of actual 5pt YM amplitudes (up to ~200 initial terms), another big improvement over CDS!



Application 3: IBP reduction

[DS 2604.05034]

- At the precision frontier, calculation of SM processes with Feynman diagrams can generate hundreds of loop integrals. These need to be reduced before numerically evaluating.
- Integration-by-parts identities are linear relations among loop integrals, parametrized by *seed* \mathbf{a} and *operation* (choice of loop momentum k_i and additional momentum v^μ):

$$I[\mathbf{a}] = \int \prod_{j=1}^L d^d k_j \prod_{i=1}^{N_p+N_s} \frac{1}{D_i^{a_i}} \quad \int \prod_{j=1}^L d^d k_j \frac{\partial}{\partial k_i^\mu} (v^\mu \cdot \text{integrand}) = 0,$$

- Can use IBP identities to reduce any loop integral to a basis of master integrals

Laporta algorithm

r: total denominator
(propagator) weight

$$w(I[\mathbf{a}]) = \left(\sum_i \max(a_i, 0), \sum_i |\min(a_i, 0)|, \mathbf{w}_3 \right)$$

s: total numerator
weight

- Basis for general purpose IBP reduction programs like **Kira**

- Make a giant linear system of IBPs
- Use Gaussian elimination to target highest weight IBP
- Continue until fully reduced to master integrals

$$\begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1k} \\ a_{21} & a_{22} & \cdots & a_{2k} \\ \vdots & \vdots & \ddots & \vdots \\ a_{k1} & a_{k2} & \cdots & a_{kk} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_k \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_k \end{bmatrix},$$

$$\left[\begin{array}{cccc|c} a'_{11} & a'_{12} & \cdots & a'_{1k} & b'_1 \\ 0 & a'_{22} & \cdots & a'_{2k} & b'_2 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & a'_{kk} & b'_k \end{array} \right].$$

- Guaranteed to work: number of IBP identities grows faster than the number of seeds
- But very computationally inefficient — **memory wall**

Self-supervised AI for Loop Integral Reduction (SAILIR)

- Learning to Unscramble applied to IBP reduction
- Some challenges unique to IBP reduction:
 - weight reduction instead of term reduction
 - much bigger action space (number of IBPs combinatorially large)
 - but set of valid actions much smaller (10-100 per expression) but variable (depends on expression)
 - much more elaborate inference

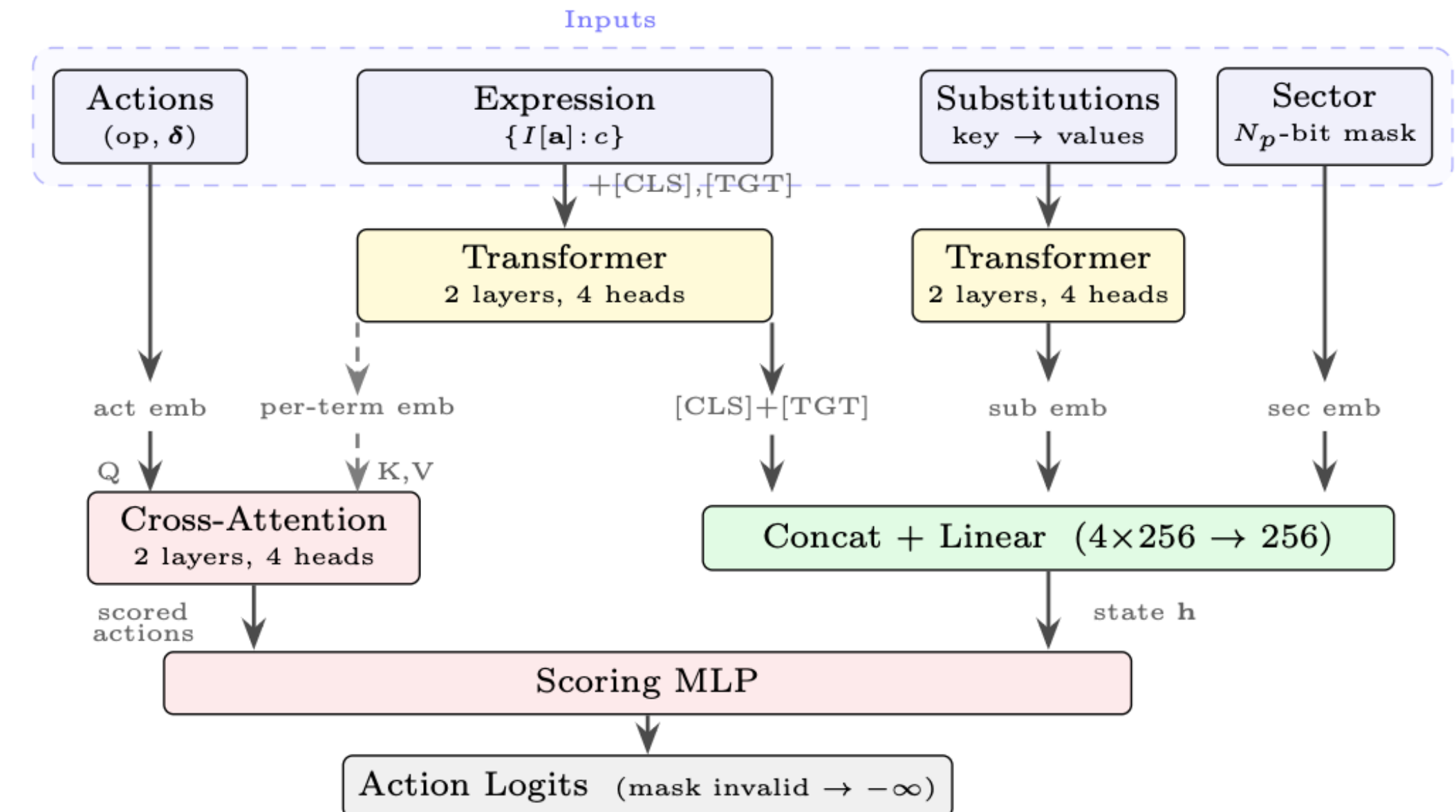
Weight vs term reduction

- Weight reordering:
 - to train the MDP to reduce by weight, we reorder the unscrambles to monotonically reduce highest weight integral in the expression at each step (can prove that this can always be done)
- Sector-wise reduction:
 - Loop integrals labeled by indices $\mathbf{a} = (a_1, a_2, \dots)$ organize into sectors — which propagator factors are present
 - Notion of subsectors $(2, 1, -1, 1) \rightarrow (1, 1, 0, 1)$
 $(-1, 0, -1, 3) \rightarrow (0, 0, 0, 1)$
 - Laporta reduction can work sectorwise: reduce to **corner integral** $I[1, 1, 0, 1]$, $I[0, 0, 0, 1]$, etc — modulo subsectors

Variable action space: learning to rank

- Used in information retrieval (ML for search engines)

- Expression \leftrightarrow question
- actions \leftrightarrow potential answers that we want to rank



- Use cross attention between encoded actions and expression to produce a per-action score
- Softmax gives classifier over all valid actions

Inference engineering

- For dialogs and scattering amplitudes, “greedy” action selection:

$$a_n = \operatorname{argmax} \pi(a | s_n)$$

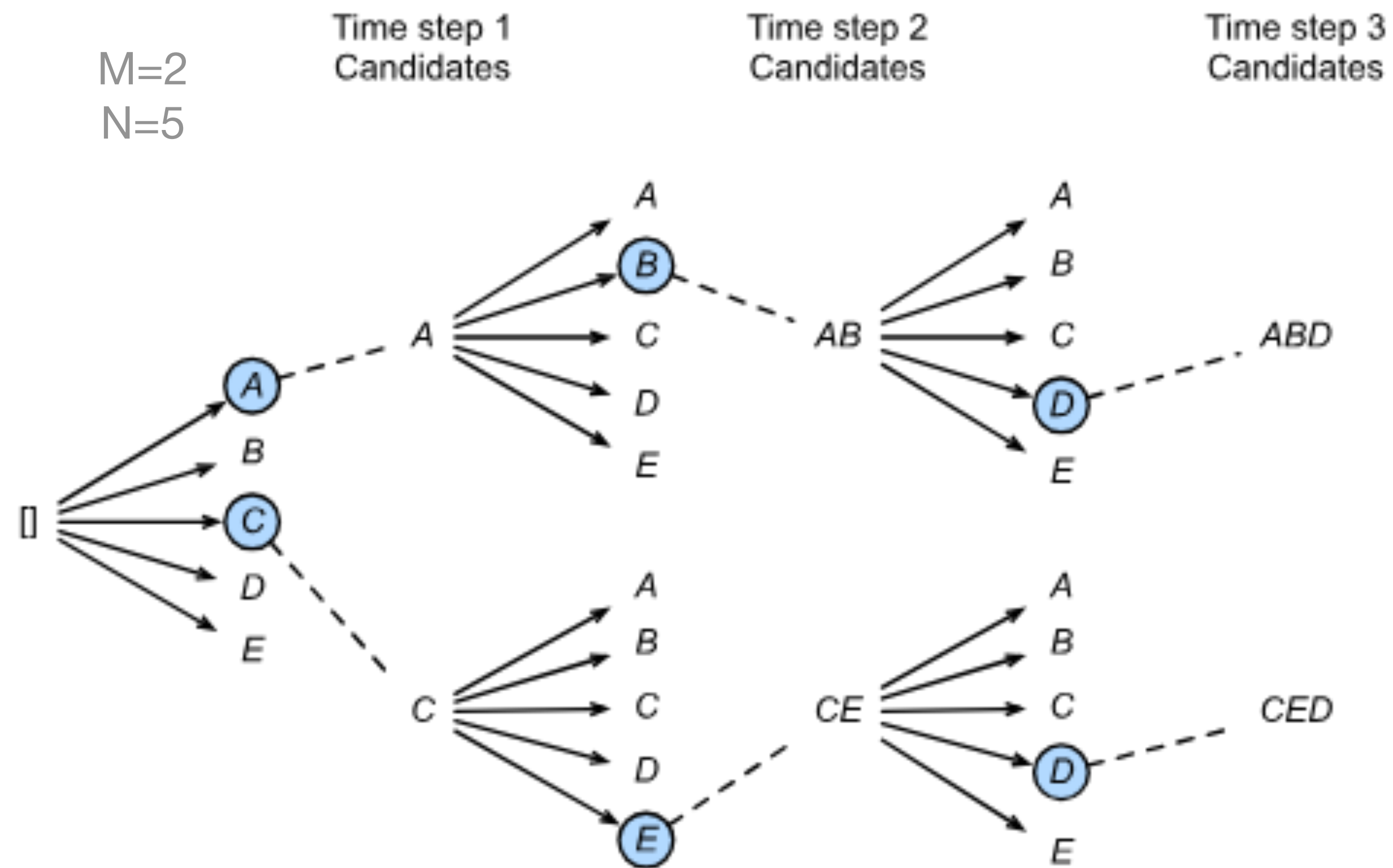
was sufficient to reduce the randomly-scrambled held-out test data

- But for IBP reduction, the train/test mismatch meant more sophisticated methods were required.

Train: sum of higher weight integrals -> single corner integral eg $I[1,1,0,1,1]$

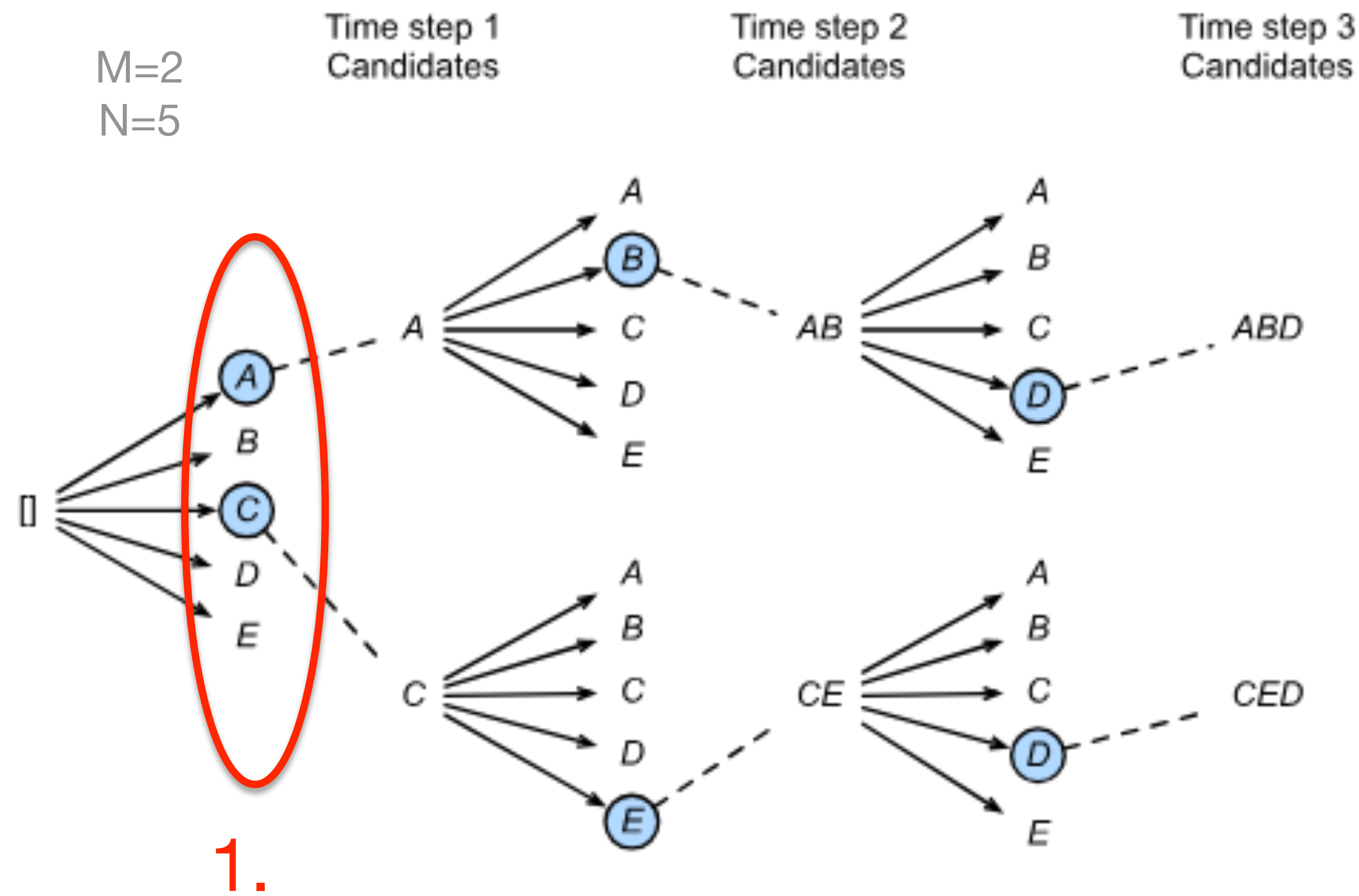
Test: single high weight integral eg $I[3,4,-2,2,2]$ -> sum of corner integrals

Inference engineering: beam search

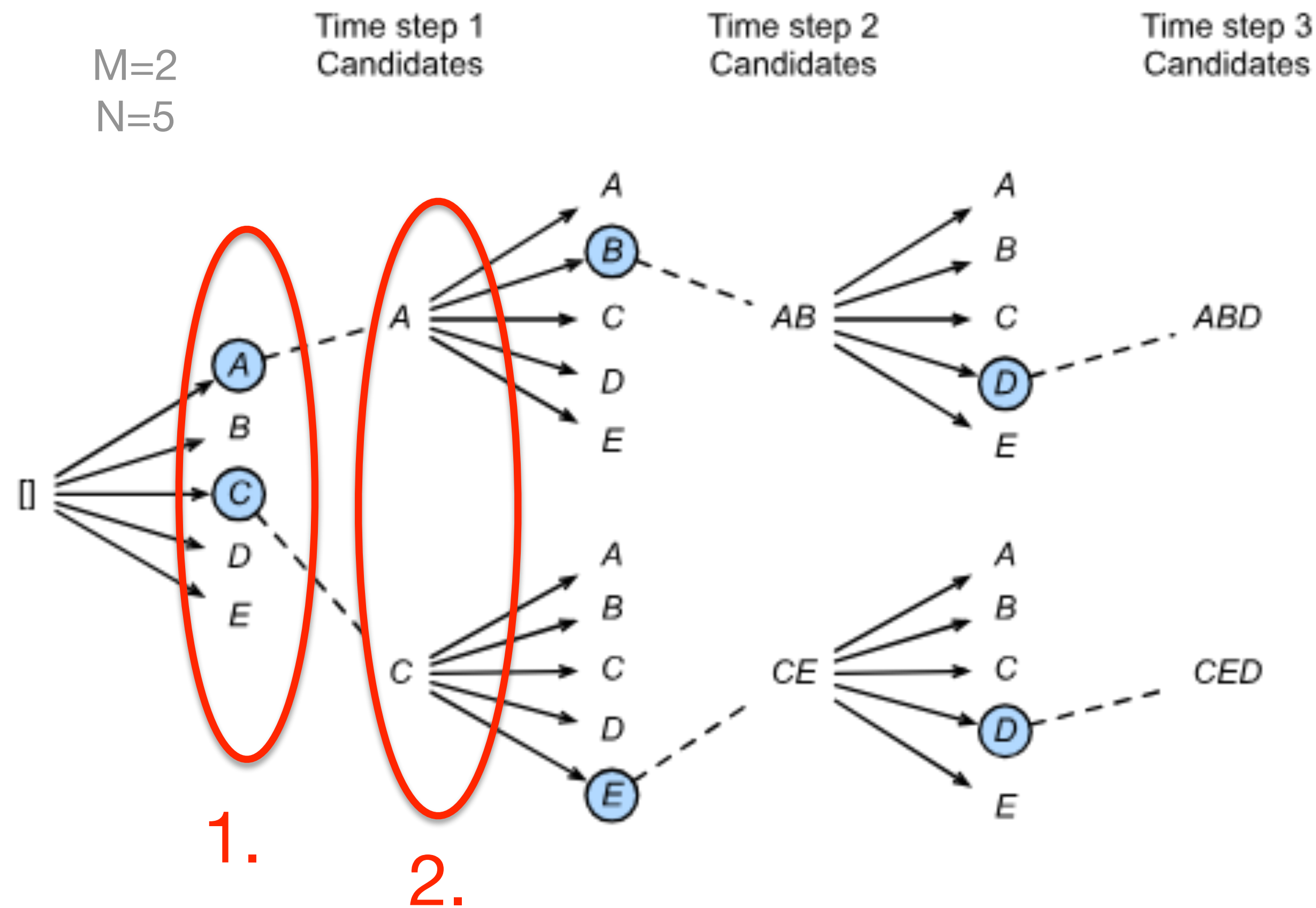


Inference engineering: beam search

1. Maintain a “beam” of $M(=20)$ promising expressions.



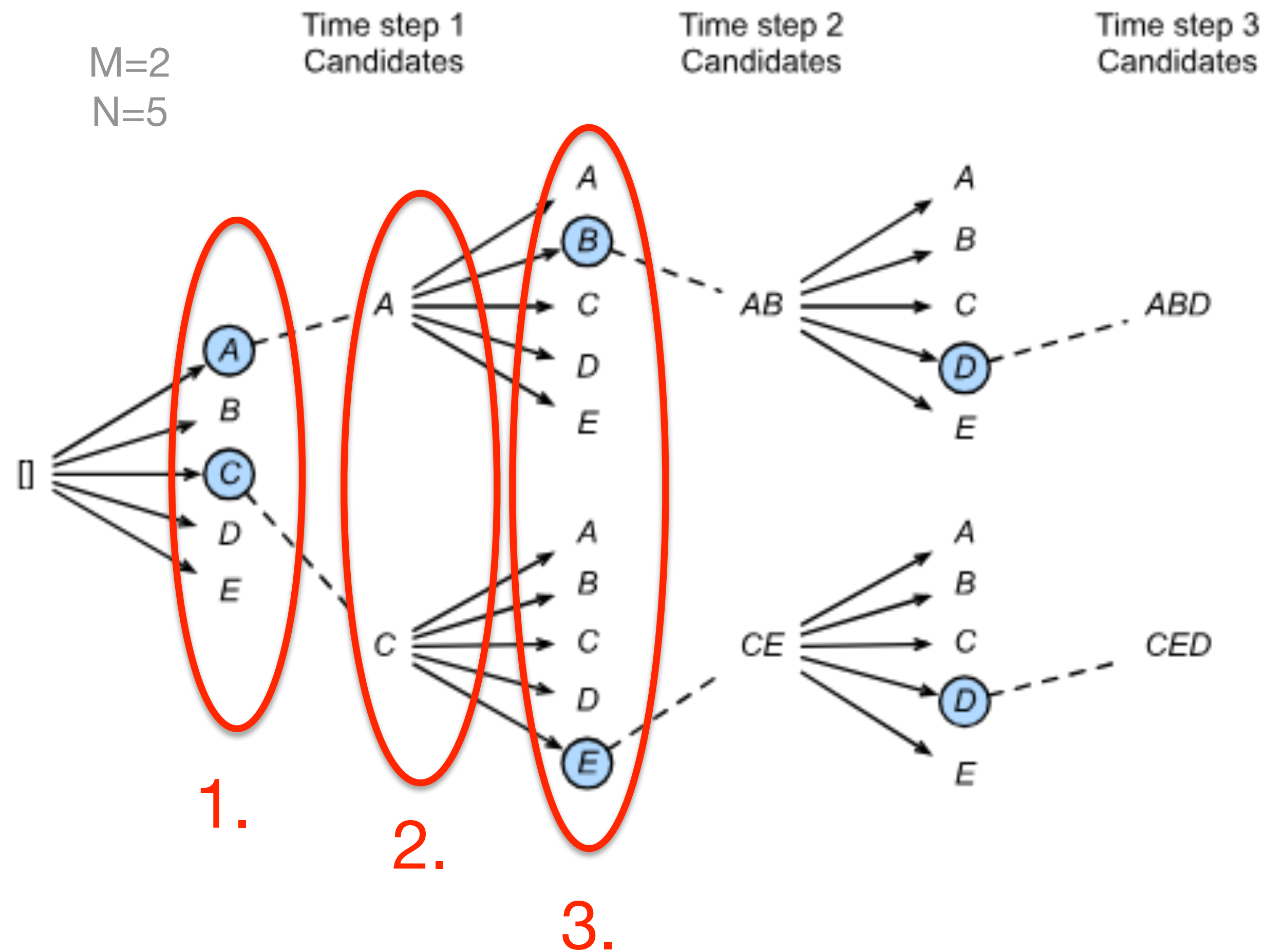
Inference engineering: beam search



1. Maintain a “beam” of $M(=20)$ promising expressions.

2. For each expression, act with the $N(=20)$ top ranked actions according to the action classifier.

Inference engineering: beam search

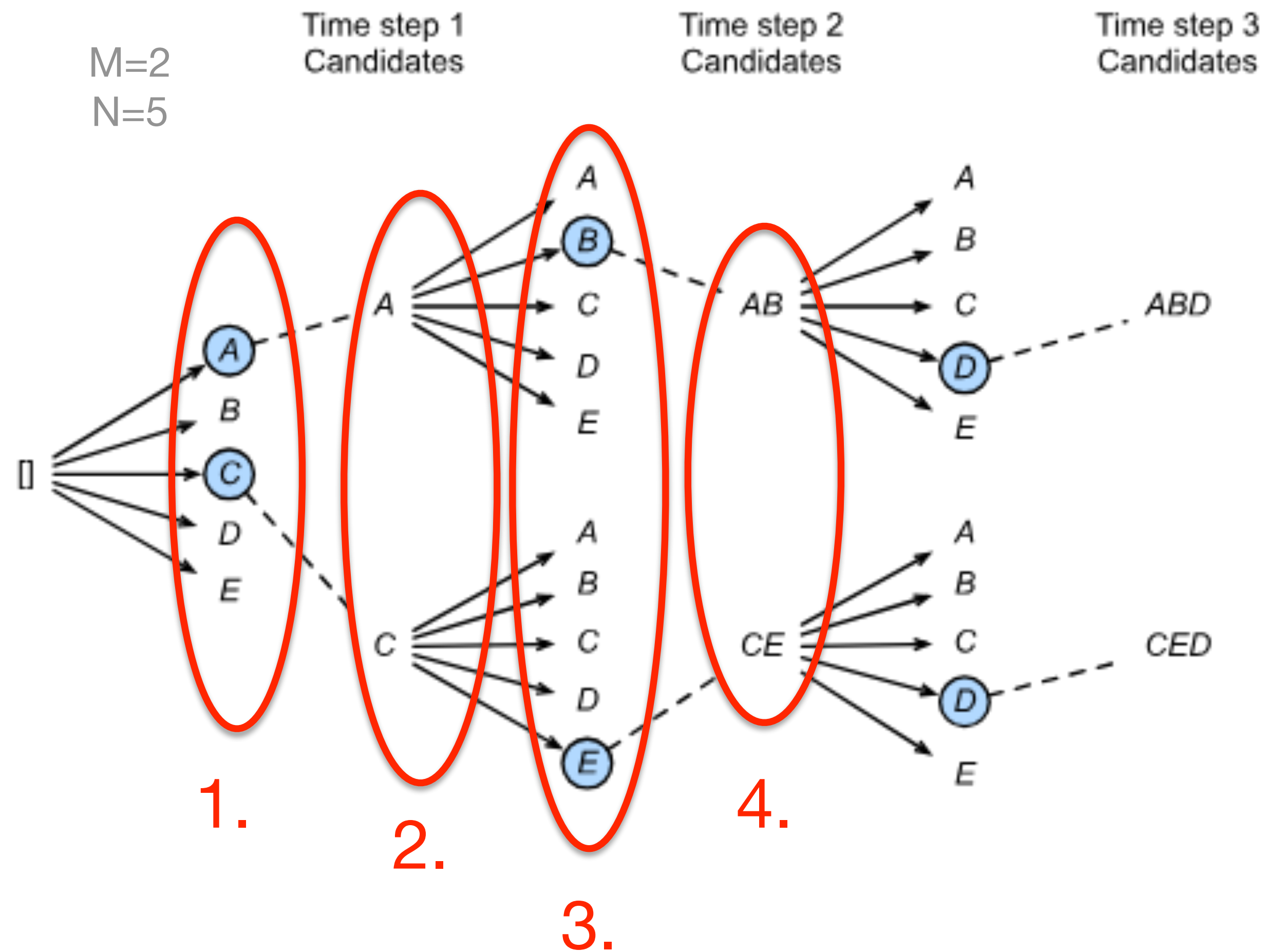


1. Maintain a “beam” of $M(=20)$ promising expressions.

2. For each expression, act with the $N(=20)$ top ranked actions according to the action classifier.

3. This gives MN candidate states.

Inference engineering: beam search



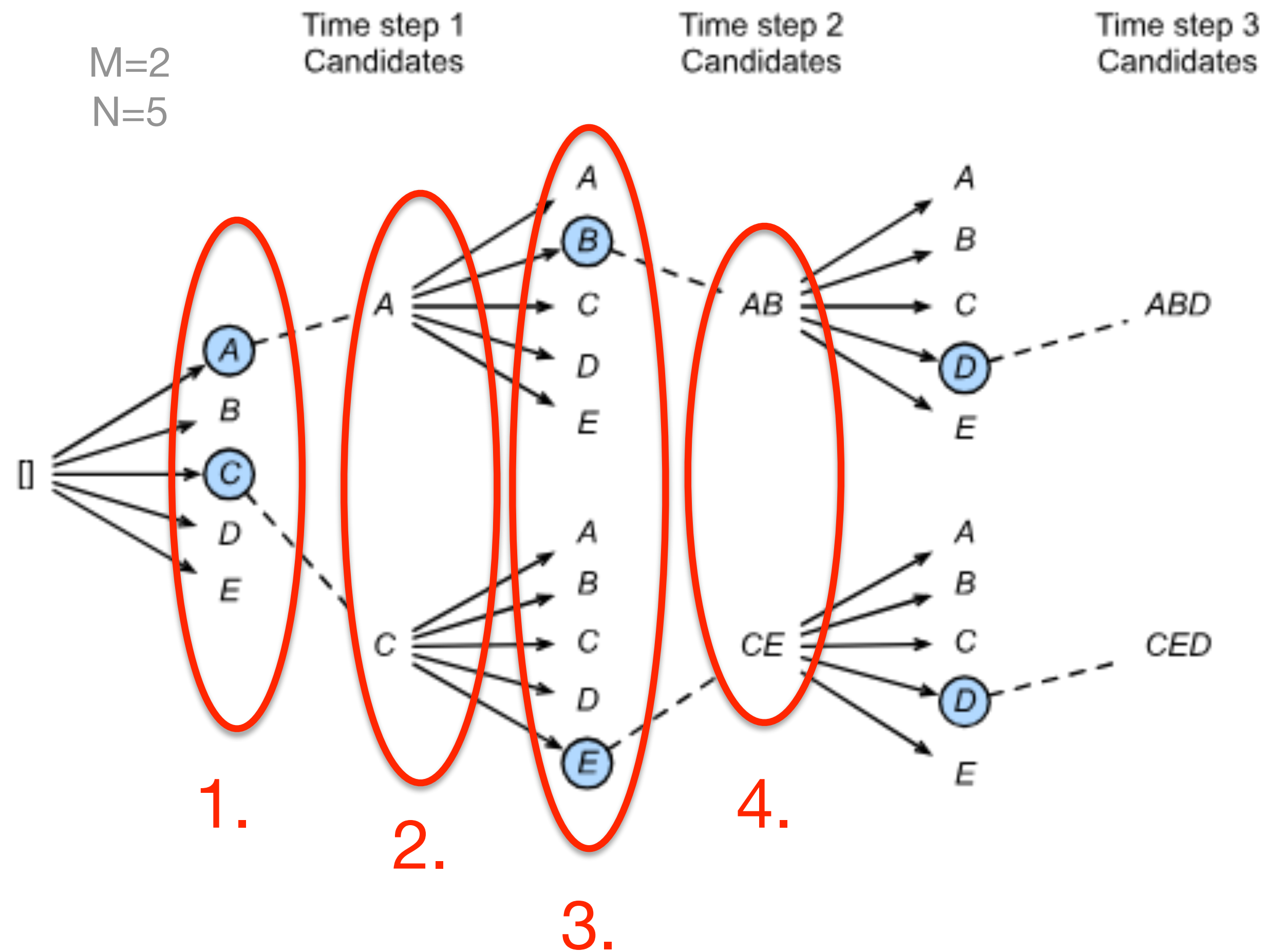
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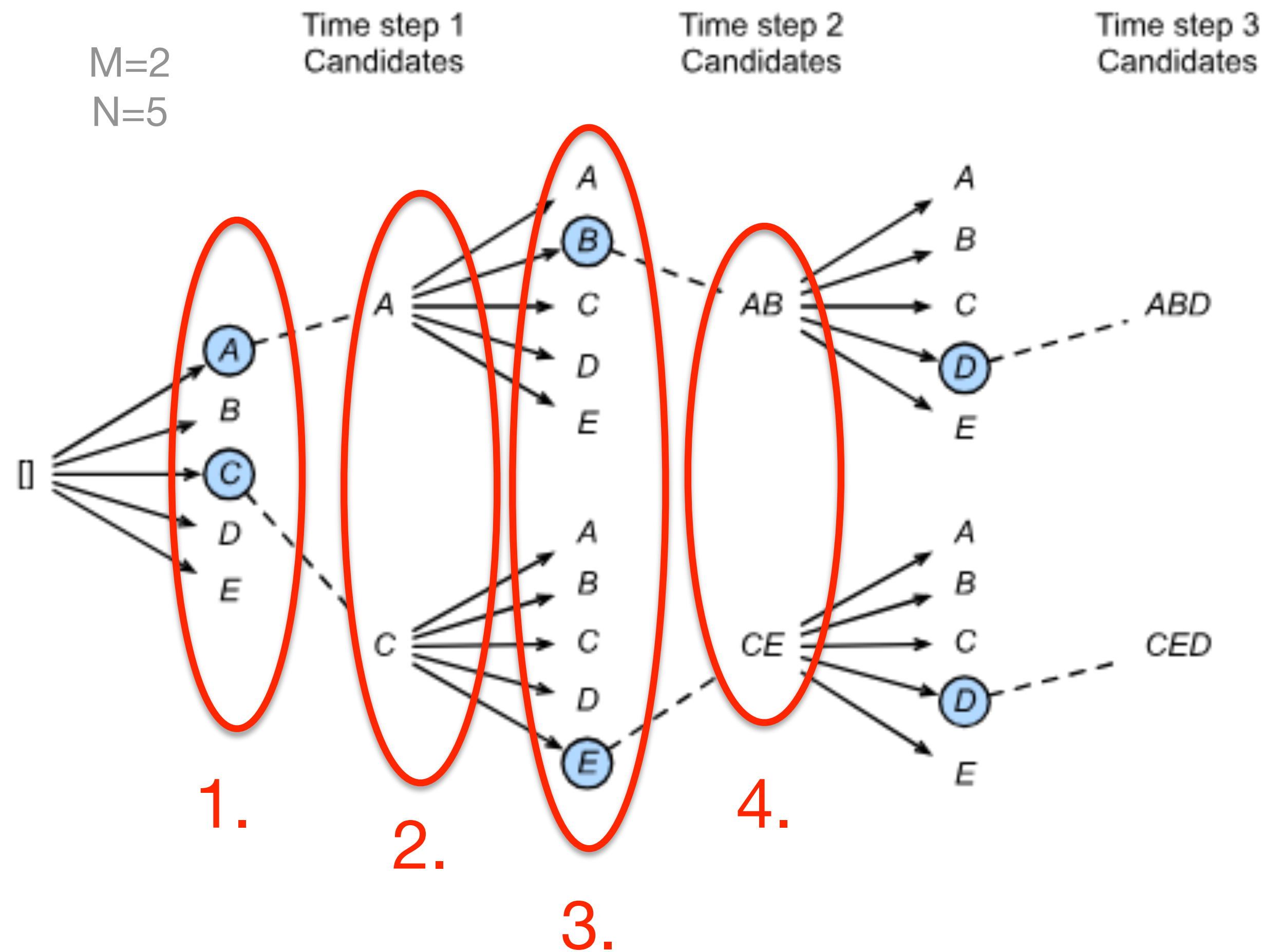
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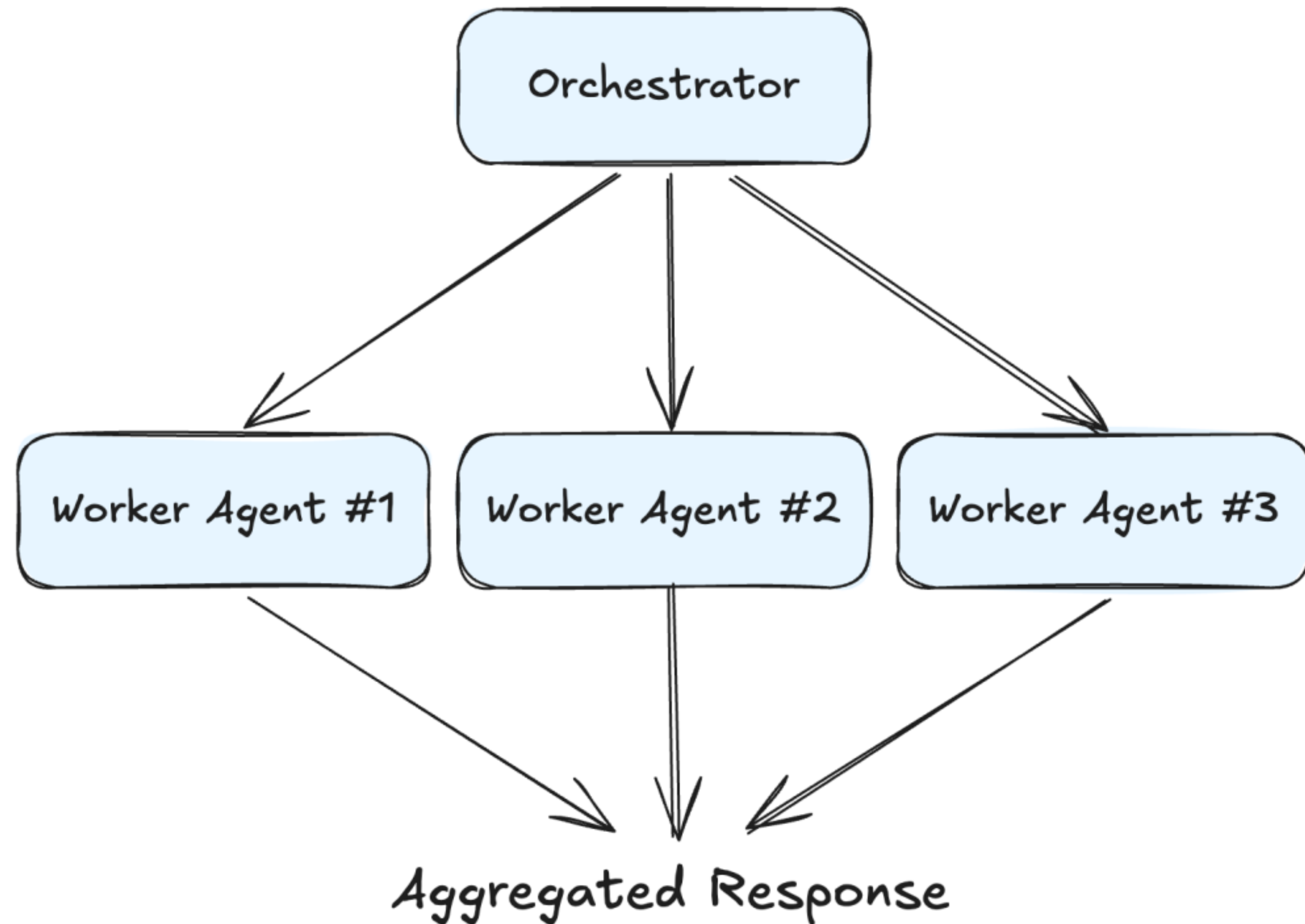
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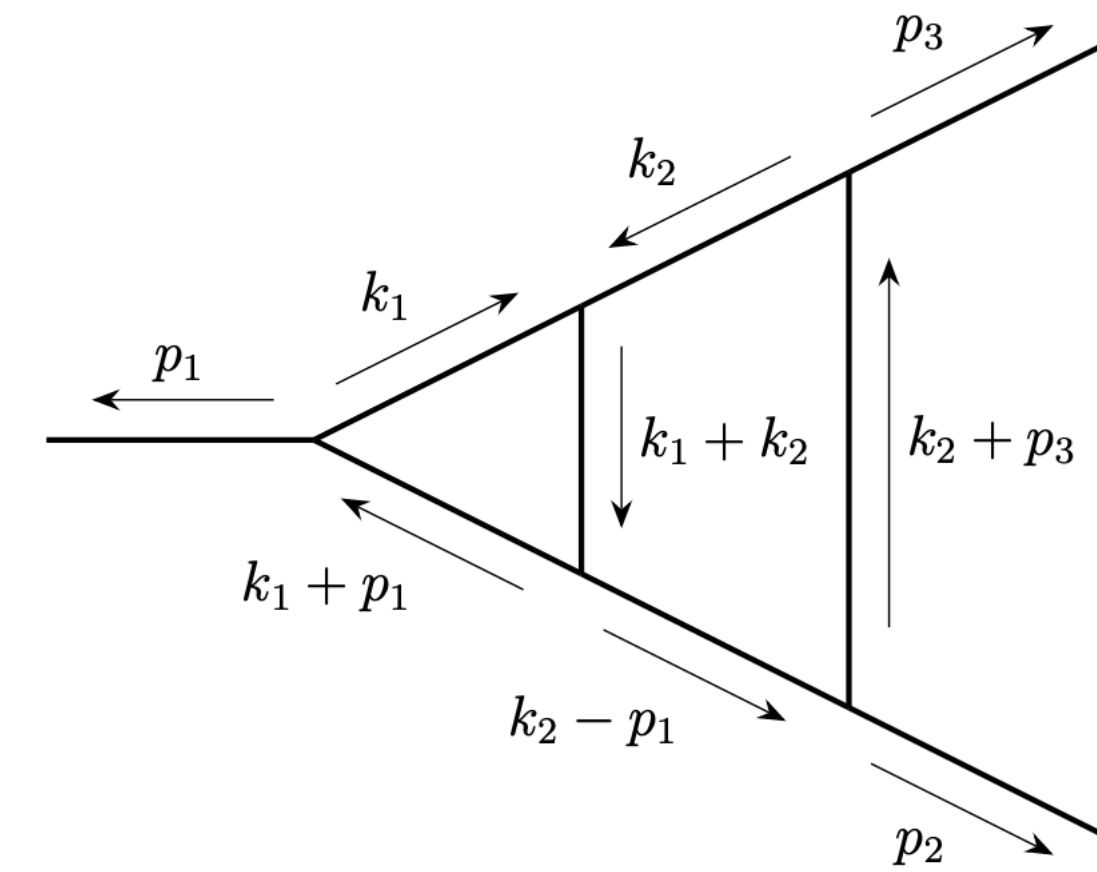
- Beam 1: criterion = min(highest weight integral in the expression)
- Beam 2: criterion = min(total summed weight of the expression)

Inference engineering: asynchronous, hierarchical, single-step reduction

- An *orchestrator* spawns asynchronous *workers*
- Each worker reduces a single high weight integral by one step, modulo subsectors, in parallel
- Reduced integrals are cached, so future workers do not reinvent wheels
- Orchestrator continues until all integrals have been reduced to masters
- CPU memory used by each worker remains bounded!



Triangle-box topology



from von Hippel & Wilhelm (2025)

- 16 master integrals

$I[0, 0, 1, 1, 1, 0, 0],$	$I[0, 1, 1, 1, 0, 0, 0],$
$I[0, 1, 1, 1, 1, 0, 0],$	$I[-1, 1, 1, 1, 1, 0, 0],$
$I[1, 0, 0, 1, 1, 1, 0],$	$I[1, 0, 1, 0, 0, 1, 0],$
$I[1, 0, 1, 0, 1, 0, 0],$	$I[1, 0, 1, 0, 1, 1, 0],$
$I[1, -1, 1, 0, 1, 1, 0],$	$I[1, 0, 1, 1, 1, 0, 0],$
$I[1, -1, 1, 1, 1, 0, 0],$	$I[1, 0, 1, 1, 1, 1, 0],$
$I[1, 1, 0, 1, 0, 1, 0],$	$I[1, 1, 0, 1, 1, 0, 0],$
$I[1, 1, 0, 1, 1, 1, 0],$	$I[1, 1, 1, 1, 1, 0, 0].$

$$I[a_0, a_1, a_2, a_3, a_4, a_5, a_6] = \int \frac{d^d k_1 d^d k_2}{D_1^{a_0} D_2^{a_1} \dots D_7^{a_6}}$$

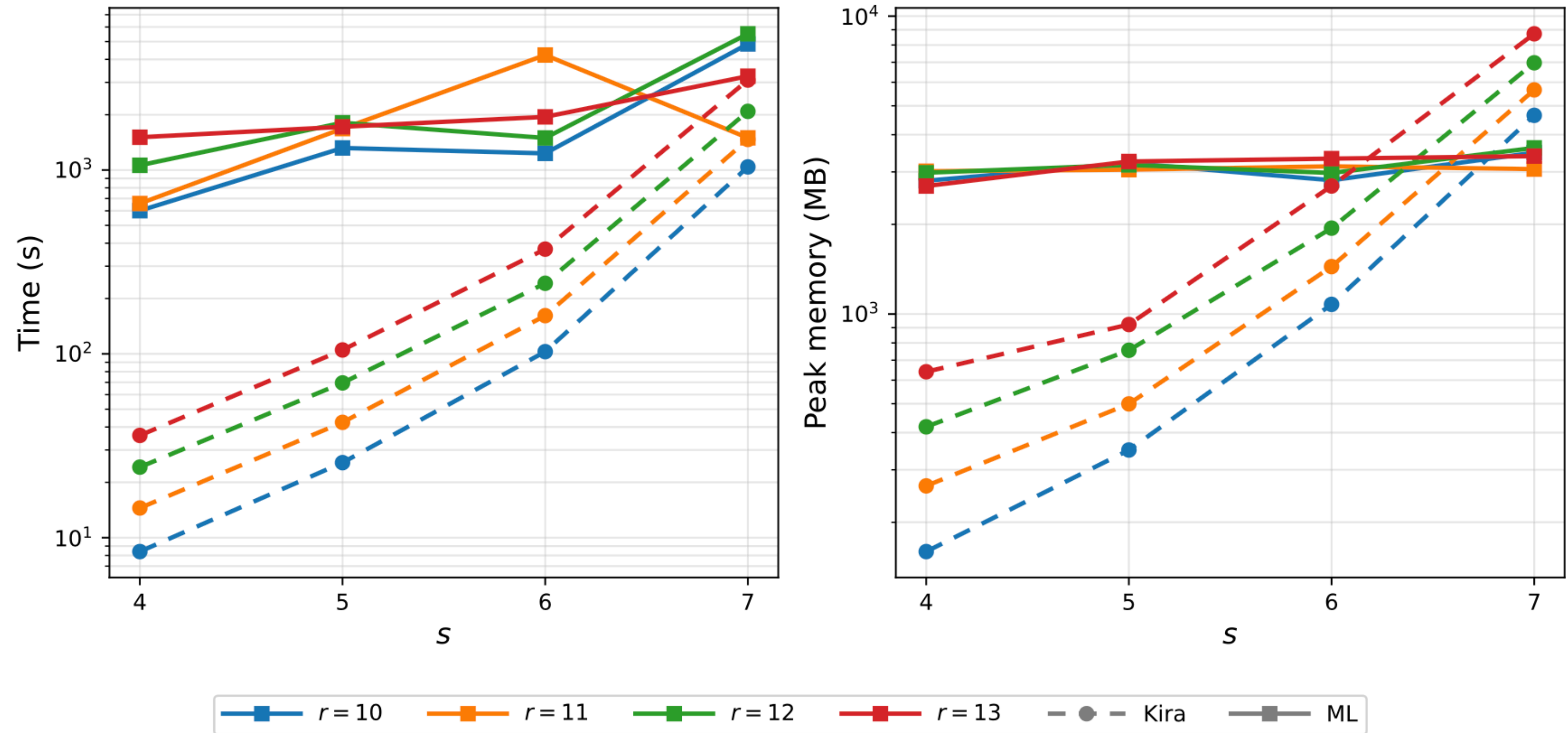
$D_1 = k_1^2,$	$D_2 = k_2^2,$
$D_3 = (k_1 + k_2)^2,$	$D_4 = (k_1 + p_1)^2$
$D_5 = (k_2 + p_3)^2,$	$D_6 = (k_2 - p_1)^2$
$D_7 = (k_1 + p_3)^2$ (ISP),	

- **Training data:** 1M training samples from randomly applying IBP identities to corner integrals

- 3 massive external momenta, 2 massless loop momenta

IBP reduction: results

r	s	Integral	r	s	Integral
10	4	$I[2, 1, 2, 1, 2, 2, -4]$	10	6	$I[1, 1, 3, 2, 2, 1, -6]$
11	4	$I[2, 2, 2, 1, 1, 3, -4]$	11	6	$I[1, 4, 2, 1, 2, 1, -6]$
12	4	$I[2, 3, 1, 3, 1, 2, -4]$	12	6	$I[3, 2, 3, 2, 1, 1, -6]$
13	4	$I[2, 3, 3, 3, 1, 1, -4]$	13	6	$I[3, 2, 1, 3, 2, 2, -6]$
10	5	$I[1, 1, 2, 2, 1, 3, -5]$	10	7	$I[2, 3, 1, 1, 2, 1, -7]$
11	5	$I[1, 1, 2, 3, 2, 2, -5]$	11	7	$I[2, 1, 1, 2, 3, 2, -7]$
12	5	$I[1, 2, 2, 2, 1, 4, -5]$	12	7	$I[3, 1, 1, 1, 1, 5, -7]$
13	5	$I[2, 2, 3, 3, 2, 1, -5]$	13	7	$I[2, 2, 3, 3, 1, 2, -7]$



- Tested on 16 triangle-box integrals with increasing weight

- SAILIR is memory stable while **Kira** memory grows rapidly with weight!

Lessons learned

- These projects were both intensely exhilarating and extremely frustrating.
- In both, Claude Code played the role of a graduate student that I interacted with entirely through text chat. Under my supervision, it wrote and ran all of the code, did all of the analysis, made all of the plots, and iterated with me on drafts of the paper.
- It was insanely fast but made tons of mistakes and kept forgetting things. Without constant close supervision and thorough validation and detailed cross checking, these projects would not have succeeded.
- Despite their flaws, I believe these agentic AI assistants will significantly lower the barrier to exploring and implementing new ideas. **Huge implications for our field!**
 - What big new questions can we now tackle that we couldn't before?
 - How do we ensure quality control? How do we handle the coming flood of papers?
 - How do we protect the future of our graduate students and postdocs? Urgently need to train them to use this amazing but flawed tool!

Summary

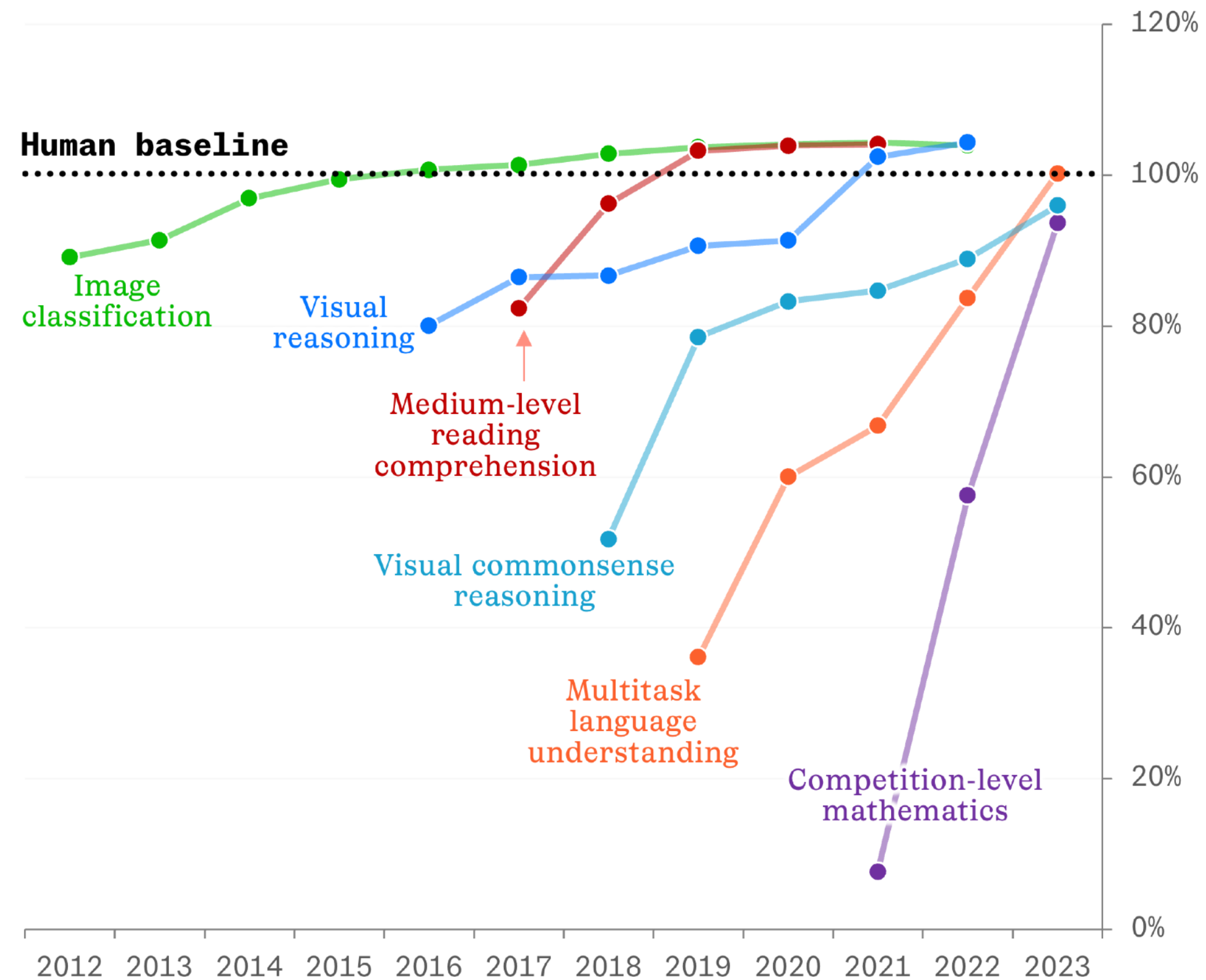
- Agentic AI is going to be a game changer for our field (and well well beyond)
- In this talk I presented two uses of agentic AI for research
 - As a hands-on research assistant -> two papers on “Learning to Unscramble”, applications to scattering amplitudes and Feynman loop integral reduction
 - As a fully automated system for reproducing LHC analyses (an important and common task in pheno research)

Where are we headed?

MAN VS. MACHINE

AI Models Are Improving Every Year

AI Technical Performance [Selected measures, 100% = human baseline]



CHARTR

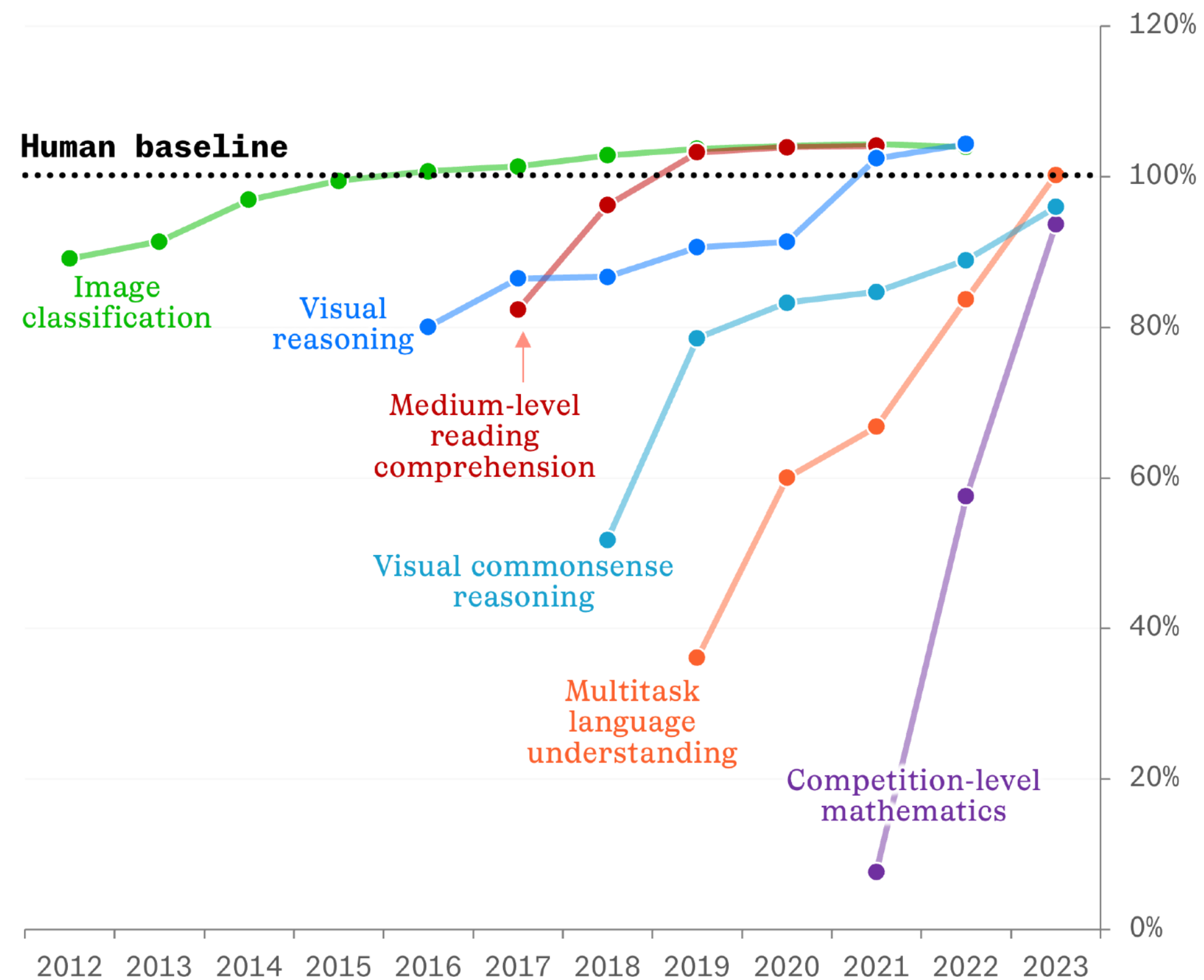
Source: Stanford University AI Index Report 2024

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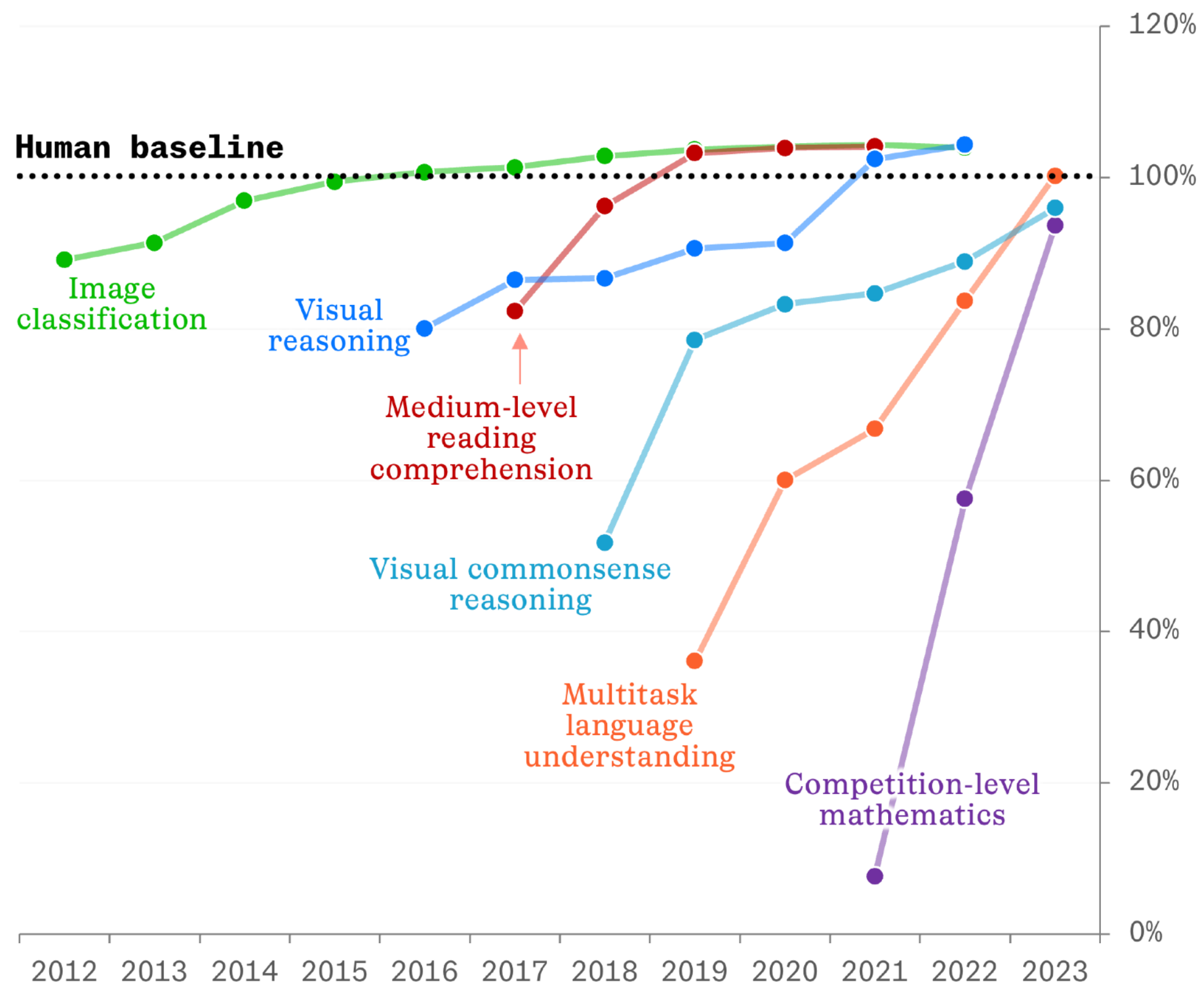
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Where are we headed?

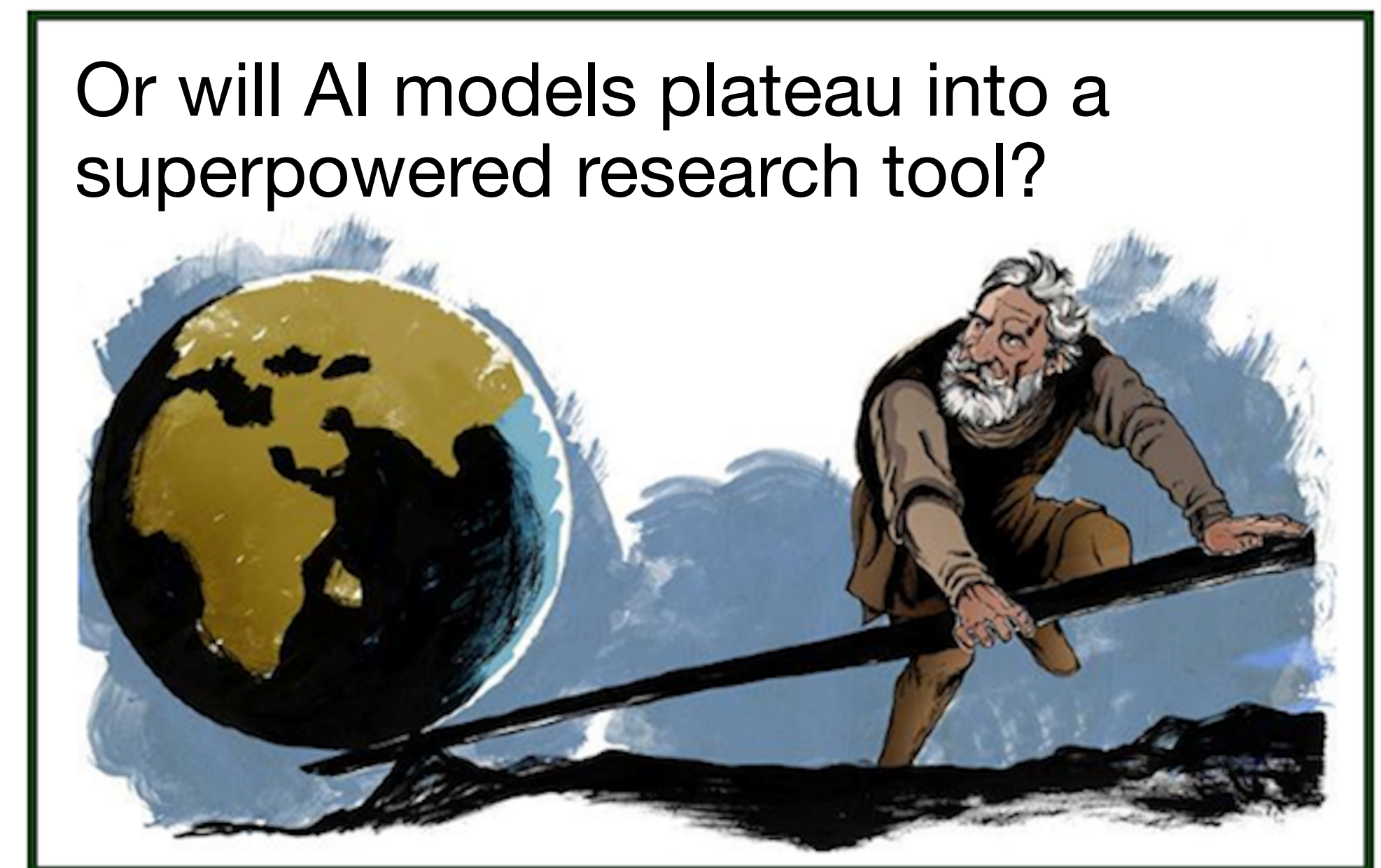
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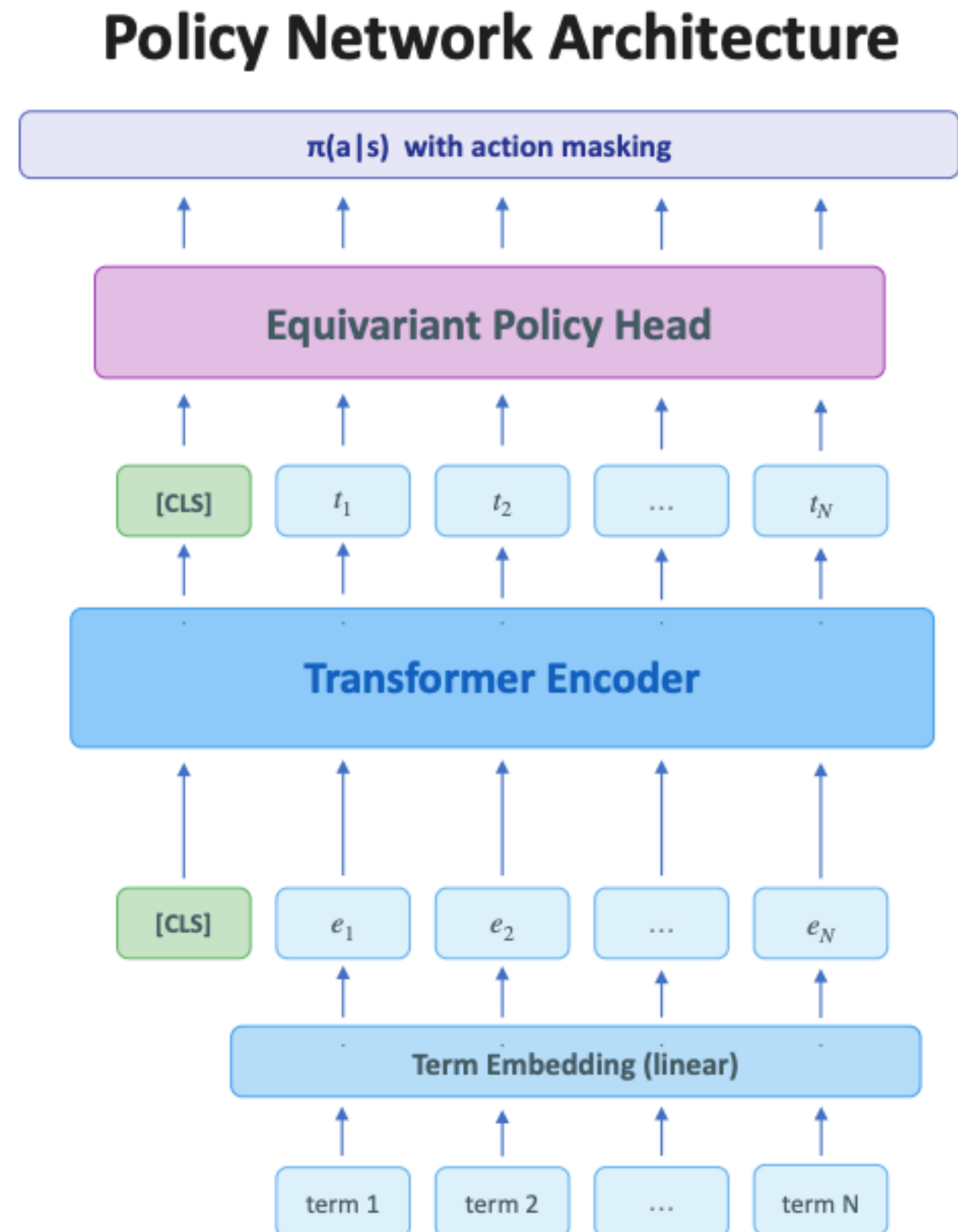
Source: Stanford University AI Index Report 2024



Thanks!

Scattering amplitudes: setup

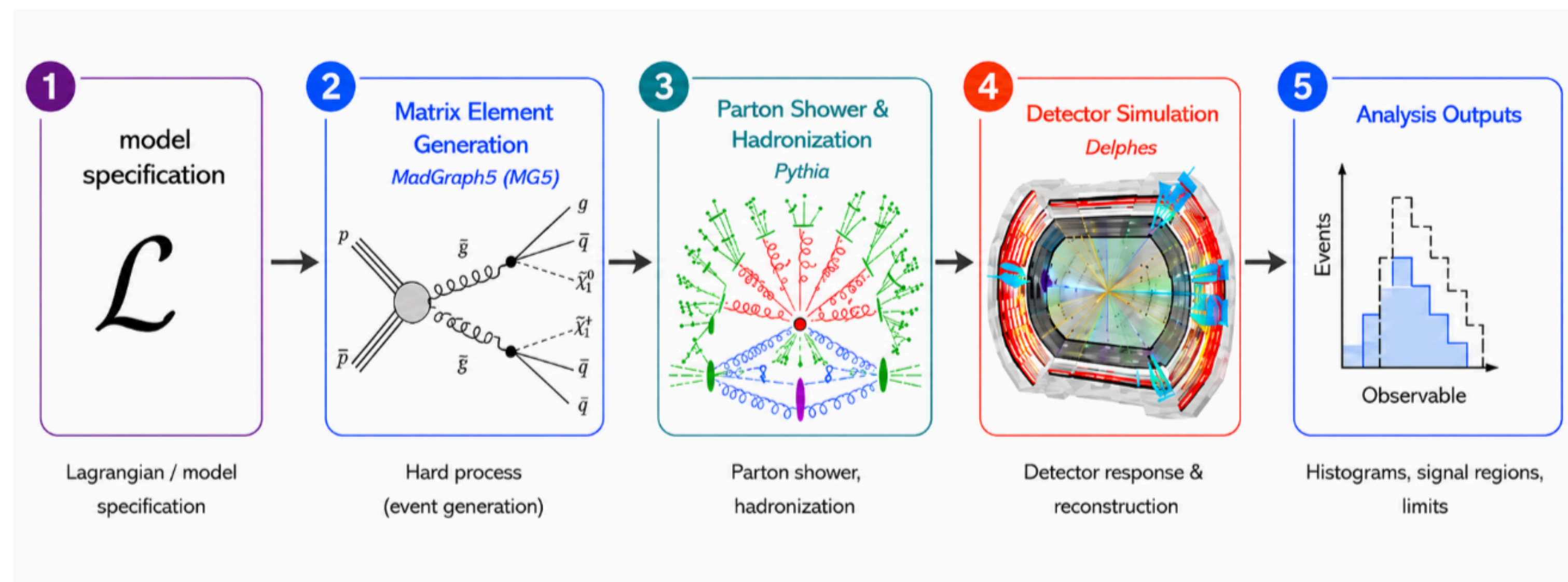
- **Permutation-equivariant action classifier:** interchanging order of terms should change action classifier output correspondingly
- **Action space** [$\sim 1.4k$ for 4 pts, $\sim 4k$ for 5 pts and $\sim 30k$ for 6 pts]
 - choice of:
 - term (up to 10 for 4-5pts, 30 for 6 pts)
 - bracket type
 - momentum
- **Term encoding** — for each factor (up to 8):
 - coefficient
 - bracket type
 - momenta
 - power



Bonus material: ColliderBench

[Faroughy, Palacios Schweitzer, Pang, Mishra Sharma, DS 2605.13950]

- A new benchmark for evaluating LLM agents on automated, long-horizon, real-world scientific tasks
- Setting: reproducing published LHC analyses (new physics searches) using public simulation tools — “recasting”



Challenges

- Unique challenges:
 - experimental papers from CMS and ATLAS often missing crucial details, inaccuracies, errors.
 - Gap between public simulation tools and proprietary CMS/ATLAS tools, correction factors, etc
 - Agent cannot get a perfect reproduction. Needs combination of physical intuition, domain knowledge, guesswork

ColliderBench: inputs

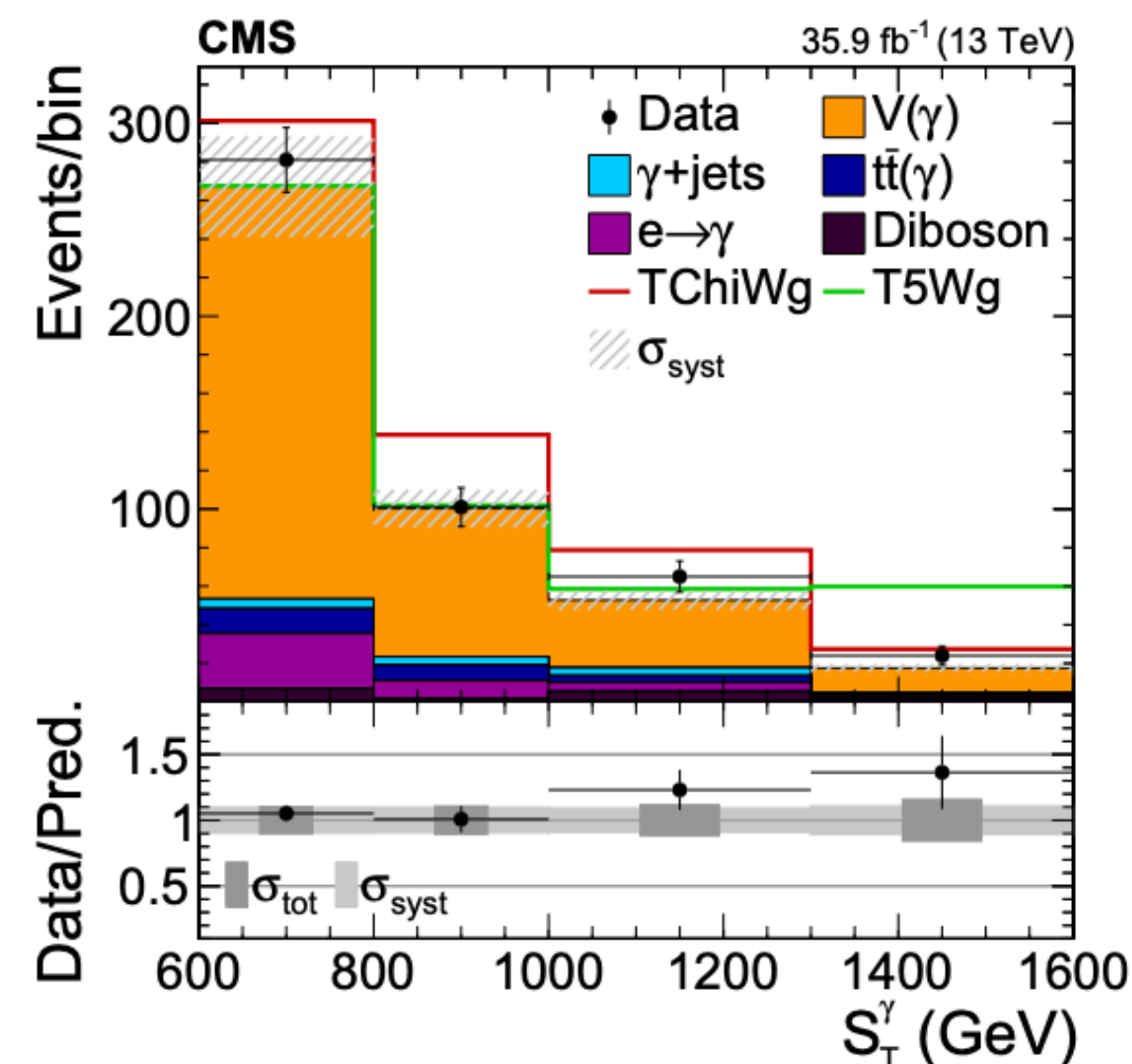
Search for gauge-mediated supersymmetry in events with at least one photon and missing transverse momentum in pp collisions at $\sqrt{s} = 13$ TeV

- Paper (PDF) from CMS/ATLAS

The CMS Collaboration*

Table 1: Summary of the event selection criteria required for the control, validation, and signal regions.

Region	Selection
Preselection	p_T^{miss} filters
	At least one reconstructed vertex
	At least one photon with $p_T > 180$ GeV
	$\Delta R(\gamma, \text{jet}) > 0.5$ $\Delta\phi(\vec{p}_T^{\text{miss}}, \text{jet}) > 0.3$ rad, if $p_T(\text{jet}) > 100$ GeV
Control region	Preselection
	$p_T^{\text{miss}} > 100$ GeV
	$M_T(\gamma, \vec{p}_T^{\text{miss}}) > 100$ GeV
	$p_T^{\text{miss}} < 300$ GeV or $M_T(\gamma, \vec{p}_T^{\text{miss}}) < 300$ GeV
Validation region	Preselection
	$p_T^{\text{miss}} > 300$ GeV
	$M_T(\gamma, \vec{p}_T^{\text{miss}}) > 300$ GeV
	$S_T^\gamma < 600$ GeV
Signal region	Preselection
	$p_T^{\text{miss}} > 300$ GeV
	$M_T(\gamma, \vec{p}_T^{\text{miss}}) > 300$ GeV
	$S_T^\gamma > 600$ GeV



Abstract

A search for gauge-mediated supersymmetry (SUSY) in final states with photons and large missing transverse momentum is presented. The data sample of pp collisions at $\sqrt{s} = 13$ TeV was collected with the CMS detector at the CERN LHC and corresponds to an integrated luminosity of 35.9 fb^{-1} . Data are compared with models in which the lightest neutralino has bino- or wino-like components, resulting in decays to photons and gravitinos, where the gravitinos escape detection. The event selection is optimized for both electroweak (EWK) and strong production SUSY scenarios. The observed data are consistent with standard model predictions, and limits are set in the context of a general gauge mediation model in which gaugino masses up to 980 GeV are excluded at 95% confidence level. Gaugino masses below 780 and 950 GeV are excluded in two simplified models with EWK production of mass-degenerate charginos and neutralinos. Stringent limits are set on simplified models based on gluino and squark pair production, excluding gluino (squark) masses up to 2100 (1750) GeV depending on the assumptions made for the decay modes and intermediate particle masses. This analysis sets the highest mass limits to date in the studied EWK models, and in the considered strong production models when the mass difference between the gauginos and the squarks or gluinos is small.

ColliderBench: inputs

- Task specification prompt
 - new physics signal to simulate
 - histogram from paper to reproduce
 - other output requirements

TASK.md

Paper: [CMS-SUS-16-046](#)

Centre-of-mass energy: 13 TeV

Luminosity: 35.9 fb^{-1}

Task type: simulation (shape-only)

Signal benchmark: TChiWg_700

Observable: S_T^γ

Task

Implement the search analysis described in **CMS-SUS-16-046** and use it to predict the normalized event distribution (shape) of S_T^γ for the signal benchmark point TChiWg_700, in the analysis's signal region.

The agent should:

1. Generate TChiWg_700 events using a matrix-element generator, parton shower, and detector simulation chain of its choice.
2. Read the paper to determine the object identification, event-selection requirements, and signal-region cuts that define the analysis, then apply them to the generated events.
3. Histogram the surviving events in S_T^γ using the bin edges already present in the `results/*.yaml` template. The bin edges must not be modified.

Definitions

- S_T^γ is the scalar sum of p_T^{miss} and the transverse momenta of all photons in the event.
- TChiWg_700 denotes electroweak associated production of mass-degenerate winos at $m(\tilde{W}) = 700 \text{ GeV}$, decaying to a massless gravitino LSP and Standard Model gauge bosons, with at least one photon in the final state through the TChiWg simplified-model topology.

Output requirements

Artifact	Purpose
<code>results/*.yaml</code>	Fill null bin values with predicted relative signal bin contents.
<code>analysis/*.py</code>	Event-selection code, runnable on the generated sample.
<code>data/*.root, sims/*.dat</code>	Selected-event files and generator/detector cards.
<code>report.md</code>	Methodological choices and deviations from the paper.

Important

The goal is to predict the signal shape from the agent's own simulation and analysis pipeline. The agent must not extract or digitize the target bin values from the paper's figures, tables, or HEPData record.

ColliderBench: inputs

- HEP toolbox
 - md files that teach agents how to use HEP software tools

```
1  √ # `feynrules` – browse and download UFO models from the FeynRules database
2
3  **Purpose.** If the bundled MadGraph UFO models (`sm`, `MSSM_SLHA2`,
4  `SMEFTsim`) don't cover your paper's BSM scenario, fetch an additional
5  model from the FeynRules wiki.
6
7  **When to use.** Only when `bin/simulate info` doesn't already list a
8  suitable UFO. For standard SUSY / SMEFT / top-EFT the bundled models are
9  usually enough.
10
11 √ ## Invocation
12
13 ```bash
14 bin/feynrules categories                # 7 top-level categories
15 bin/feynrules list --category SusyModels # browse one category
16 bin/feynrules list --search "vector-like quark" # substring search over slug/title/description
17 bin/feynrules info <model-slug>        # show all attachments for a model
18 bin/feynrules fetch <model-slug> [--file <name>] [--all] [--dest <dir>] [--extract]
19 bin/feynrules refresh-catalog          # re-scrape the wiki (catalog is cached)
20 ```
21
```

```
1  √ # Simulation stack – MadGraph5 / Pythia8 / Delphes
2
3  **Purpose.** Generate signal events end-to-end (parton-level → parton
4  shower → detector simulation) when no matching MC is available in CMS
5  Open Data. The CLIs are simple enough that there's no wrapper; you call
6  them directly. `bin/simulate info` lists installed models and cards;
7  `bin/simulate --doc` shows this page.
8
9  **When to use.** For BSM signals the paper defines but nobody has
10 produced for Open Data (SUSY benchmark points, EFT signals, etc.). For
11 SM backgrounds you usually want `cms-opendata` instead – save compute.
12
13 ---
14
15 √ ## Quick discovery
16
17 ```bash
18 bin/simulate info          # installed UFO models + Delphes cards + tool paths
19 bin/simulate --doc        # this page
20 ```
21
22 The relevant env vars (set inside the bench image; fall back to the
23 in-repo paths otherwise):
24
```

ColliderBench: metrics

$$d(\hat{y}, y^*) = \sqrt{\frac{\sum_{k=1}^K (\hat{y}_k - y_k^*)^2}{\sum_{k=1}^K y_k^{*2}}}.$$

L2 histogram distance

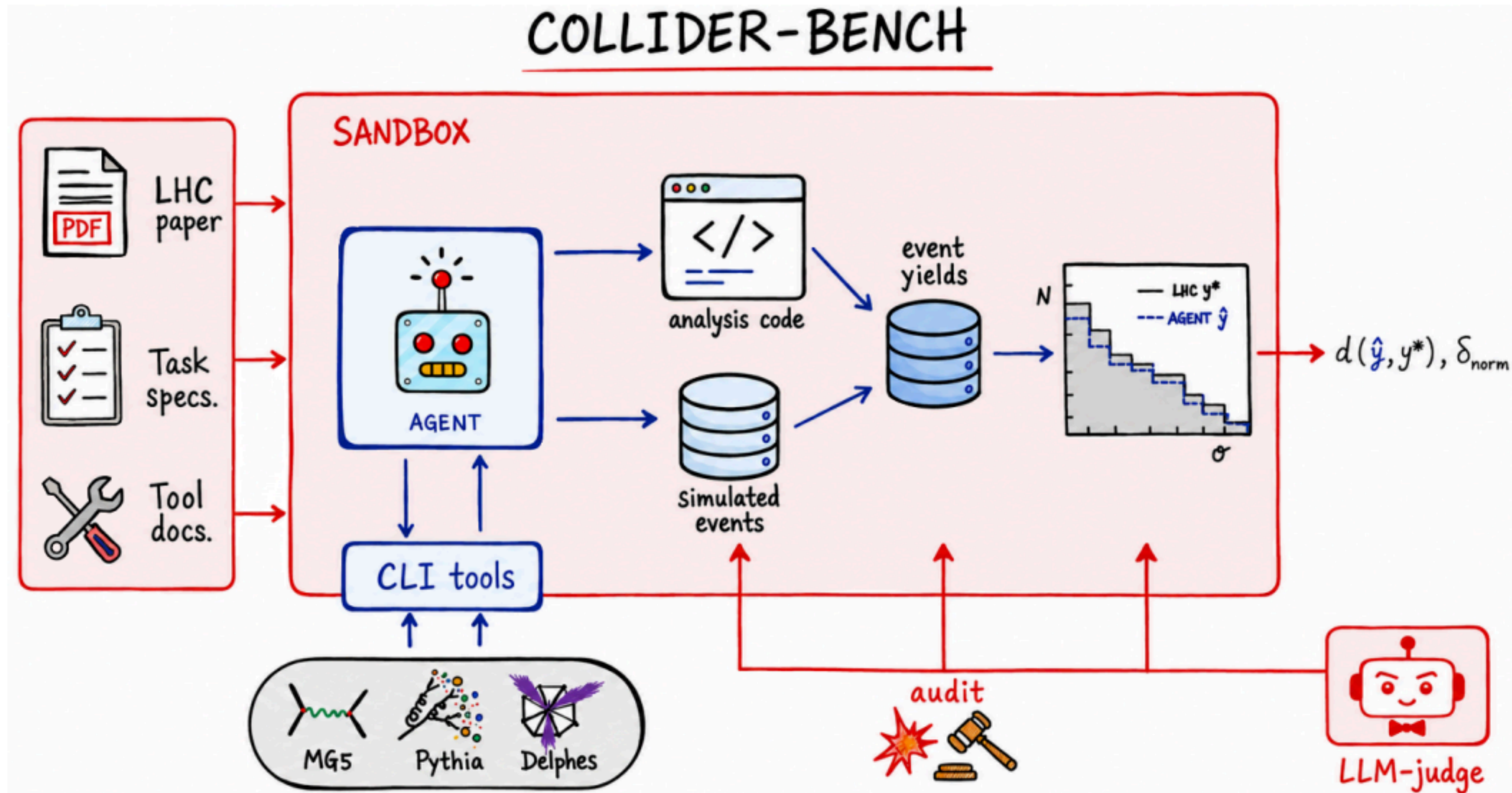
$$\delta_{\text{norm}} = \frac{|\hat{Y} - Y^*|}{Y^*}.$$

normalization error

$$\text{Acc}_\tau = \mathbb{I}[d_{\text{task}} < \tau],$$

pass/fail metric

ColliderBench: overview



LLM judge to catch cheating, hallucinations

ColliderBench V1

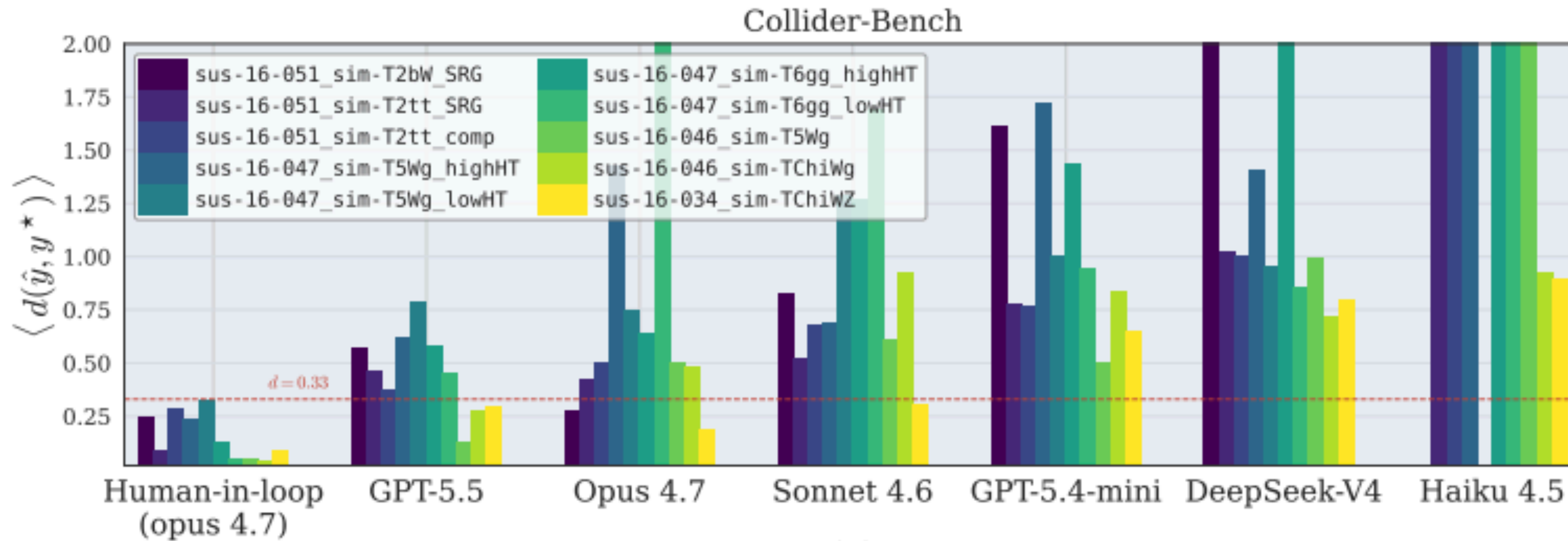
- 10 tasks over 4 CMS supersymmetry searches from ~2016 (13 TeV, 36/fb)

Table 1: Source analyses and simulation tasks in COLLIDER-BENCH. Each task fixes a paper, signal benchmark, target observable or signal region, and output template. Difficulty is graded from the relative- L^2 residual of our physicist-in-the-loop reproduction of each task: ★ (easy), ★★ (medium), ★★★ (hard).

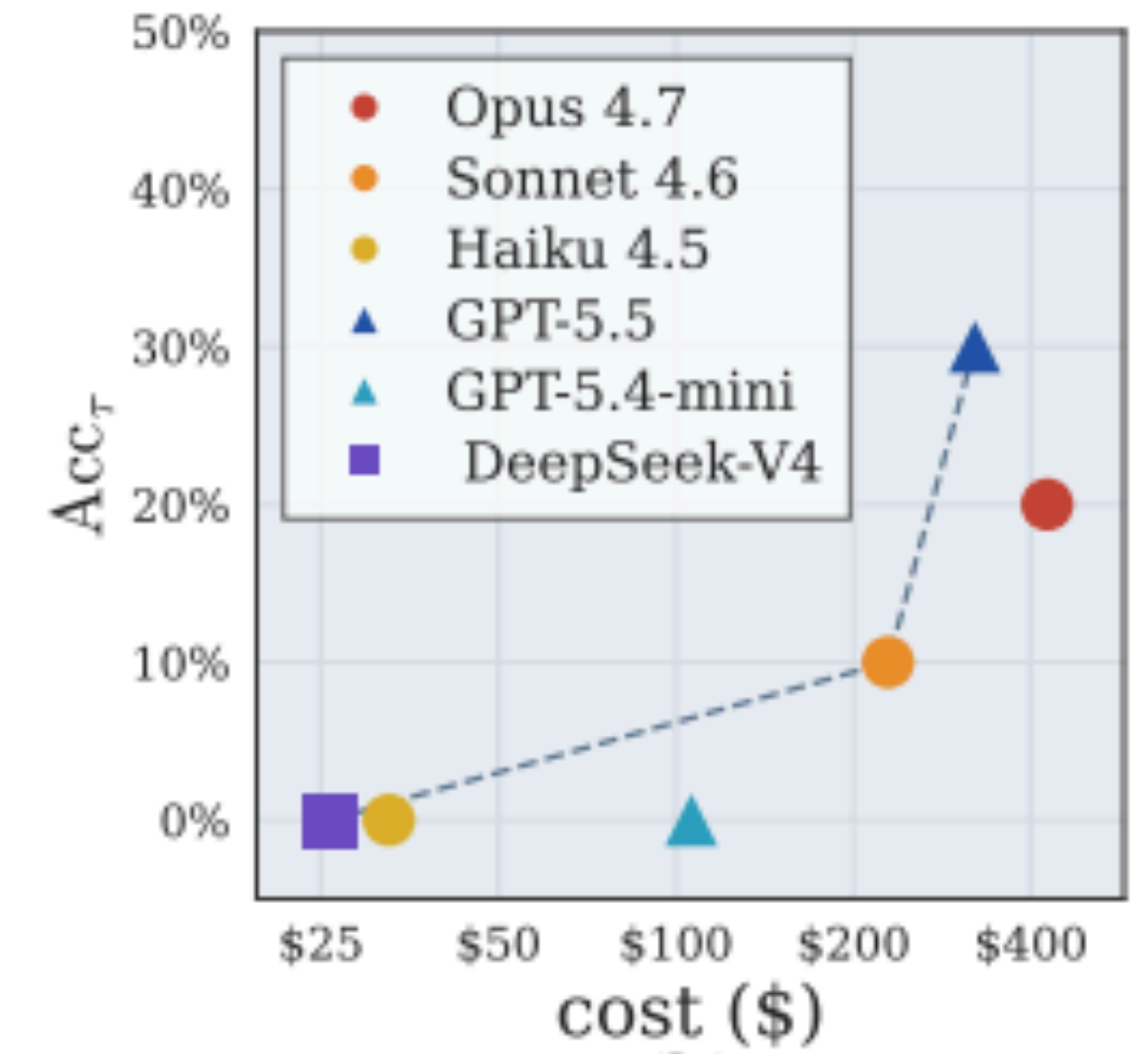
Task	Analysis target	Signal s	obs. \mathcal{O}	LHC search	Reference	Diff.
sus-16-034_sim-TChiWZ	leptons + jets	TChiWZ	E_T^{miss}	CMS-SUS-16-034	Sirunyan et al. [2018b]	★
sus-16-046_sim-T5Wg	photons	T5Wg	S_T^γ	CMS-SUS-16-046	Sirunyan et al. [2018a]	★
sus-16-046_sim-TChiWg	photons	TChiWg	S_T^γ	CMS-SUS-16-046	Sirunyan et al. [2018a]	★
sus-16-047_sim-T5Wg_highHT	photons	T5Wg, high- H_T	p_T^{miss}	CMS-SUS-16-047	Sirunyan et al. [2017b]	★★
sus-16-047_sim-T5Wg_lowHT	photons	T5Wg, low- H_T	p_T^{miss}	CMS-SUS-16-047	Sirunyan et al. [2017b]	★★★
sus-16-047_sim-T6gg_highHT	photons	T6gg, high- H_T	p_T^{miss}	CMS-SUS-16-047	Sirunyan et al. [2017b]	★★
sus-16-047_sim-T6gg_lowHT	photons	T6gg, low- H_T	p_T^{miss}	CMS-SUS-16-047	Sirunyan et al. [2017b]	★
sus-16-051_sim-T2tt	single lepton	T2tt	E_T^{miss}	CMS-SUS-16-051	Sirunyan et al. [2017a]	★
sus-16-051_sim-T2tt_comp	single lepton	T2tt, compressed	E_T^{miss}	CMS-SUS-16-051	Sirunyan et al. [2017a]	★★★
sus-16-051_sim-T2bW	single lepton	T2bW	E_T^{miss}	CMS-SUS-16-051	Sirunyan et al. [2017a]	★★

- Hundreds of more tasks and searches available, will be added for V2!

ColliderBench: results

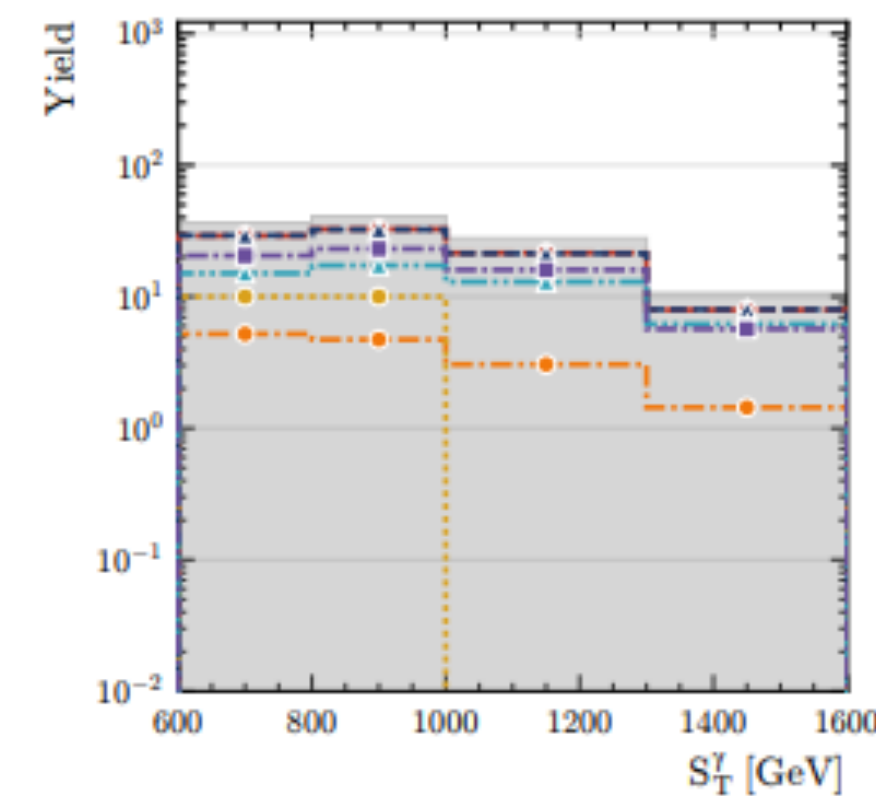


(a)

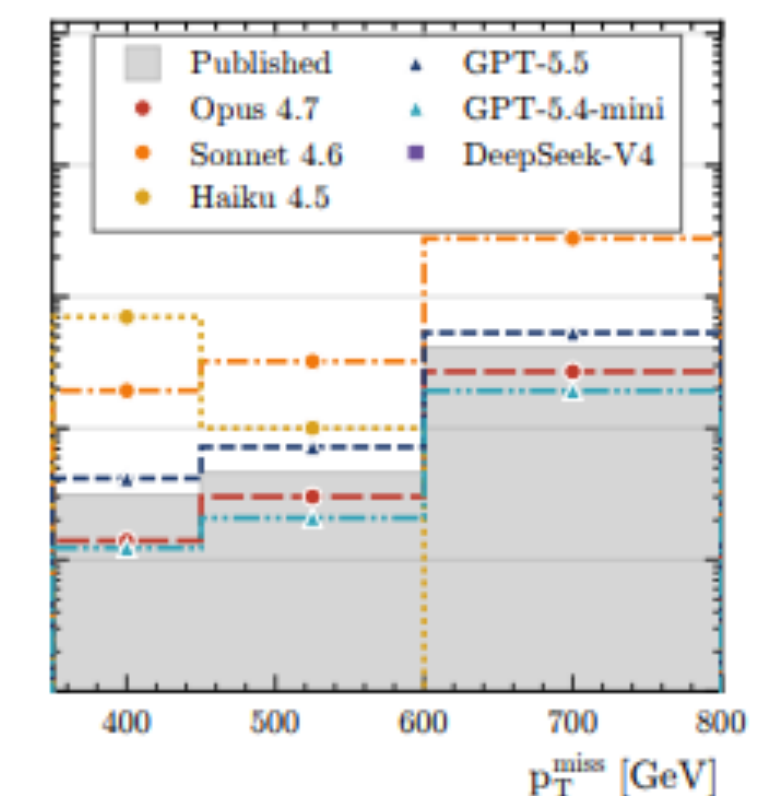


(b)

- Clear capability ladder
(Opus>Sonnet>Haiku; GPT5.5>GPT-5.4-mini)
- Clear Pareto front in pass/fail vs cost
- No LLM agent beats human-in-the-loop



(a)



(b)