Learning to Reason and Align via Self-Play

In pursuit of Superhuman Intelligence

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Research Goal: In Pursuit of Superhuman Intelligence





Agenda for Today's Talk



Intro: Learning as an Infinite Game

"a paradigm shift for training large models"





The Vision: "Universality of Computation"

6. The universal computing machine.

It is possible to invent a single machine which can be used to compute any computable sequence. If this machine \mathfrak{N} is supplied with a tape on the beginning of which is written the S.D of some computing machine \mathcal{M} , then \mathfrak{N} will compute the same sequence as \mathcal{M} .

– Alan M. Turing, 1936

"what a *human* can think or know"

"what a machine can compute"

The Challenge: Gaps in Achieving Human-Level Performance





2% accuracy on challenging contemporary mathematics problems on <u>FrontierMath</u>.

• >3.5x performance drop as coding problems get harder on <u>LiveCodeBench</u>.

What may go wrong in conventional ways of training AI models?

The Challenge: Scaling Law is Hitting the Wall? ≼

"Ilya Sutskever, co-founder of AI labs Safe Superintelligence (SSI) and OpenAI, told Reuters recently that results from scaling up pre-training - **the phase of training an AI model** that use s a vast amount of unlabeled data to understand language patterns and structures - **have plateaued**."

"The 2010s were the age of scaling, now we're back in the age of wonder and discovery once again. Everyone is looking for **the next thing**," Sutskever said. "**Scaling the right thing matters more now than ever.**"

- Ilya Sutskever with Reuters, Nov 2024

What are the next right things to scale?

Conventional Way of Agent Training



- Intelligence: Agents that are able to *learn* to *make decisions* to *achieve goals*.
- ▲ **Reasoning:** The process of *making decisions* by evaluating information.
- **Alignment:** The process of *<u>achieving goals</u>* by reward maximization.

Myth 1: Learning is Purely Solving (under a given world)

a given world



Conventional way: 🏷

Design agents that **find solutions** in a fixed environment, then **stop learning**.

the open-ended worlds



Better way:

Design agents that create new tasks/environments, then continuously learn to self-improve.

Myth 2: Reasoning is Step-by-Step (by a single policy)



Better way:

Learn policies with a hierarchy of abstract models, and roll out at different levels for optimization.

Conventional way: 🏷

Learn a policy that operates under a **one-step model**, and roll it out (with tree search) in training.

Fig 1. A world can be divided at different levels in certain hierarchy (<u>Dayan and Hinton, 1992</u>).

A New, Scalable Training Paradigm

"There are at least 2 kinds of games. One could be called finite; the other infinite."

- A finite game is played for the purpose of winning.
- An **infinite game** is for the purpose of continuing the play.

– James P. Carse, 2011

hierarchical policies





A New, Scalable Training Paradigm

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Recap on Agenda



Solving Myth 1: Going Beyond Static World *Solving Myth 2:* Hierarchical Planning

Self-Play to Align: The Creator-Solver Game

"Scalable language model training beyond human prompts."

Gratitude to every wonderful co-author of this project (<u>link</u>): Rishabh Agarwal, Tianqi Liu, Rishabh Joshi, Sarmishta Velury, Quoc V. Le, Qijun Tan, Yuan Liu. Google DeepMind

TL; DR

We identify **learnable**, worth-learning prompts by reward signals, then evolve new prompts for open-ended continual RLHF training.



Artificial Intelligence May Be Bottlenecked by Static Data



Fig 4. The scale, quality and growth of human knowledge is bottlenecked.



Fig 5. The **imbalance distribution** of static training data.

Can language models identify and self-create **new**, **learnable**, and **worth-learning** tasks, to self-improve to generalize better for alignment?

Classical RLHF

Alignment by RLHF. Classical RLHF (Ouyang et al., 2022) optimizes on a fixed distribution \mathcal{D} : $\max_{\pi_{\theta}} \mathbb{E}_{\mathbf{x} \sim \mathcal{D}, \mathbf{y} \sim \pi_{\theta}(\cdot | \mathbf{x})} \left[r(\mathbf{x}, \mathbf{y}) \right] - \mathbb{E}_{\mathbf{x} \sim \mathcal{D}} \left[\beta \cdot \mathbb{D}_{\mathrm{KL}} \left[\pi_{\theta}(\mathbf{y} | \mathbf{x}) \| \pi_{\mathrm{SFT}}(\mathbf{y} | \mathbf{x}) \right] \right], \quad (1)$

where x and y denote the prompts and responses, and $r(\cdot, \cdot)$ is the reward function.

Our Perspective: RLHF Should Be Made Open-Ended

Definition 1 (Open-Ended RLHF) We define evolving alignment as the open-ended joint optimization on the prompt and response policy for alignment w.r.t the joint reference policy: $\max_{\phi,\theta} \mathbb{E}_{\mathbf{x}\sim\pi_{\phi}(\cdot), \ \mathbf{y}\sim\pi_{\theta}(\cdot|\mathbf{x})} \left[r(\mathbf{x},\mathbf{y}) \right] - \beta \cdot \mathbb{D}_{KL} \left[\pi_{\phi,\theta}(\mathbf{x},\mathbf{y}) \parallel \pi_{ref}(\mathbf{x},\mathbf{y}) \right], \quad (7)$ where $\pi_{\phi,\theta}(\mathbf{x},\mathbf{y}) := \pi_{\phi}(\mathbf{x}) \cdot \pi_{\theta}(\mathbf{y} \mid \mathbf{x})$ and $\pi_{ref}(\mathbf{x},\mathbf{y}) := p_{ref}(\mathbf{x}) \cdot \pi_{SFT}(\mathbf{y} \mid \mathbf{x})^{a}$. $\max_{\phi,\theta} \mathbb{E}_{\mathbf{x}\sim\pi_{\phi}(\cdot)} \left[\mathbb{E}_{\mathbf{y}\sim\pi_{\theta}(\cdot|\mathbf{x})} \left[r(\mathbf{x},\mathbf{y}) \right] - \beta_{1} \mathbb{D}_{KL} \left[\pi_{\theta}(\mathbf{y}|\mathbf{x}) \parallel \pi_{SFT}(\mathbf{y}|\mathbf{x}) \right] \right] - \beta_{2} \mathbb{D}_{KL} \left[\pi_{\phi}(\mathbf{x}) \parallel p_{ref}(\mathbf{x}) \right]. \quad (8)$

However, directly optimizing this can be *intractable* or *unstable*... 🔗

Our Method: Open-Ended RLHF via Creator-Solver Games



What? The **Regret** of the Solver's Policy

$$\operatorname{Regret}(\pi_{\phi}, \pi_{\theta}) = \mathbb{E}_{\mathbf{x} \sim \pi_{\phi}(\cdot)} \Big[\mathbb{E}_{\mathbf{y} \sim \pi_{\theta}(\mathbf{y}|\mathbf{x})} \big[r(\mathbf{x}, \mathbf{y}) \big] - \mathbb{E}_{\mathbf{y} \sim \pi_{\mathsf{KL}}^{\star}(\mathbf{y}|\mathbf{x})} \big[r(\mathbf{x}, \mathbf{y}) \big] \Big]$$

Why? The Minimax Regret Strategy at the Nash Equilibrium $\pi_{\mathcal{Y}|\mathcal{X}}^{\star} \in \operatorname*{arg\,min}_{\pi_{\mathcal{Y}|\mathcal{X}}} \max_{\pi_{\mathcal{X}}} \mathbb{E}_{\mathbf{x} \sim \pi_{\mathcal{X}}} \left[\operatorname{Regret}(\mathbf{x}, \pi_{\mathcal{Y}|\mathcal{X}}) \right]$

However, w/o access to the true π^* , we must **approximate** this regret...



Our Method: Open-Ended RLHF via Creator-Solver Games

• How to approximate the **regret**? Simply use the **stochastic policy...**

Sample *N* times from the policy, then choosing the *reward gap* between *the best* and *the baseline*.

 $|\hat{\operatorname{Regret}}(\mathbf{x}, \pi_{\theta})| \leftarrow \operatorname{info}_{\theta}(\mathbf{x}) := r(\mathbf{x}, \mathbf{y}_{+}) - r(\mathbf{x}, \mathbf{y}_{\operatorname{baseline}}),$

$$\begin{split} \mathbf{y}_{+} &:= \arg \max_{\mathbf{y}_{i}} r(\mathbf{x}, \mathbf{y}), \\ \mathbf{y}_{\text{baseline}} &:= \arg \min_{\mathbf{y}_{i}} r(\mathbf{x}, \mathbf{y}) \text{ or } \mathbf{y}_{\text{baseline}} := \operatorname{avg}_{\mathbf{y}_{i}} r(\mathbf{x}, \mathbf{y}) \end{split}$$



Learning potential.

eva picks the prompts that are learnable but not learned yet.

Worst-case guarantee.

The minimax objective incentivizes the solver to perform well in all cases.

Auto-curricula for the solver player.

The optimal strategy of the creator is to create prompts just beyond solvers' current capability .

Auto-curricula inherent to contrastive learning.

eva prioritizes prompts with lower contrastive loss by design, thus accelerating learning.

See also: PAIRED: A New Multi-Agent Framework for Adversarial Environment Generation

The eva Algorithm

Algorithm 1 eva: Evolving Alignment via Asymmetric Self-Play

Input: initial policy π_{θ_0} , initial prompt set \mathcal{X}_0

1: for iteration t = 1, 2, ... do

∇ /* creator step */

- 2: sample subset: self-evolve prompts: $\mathcal{X}_t \leftarrow \texttt{evolve}(\mathcal{X}_{t-1}^{\texttt{info}})$
- estimate informativeness: $\mathcal{X}_{t-1} \leftarrow \{(\mathbf{x}_i, \mathtt{info}(\mathbf{x}_i)) \mid \mathbf{x}_i \in \mathcal{X}_{t-1}\}$ $\mathcal{X}_{t-1}^{ ext{info}} \leftarrow \texttt{sample}(\mathcal{X}_{t-1})$

\bigtriangledown /* solver step */

- 3: annotate rewards:
- self-generate responses: $\forall x_i \in \mathcal{X}_t$, generate $\{y_i^{(j)}\} \sim \pi_{\theta_{t-1}}(\cdot \mid x_i)$ $\mathcal{X}'_t \leftarrow \mathcal{X}_t \cup \{(\boldsymbol{u}^{(j)}_i, r^{(j)}_i)\}$ preference optimization: $\boldsymbol{\theta}_t \leftarrow \boldsymbol{\theta}_{t-1} - \eta \nabla_{\boldsymbol{\theta}} \mathcal{L}_{\mathcal{X}'}(\boldsymbol{\theta})$

4: end for 5: return final solver policy $\pi_{\theta_{T}}$

Fig 6. eva requires only a creator module addition to make current RLHF pipeline open-ended.

The Creator Step: Estimate, Sample then Evolve



Fig 7. eva currently uses the estimate, sample then evolve procedure for the creator. Here, $info(\cdot)$ is the reward gap, and $evol(\cdot)$ can be any prompt creation method.

Example Evolving Method: evol(·)

We use EvolInstruct (Can et al., 2023) for in-depth evolving and in-breadth-evolving.

Initial prompt \downarrow

If a man smokes <u>1000 cigarettes a day</u>, why is he getting healthier?

Evolved #1 \ (*in-depth* evolving)

Elaborate on the seemingly <u>paradoxical situation</u> where an individual consumes <u>1000 cigarettes daily</u> yet exhibits signs of improving health, <u>delineating the factors</u> that could underlie such an unexpected outcome.

Evolved #2 \ (*in-breadth* evolving)

Discuss the conundrum of a person drinking <u>a gallon of</u> <u>caffeinated coffee</u> every hour but displaying unusually deep and restful sleep patterns, exploring possible explanations for this unusual phenomenon.

UTATION_TEMPLATES = { #
" # >>>>>> In-depth evolving <<<<<< #
" "CONSTRAINTS": prompt.format("Add one more constraints into '#The Given Prompt#'"), "STRETERTING"
"DEEPENING": prompt.format("If #The Given Prompt# contains inquiries about certain issues, the depth and breadth of the inquiry can be increased."
), "CONCRETIZING": prompt.format("Please replace general concepts with more specific concepts."
<pre>>, "INCREASED_REASONING_STEPS": prompt.format("If #The Given Prompt# can be solved with just a few simple thinking processes, you can rewrite it to explicitly request multiple-step reasoning."</pre>
), # # >>>>>> In-breadth evolving <<<<<
"BREADTH": prompt.format("By inspiration from #The Given Prompt#, create a new prompt. This new prompt should belong the the same domain as it, but be even more rare. The length and complexity should be similar. The #Created Prompt# must be reasonable and must be understood and responded by humans."
)

Results: Remarkable Gains on Hard Benchmarks*!



Figure. **eva** achieves concrete performance gain especially on **hard benchmarks**, without relying on any additional human prompts.

Results: Remarkable Gains on Hard Benchmarks*!

$\overline{\textbf{Model Family}} (\rightarrow)$			Gемма	-2-9B-IT		
Benchmark (\rightarrow)	Arena-Hard		MT-Benc	h	AlpacaEv	al 2.0
Method (\downarrow) / Metric ($ ightarrow$)	WR (%)	avg. score	1 st turn	2 nd turn	LC-WR (%)	WR (%)
$\overline{oldsymbol{ heta}_0: \text{SFT}}$	41.3	8.57	8.81	8.32	47.11	38.39
$\overline{\boldsymbol{\theta}_{0 \to 1}}$: DPO	51.6	8.66	9.01	8.32	55.01	51.68
$oldsymbol{ heta}_{1 ightarrow ilde{1}}$: +eva	60.1 (+8.5)	8.90	9.04	8.75 (+0.43)	55.35	55.53
$ heta_{1 ightarrow 2}$: +new human prompts	59.8	8.64	8.88	8.39	55.74	56.15
$\overline{\boldsymbol{\theta}_{0 \to 1}}$: SPPO	55.7	8.62	9.03	8.21	51.58	42.17
$oldsymbol{ heta}_{1 ightarrow ilde{1}}$: +eva	58.9 (+3.2)	8.78	9.11	8.45 (+0.24)	51.86	43.04
$ heta_{1 ightarrow 2}$: +new human prompts	57.7	8.64	8.90	8.39	51.78	42.98
$\overline{\boldsymbol{\theta}_{0 \to 1}}$: SimPO	52.3	8.69	9.03	8.35	54.29	52.05
$oldsymbol{ heta}_{1 ightarrow ilde{1}}$: +eva	60.7 (+8.4)	8.92	9.08	8.77 (+0.42)	55.85	55.92
$ heta_{1 ightarrow 2}$: +new human prompts	54.6	8.76	9.00	8.52	54.40	55.72
$\overline{\boldsymbol{\theta}_{0 \to 1}}$: ORPO	54.8	8.67	9.04	8.30	52.17	49.50
$oldsymbol{ heta}_{1 ightarrow ilde{1}}$: +eva	60.3 (+5.5)	8.89	9.07	8.71 (+0.41)	54.39	50.88
$ heta_{1 ightarrow 2}$: +new human prompts	57.2	8.74	9.01	8.47	54.00	51.21

Table 1: Main results. Our eva achieves notable alignment gains and can surpass human prompts on major benchmarks across a variety of representative direct preference optimization algorithms.

^{*} All experiments are conducted with external open-source frameworks and models on HuggingFace. We use 10K prompts from <u>UltraFeedback</u> for training, and use <u>ArmoRM-8B</u> as the default reward model.

Additional Results – **eva** creates meaningful curriculum.



model

- --- gemma-2-9b-it
- gemma-2-9b-it-dpo
- 🕶 gemma-2-9b-it-dpo-eva-iter-1
- --- gemma-2-9b-it-dpo-eva-iter-2
- gemma-2-9b-it-dpo-eva-iter-3

Prompt Set (\downarrow) / Metric (\rightarrow)	Complexity (1-5)	Quality (1-5)
UltraFeedback (seed)	2.90	3.18
UltraFeedback-eva-Iter-1	3.84	3.59
UltraFeedback-eva-Iter-2	3.92	3.63
UltraFeedback-eva-Iter-3	3.98	3.73

Ablation #1 – eva's minimax design outperforms alternatives.

Metric	$info(\mathbf{x})$	Related Interpretations
A^{\star}_{\min} : worst-case optimal advantage	$ \min_{\mathbf{y}} r(\mathbf{x},\mathbf{y}) - \max_{\mathbf{y}'} r(\mathbf{x},\mathbf{y}') $	minimax regret (Savage, 1951)
A^{\star}_{avg} : average optimal advantage	$ rac{1}{N}\sum_{\mathbf{y}}r(\mathbf{x},\mathbf{y})-\max_{\mathbf{y}'}r(\mathbf{x},\mathbf{y}') $	Bayesian regret (Banos, 1968)
A^{\star}_{dts} : dueling optimal advantage	$ \max_{\mathbf{y} eq \mathbf{y}^{\star}} r(\mathbf{x}, \mathbf{y}) - \max_{\mathbf{y}'} r(\mathbf{x}, \mathbf{y}') $	dueling regret (Wu and Liu, 2016)

Table 2: The reward-advantage-based metrics that serve as the informativeness proxies for prompts.

Model	Family $(ightarrow)$	Gemma-2-9B-it					
Benchn	nark ($ ightarrow$)	Arena-Hard		MT-Benc	ch 🛛	AlpacaEva	al 2.0
Method	l (\downarrow) / Metric ($ ightarrow$)	WR (%)	avg. score	1 st turn	2 nd turn	LC-WR (%)	WR (%)
$oldsymbol{ heta}_{0 ightarrow 1}$: I	OPO	51.6	8.66	9.01	8.32	55.01	51.68
$oldsymbol{ heta}_{1 ightarrow ilde{1}}$:	+ eva (uniform)	57.5	8.71	9.02	8.40	53.43	53.98
$ \begin{array}{c} \boldsymbol{\theta}_{1 \to \tilde{1}} \\ \boldsymbol{\theta}_{1 \to \tilde{1}} \\ \boldsymbol{\theta}_{1 \to \tilde{1}} \\ \boldsymbol{\theta}_{1 \to \tilde{1}} \end{array} $	+ eva $(var(r))$ + eva $(avg(r))$ + eva $(1/avg(r))$	54.8 58.5 56.7	8.66 8.76 8.79	9.13 9.13 9.13	8.20 8.40 8.45	54.58 55.01 55.04	52.55 55.47 54.97
$\frac{1 \rightarrow 1}{\boldsymbol{\theta}_{1 \rightarrow \tilde{1}}}$:	+ eva $(1/A_{\min}^{\star})$	52.3	8.64	8.96	8.31	53.84	52.92
$\overline{oldsymbol{ heta}_{1 ightarrow ilde{1}}}_{oldsymbol{ heta}_{1 ightarrow ilde{1}}}$:	+ eva (A^{\star}_{avg}) (our variant) + eva (A^{\star}_{dts}) (our variant)	60.0 60.0	8.85 8.86	9.08 9.18	8.61 8.52	56.01 55.96	56.46 56.09
$\theta_{1 \rightarrow \tilde{1}}$:	+ eva (A^{\star}_{\min}) (our default)	60.1 (+8.5)	8.90	9.04	8.75 (+0.43)	55.35	55.53

Table 3: Choice of informativeness metric. Our informativeness metric by *advantage* achieves the best performances, comparing with others as the weight to sample prompts to evolve by the creator.

Ablation #2 – **eva**'s design of evolving is meaningful.

Benchn	nark ($ ightarrow$)	Arena-Hard	Μ	IT-Bench		AlpacaEva	al 2.0
Method	l (\downarrow) / Metric ($ ightarrow$)	WR (%)	avg. score	1 st turn	2 nd turn	LC-WR (%)	WR (%)
$\overline{oldsymbol{ heta}_{0 ightarrow 1}}$: I	DPO	51.6	8.66	9.01	8.32	55.01	51.68
$egin{aligned} & m{ heta}_{1 ightarrow ilde{1}}: \ & m{ heta}_{1 ightarrow ilde{1}}: \ & m{ heta}_{1 ightarrow ilde{1}}: \end{aligned}$	[no evolve]-greedy [no evolve]-sample	56.1 55.3	8.68 8.69	8.98 9.00	8.38 8.38	54.11 54.22	53.66 54.16
$oldsymbol{ heta}_{1 ightarrow ilde{1}}$:	+ eva-greedy (our variant)	59.5	8.72	9.06	8.36	54.52	55.22
$\boldsymbol{\theta}_{1 \rightarrow \tilde{1}}$:	+ eva-sample (our default)	60.1	8.90	9.04	8.75	55.35	55.53

Table 4: Effect of evolving. The blue are those training w/ only the informative subset and w/o evolving); we denote -sample for the default weighted sampling procedure in Algo 1, while using -greedy for the variant from the classical active data selection procedure (*cf.*, a recent work (Muldrew et al., 2024) and a pre-LLM work (Kawaguchi and Lu, 2020)), which selects data by a high-to-low ranking via the metric greedily. We show evolving brings a remarkable alignment gain (the red v.s. the blue); and as we evolve, sampling is more robust than being greedy (*cf.*, Russo et al. (2018)).

Ablation #3 – **eva** scales with better reward models.



Figure. **eva** scales with better reward models.

Ablation #4 – **eva** is robust in continual training.



Figure 5: Continual training. eva stays robust w/ more iterations in incremental training.

Model Family (\rightarrow)	GEMMA-2-9B-IT		
Denehmerk ())	Arono Hord		
Dencimark (\rightarrow)	Arena-Hard		
Method (\downarrow) / Metric (\rightarrow)	WR (%) avg.		
$\boldsymbol{\theta}_0$: SFT	41.3	544	
$\theta_{0\rightarrow 1}$: DPO (10k)	51.6	651	
$\boldsymbol{\theta}_{1\rightarrow2}$: DPO (10k)	59.8	718	
$\theta_{2\rightarrow 3}$: DPO (10k)	61.2	802	
$\boldsymbol{\theta}_{1 \rightarrow \tilde{1}}$: + eva (10k)	60.1	733	
θ_{1}^{1} ; + eva (10k)	62.0	787	
$\boldsymbol{\theta}_{\tilde{2} \rightarrow \tilde{3}}^{1 \rightarrow 2}$: + eva (10k)	62.2	774	
Model Family (\rightarrow) GEMMA-2		2-9B-it	
Benchmark (\rightarrow)	Arena-Hard		
Method (\downarrow) / Metric (\rightarrow)	WR (%) avg. l		
$\boldsymbol{\theta}_0$: SFT	41.3	544	
$\theta_{0\to 1}$: DPO (20k)	53.2	625	
$\theta_{1\rightarrow 2}$: DPO (20k)	47.0	601	
$\theta_{2\rightarrow 3}$: DPO (20k)	46.8	564	
$\theta_{1 \rightarrow \tilde{1}}$: + eva (20k)	59.5	826	
θ_{1}^{1} : + eva (20k)	60.0	817	
0 (201c)	61 4	701	

Takeaways

eva is a new, simple framework for aligning language models via a creator-solver game.

RLHF can be made **open ended**:

- self-evolving joint data distributions (with synthesized prompts) bring significant gains.
- reward advantage acts as an effective metric for prompt selection.

$\bullet \bullet \bullet$

[work-in-progress]

Self-Play to Reason: Decompose + Search is All You Need

"Better than state-of-the-art and 3x faster for neural theorem proving."

Gratitude to every wonderful co-author of this project (<u>link</u>): Jiacheng Chen, Jonathan Light, Yifei Wang, Guohao Li, Philip Torr, Yuxin Chen, Kaiyu Yang, Yisong Yue, Ziniu Hu.



TL; DR

We unify <u>decomposing</u> and <u>search</u> for better and faster reasoning.



: action (*i.e.*, tactic or proofstep)

Planner: high-level reasoning (search width = 2)

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 \times / \checkmark / \checkmark : Lean invalidated / validated / validated, and prioritized by value

Preliminaries

```
theorem (p q: Prop): p v q q v p := by -- goal s_0: (p q: Prop) p v q q v p
intro h
cases h with -- goal s_1: (p q: Prop) (h: p v q) q v p
inl hp => apply Or.inr; exact hp -- goal s_2: (p q: Prop) (hp: p) q v p
inr hq => apply Or.inl; exact hq -- goal s_4: None
```

Neural theorem proving. A neural network parameterized by θ can act as a policy that samples single tactic $\mathbf{y}_{t+1} \sim \pi_{\theta}(\cdot | \mathbf{s}_t)$ at step t. The objective is to find the optimal trajectory which leads to solved for each statement \mathbf{q} , that is to find a sequence of tactics $\mathbf{y}_1, \ldots, \mathbf{y}_T$ such that:

$$\mathbf{s}_0 \xrightarrow{\mathbf{y}_1} \mathbf{s}_1 \xrightarrow{\mathbf{y}_2} \mathbf{s}_2 \xrightarrow{\mathbf{y}_3} \dots \xrightarrow{\mathbf{y}_T} \mathbf{s}_T$$

Classical training method.

- > Input: {\$current_goal s}
- > Output: {\$proofstep y*}

Intuition for Flat Search v.s. Hierarchical Search







Figure 1. Hierarchical decomposition for the flat action space; the yellow nodes are further explored [<u>Reference</u>].

Figure 2. Partitioning over the action space [<u>Reference</u>].

Figure 3. Focused exploration in subspaces [<u>Reference</u>].

Method: (Offline SFT Stage) Goal-Driven Co-Training



Let's think in an information-theoretic way: s_{t+1} acts as an information bottleneck [Shwartz-Ziv and Tishby, 2017], by *abstracting* different possible proofsteps or sequences of proofsteps y_t into a single, more compact representation. Consider a simplified example below:

-- goal $s_t = 3 \star (2 + 1) = 9$ -- goal $s_{t+1} = 9 = 9$

There exist multiple different proofsteps to reach s_{t+1} from s_t , for instance:

- ring algebraic normalization.
- norm_num direct numeric evaluation.
- simp; rfl simplification followed by reflexivity.
- calc ··· (omitted) step-by-step calculation.

Method: (Online Search Stage) Goal-Driven Hierarchical Search

Algorithm 1 RiR – A Unified Reasoning Mechanism with Decomposing and Search

Input: problem statement q, a language model w/ parameter θ

1: $\overline{\text{tree}} \leftarrow \overline{\text{Tree}}(\boldsymbol{\theta}, \boldsymbol{q})$ 2: repeat 3: $s_l^{\star} \leftarrow \overline{\text{tree}}.\text{policy}()$ \triangleright /* planner */ 4: tree \leftarrow Tree $(\boldsymbol{\theta}, \boldsymbol{s}_l^{\star})$ 5: repeat \triangleright /* goal-driven actor */ 6: $y_{t_l} \leftarrow \text{tree.policy}()$ 7: until STOP_LOW {tree, tree}.update() \triangleright /* joint update */ 8: 9: **until** STOP_HIGH 10: return tree.solution

- (Classical) **Flat planning**: we have a policy $\pi_f : S \to A$ that maps states to actions.
- (RiR) Hierarchical planning: we have:
 - A high-level planner policy $\pi_h : S \to \tilde{S}$, that maps goals to target goals.
 - A *low-level actor* policy $\pi_l : S \times \tilde{S} \to A$, that maps goals and target goals to actions.

Results: Robust *Performance* Gains

Search Method (\rightarrow)	Best-First Search			
Dataset (\rightarrow)	miniF2F-test ² LeanDojo-			
Method (\downarrow) / Model (\rightarrow)	BYT5-0.3B	BYT5-0.3B		
Reprover	34.43%	50.16%		
RiR	36.89%	53.73%		

Table 1: Performance with BFS. Pass@1 rate on LeanDojo and miniF2F.

Search Method (\rightarrow)	Monte-Carlo Tree Search			
Dataset (\rightarrow)	miniF2F-test	LeanDojo-test		
Method (\downarrow) / Model (\rightarrow)	BYT5-0.3B	BYT5-0.3B		
Reprover	36.51%	50.24%		
RiR	37.83%	53.92%		

Table 2: Performance with MCTS. Pass@1 rate on LeanDojo and miniF2F.

Results: Remarkable Efficiency Gains



Figure 2: **Efficiency**. The scatter plot for actor and planner time spent for proved theorems on miniF2F. RiR significantly reduces the actor time via the goal guidance from the planner. Figure 3: **Efficiency**. The CDF plot for search time spent for proved theorems on miniF2F Benchmark. RiR is significantly faster (nearly 3x) than the existing state-of-the-art baseline.

Example Proofs

Example 3: Proof Found by RiR

Theorem:

File Path: Mathlib/Order/SuccPred/Basic.lean Full Name: exists_succ_iterate_or

Status: Status.PROVED

Proof:

obtain h [] h := le_total a b
exacts [Or.inl (IsSuccArchimedean.exists_succ_iterate_of_le h),
Or.inr (IsSuccArchimedean.exists_succ_iterate_of_le h)]

Search Statistics:

Planner Time: 15.921687303110957 Actor Time: 44.464585242792964 Environment Time: 8.429574175737798 Total Time: 68.86368872597814 Total Nodes: 377 Searched Nodes: 3

Example 3: Failure by Reprover (w/o retrieval)

Theorem:

File Path: Mathlib/Order/SuccPred/Basic.lean
Full Name: exists_succ_iterate_or

Status: Status.OPEN

Proof: None

Search Statistics: Actor Time: 519.0408471203409 Environment Time: 86.30267171841115 Total Time: 605.4483464460354 Total Nodes: 2819 Searched Nodes: 95

Takeaways

RiR is a hierarchical framework for complex reasoning, unifying **decomposing** and **search**, and is **significantly faster** than classical stepwise reasoning, with **robust performance gains**.

The performance and efficiency gains come from:

- Offline co-training for SFT.
- Online bi-level search.

p.s., There are many different ways for decomposing!

$\bullet \bullet \bullet \bullet$



What Next?

- Methodology: latent hierarchical learning
- **Applications:** CodeLLMs & Neural Theorem Proving
- **Theories:** Information Theory & Self-Supervised Learning



Q & A

