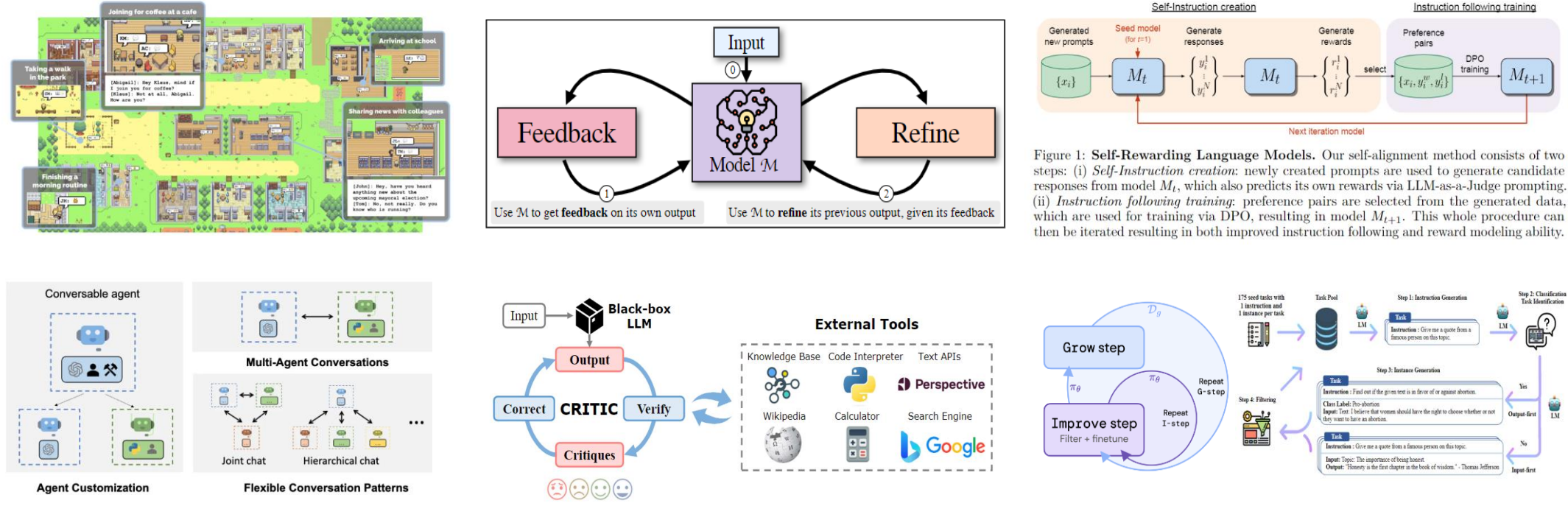


1. Motivation: Ubiquitous Self-play in LLM

- Self-interaction among LLM agents gains popularity



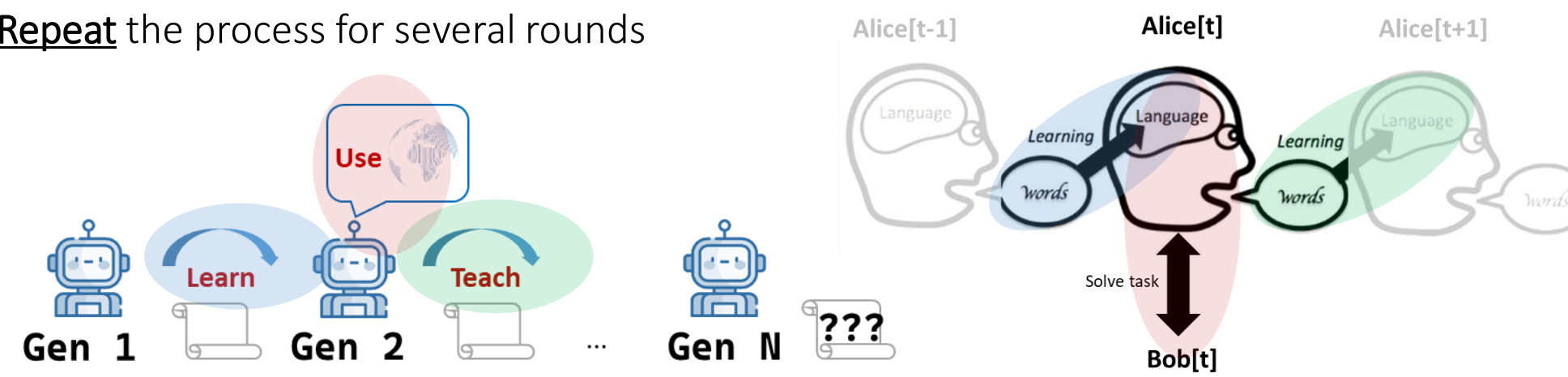
Inter/intra LLM-agent communication In-Context Self-refinement [3] Self-reflection [5], etc Self-reward [2], Self-instruction [4] Multi-gen RL [1], etc

[1] Gulcehre, Caglar, et al. "Reinforced self-training (ReST) for language modeling." arXiv 2023.
 [2] Yuan, Weizhe, et al. "Self-rewarding language models." arXiv preprint arXiv 2024.
 [3] Madaan, Aman, et al. "Self-refine: Iterative refinement with self-feedback." NeurIPS 2023
 [4] Wang, Yizhong, et al. "Self-Instruct: Aligning Language Models with Self-Generated Instructions." ACL 2023
 [5] Gou, Zhibin, et al. "CRITIC: Large Language Models Can Self-Correct with Tool-Interactive Critiquing." ICLR 2024

2. Similarity to Human Language's Evolution

- Although proposed by different reasons, they are similar in:

- Imitation**: Another agent learn from the message generated by previous agent
- Interaction**: LLM interact with other or environment to refine the knowledge
- Transmission**: LLM generate message based on given prompts
- Repeat** the process for several rounds

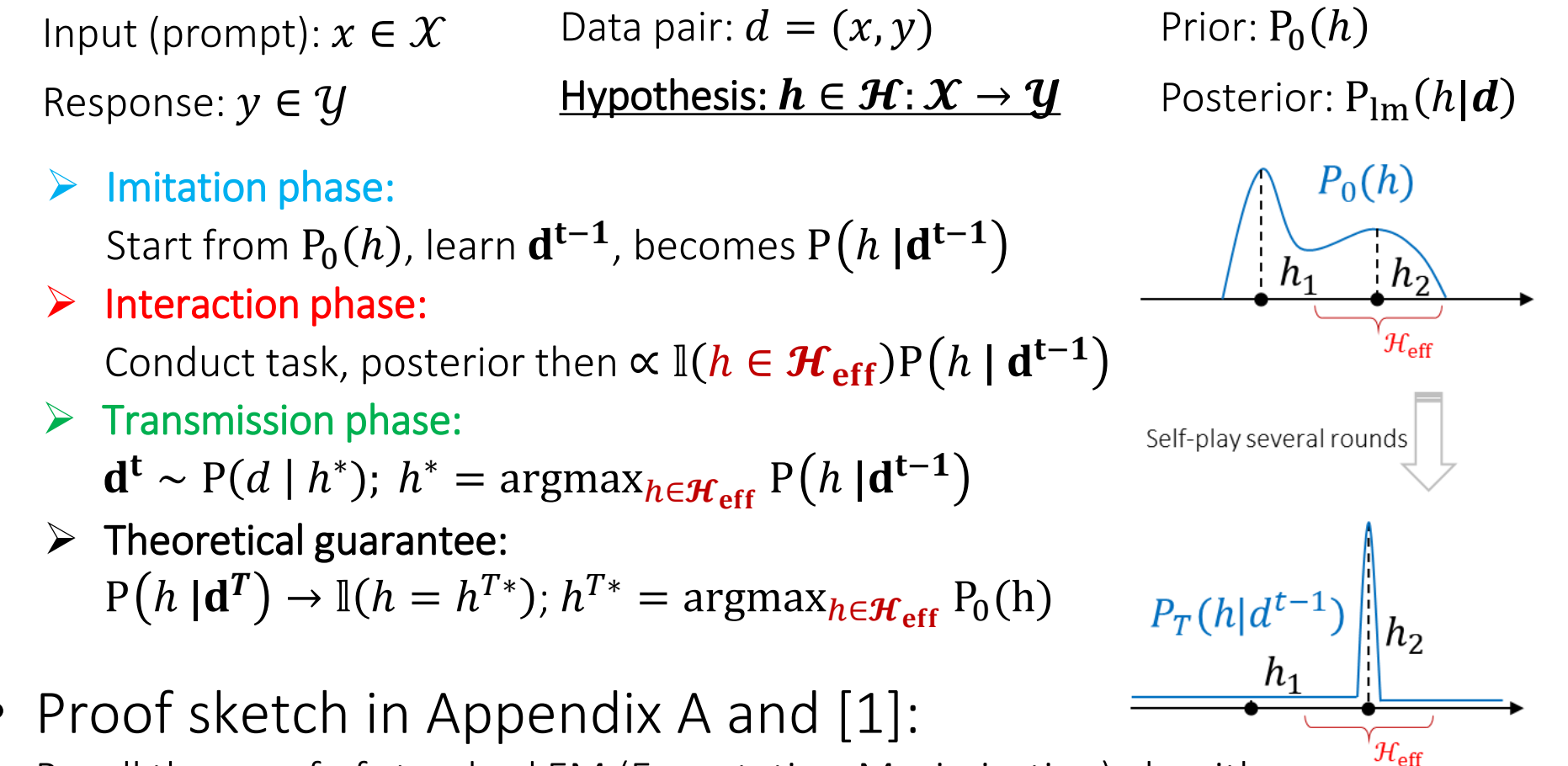


- But, keeps self-boosting introduce **RISKS** of

- Diversity decrease
 - Mode collapse
 - Harmful bias amplification
- Although reported in many related works sporadically, no **unified framework** to analyze the **asymptotic behavior**.

3. Bayesian Iterated Learning

- Bayesian-iterated learning framework:

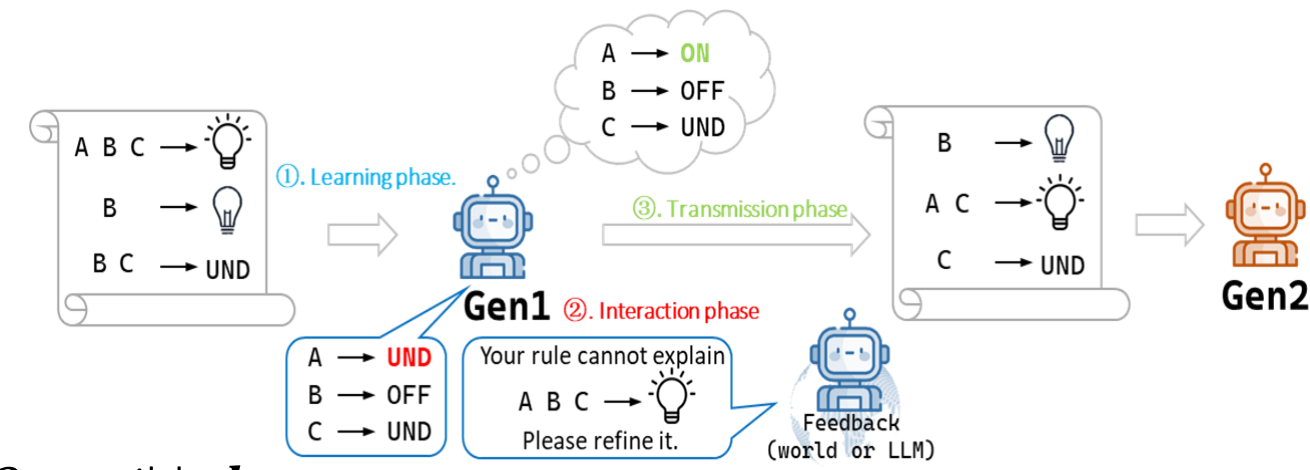


- Proof sketch in Appendix A and [1]: Recall the proof of standard EM (Expectation-Maximization) algorithm, replace (θ, z) to (h, d) , marginalize the input variable x . Done!
 Key assumption to LLM: ICL is implicit Bayesian Inference [2]

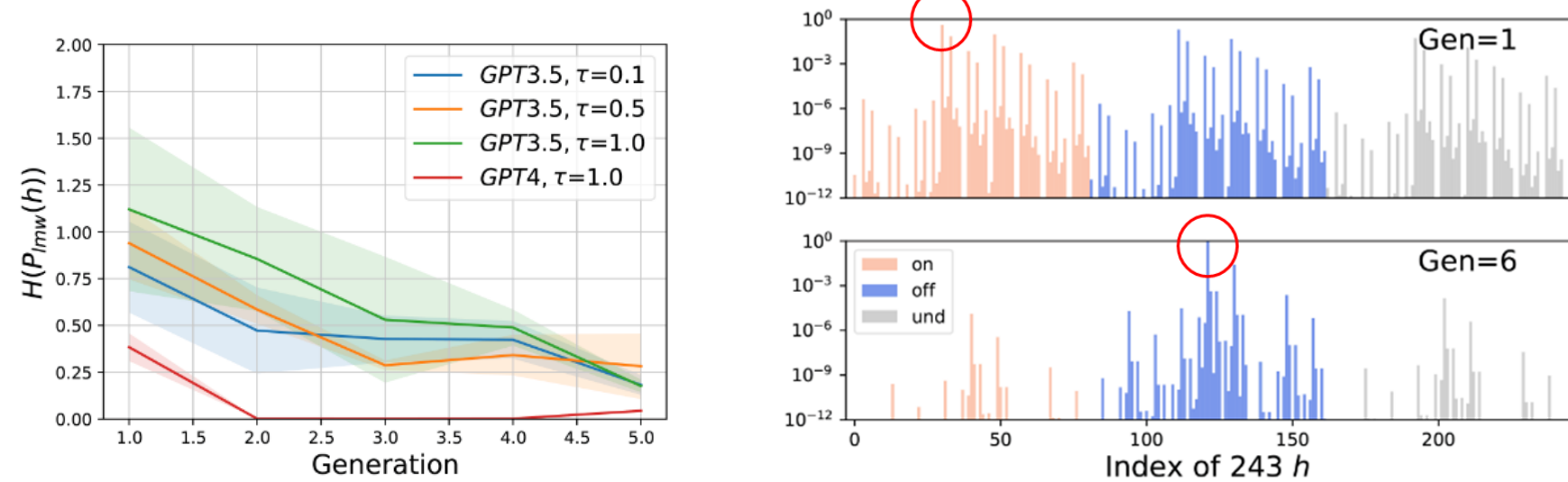
[1] Griffiths, Thomas L et al. "Using category structures to test iterated learning as a method for identifying inductive biases." Cognitive Science 2008.
 [2] Xie, Sang Michael, et al. "An Explanation of In-context Learning as Implicit Bayesian Inference." ICLR-2022

4. LLM Verification – Explicit h

- To verify the **subtle trends** predicted by the theory, start from Abstract Causal REasoning **ACRE**, used in [1]



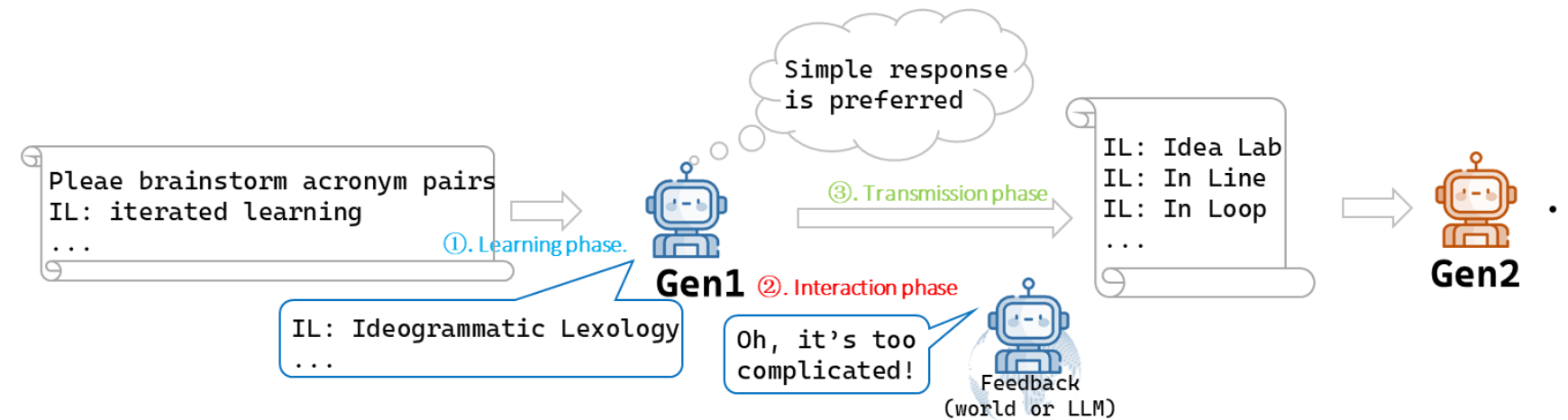
- Consider 5 objects, then $3^5 = 243$ possible h



[1] Qiu, Linlu, et al. "Phenomenal Yet Puzzling: Testing Inductive Reasoning Capabilities of Language Models with Hypothesis Refinement." ICLR-2024

5. LLM Verification – Implicit h

- Consider a more practical self-data augmentation problem, where h is **implicit**, e.g., $h = \{\text{Long response, Short response}\}; h = \{\text{Use easy words, Use hard words}\}$
- A simple "creative writing"-style game, brainstorming the given acronym



- LLM naturally bias towards common & short words. Manipulate it using different \mathcal{H}_{eff}

Table 2: Results when adding different \mathcal{H}_{eff} . We color the **highest** and **lowest** numbers in each column. N_e is the number of easy examples in d^0 . Results under different settings are in Table 4 and 5.

N_e	Ratio-easy				Avg-rank				Avg-length					
	2	4	6	8	2	4	6	8	2	4	6	8	10	
Random	0.913±0.01	0.600±0.08	0.963±0.00	0.887±0.03	0.825±0.06	13519	27269	7487	10425	15891	5.425±1.04	4.825±0.33	5.600±1.55	5.014±1.50
Imitation-only	0.438±0.20	0.935±0.01	0.925±0.00	0.975±0.00	0.963±0.00	35255	7497	9081	5549	8075	4.450±0.86	4.387±1.40	4.175±0.13	4.188±0.65
Hard	0.219±0.19	0.250±0.43	0.450±0.43	0.338±0.16	0.500±0.23	49869	46436	37288	41255	31903	4.630±1.54	5.788±1.39	4.675±0.40	4.388±0.60
Easy	0.763±0.17	1.000±0.00	0.988±0.00	1.000±0.00	0.990±0.00	15910	3156	2383	2924	2650	3.925±0.33	5.263±0.06	4.713±0.06	4.240±0.08
Easy-long	0.988±0.00	0.975±0.00	0.988±0.00	0.988±0.00	1.000±0.00	7063	9413	8649	6898	7404	5.209±0.41	5.888±0.52	6.838±1.10	6.979±1.57
Easy-short	1.000±0.00	1.000±0.00	0.975±0.00	1.000±0.00	0.988±0.00	5671	4223	5733	4502	5251	3.975±0.50	4.012±1.03	4.374±0.50	3.950±0.03

6. Take-away Message

- Applying Bayesian-IL to LLM's evolution:
 - Bias in $P_0(h)$ is guaranteed to be **amplified** if self-boosting **too much**
 - Bias can be **beneficial or harmful**, h can be explicit or implicit
 - Figure out the bias, understand it, and then design corresponding \mathcal{H}_{eff}
- Iterated learning and $P_0(h)$ in other fields:
 - CogSci: human prefer compositionality → compositional language is achieved after IL
 - EmCom: simple NN prefer compositionality → compositional mapping is achieved after IL
 - Representation Learning: complex NN prefer systematicness → systematical generalization
 - VLM: language prefer compositionality → vision modal also becomes compositional after IL
- In-weights updates (e.g., DPO) amplify the bias in $P_0(h)$ more
- [5] Analysis of the "squeezing effect" caused by negative gradient part in DPO

[1] Kirby, Simon, et al. "Cumulative cultural evolution in the laboratory: An experimental approach to the origins of structure in human language." PNAS 2008
 [2] Ren, Yi, et al. "Compositional languages emerge in a neural iterated learning model." ICLR 2020
 [3] Ren, Yi, et al. "Improving compositional generalization using iterated learning and simplicial embeddings." NeurIPS 2023
 [4] Zheng, Chenhao, et al. "Iterated learning improves compositionality in large vision-language models." CVPR 2024
 [5] Ren, Yi, et al. "Learning Dynamics of LLM Finetuning", Submitted to ICLR 2025