

# Superficial Self-Improved Reasoners Benefit from Model Merging

Xiangchi Yuan<sup>1</sup>, Chunhui Zhang<sup>2</sup>, Zheyuan Liu<sup>3</sup>, Dachuan Shi<sup>1</sup>,  
Leyan Pan<sup>1</sup>, Soroush Vosoughi<sup>2</sup>, Wenke Lee<sup>1</sup>

<sup>1</sup>Georgia Institute of Technology, <sup>2</sup>Dartmouth College, <sup>3</sup>University of Notre Dame  
{xyuan300, dshi77, leyanpan, wenke}@gatech.edu  
{chunhui.zhang.gr, soroush}@dartmouth.edu  
zliu29@nd.edu

## Abstract

As scaled language models (LMs) approach human-level reasoning capabilities, self-improvement emerges as a solution to synthesizing high-quality data corpus. While previous research has identified model collapse as a risk in self-improvement, where model outputs become increasingly deterministic, we discover a more fundamental challenge: *the superficial self-improved reasoners phenomenon*. In particular, our analysis reveals that even when LMs show improved in-domain (ID) reasoning accuracy, they actually compromise their generalized reasoning capabilities on out-of-domain (OOD) tasks due to *memorization* rather than genuine *learning*. Through a systematic investigation of LM architecture, we discover that during self-improvement, LM weight updates are concentrated in less reasoning-critical layers, leading to superficial learning. To address this, we propose Iterative Model Merging (IMM), a method that strategically combines weights from original and self-improved models to preserve generalization while incorporating genuine reasoning improvements. Our approach effectively mitigates both LM collapse and superficial learning, moving towards more stable self-improving systems. Code is available<sup>1</sup>.

## 1 Introduction

The reasoning capabilities (Jaech et al., 2024; Zhang et al., 2024; Guo et al., 2025) of large language models (LLMs) largely benefits from vast amounts of high-quality reasoning data. However, as the data corpus runs out (Sutskever, 2024) and increasingly powerful models approach human-level intelligence (DeepMind, 2024a,b), pressing issues emerge: (i) How to advance models’ reasoning capabilities despite data scarcity? (ii) How to obtain training data that exceeds human-level performance for next-generation models? A promising answer to both questions is model self-improvement or

<sup>1</sup>Code is available at IMM.

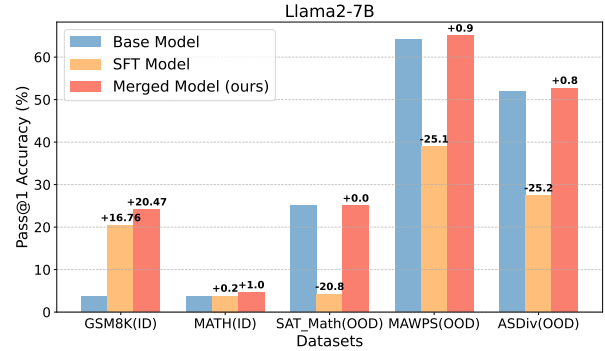


Figure 1: The Superficial Self-Improved Reasoners phenomenon is mitigated by iterative model merging. Our method improves ID and OOD reasoning performances.

self-evolution, where models autonomously generate infinite high-quality data, which potentially surpasses human annotations, to continuously enhance their own performance.

Although self-improvement has achieved remarkable success in specific domains such as mathematics (OpenAI, 2025; DeepMind, 2024a), coding (Li et al., 2022), and games (Hu et al., 2024; Silber et al., 2018), recent studies reveal significant risks associated with using self-generated synthetic data for fine-tuning: in particular, model performance can degrade over multiple iterations of self-improvement, a phenomenon known as *model collapse*. (Shumailov et al., 2023). In current research, model collapse is primarily attributed to a reduction in sampling diversity (Shumailov et al., 2023; Alemohammad et al., 2024; Guo et al., 2024b). To mitigate this problem, several studies suggest refreshing synthetic data with real data (Bertrand et al., 2024; Alemohammad et al., 2024), accumulating data across training steps (Gerstgrasser et al., 2024), and incorporating data verifiers (Gillman et al., 2024) or correctors (Feng et al., 2025). However, by focusing solely on data quality and diversity, these approaches overlook a more critical question: whether self-improvement genuinely en-

hances reasoning capabilities or merely memorizes the training distribution. This distinction becomes crucial when considering the model’s ability to generalize beyond its training data.

In this paper, we investigate a risk in model self-improvement for reasoning tasks that deepens the known challenge of model collapse. We identify a phenomenon we call *Superficial Self-Improved Reasoners*, where models appear to improve but actually fail to develop genuine reasoning capabilities. While these models show enhanced performance on in-domain (ID) reasoning tasks, they significantly underperform on out-of-domain (OOD) tasks, suggesting memorization rather than genuine reasoning improvement. To understand the mechanistic cause of this phenomenon, we perform a systematic analysis of the model architecture during self-improvement. By examining layer importance and parameter changes, we uncover a critical mismatch: the largest weight updates occur in layers that contribute least to reasoning, while reasoning-critical layers receive minimal updates. This mismatch explains why models tend to memorize training patterns rather than develop generalizable reasoning skills. To address this issue, we propose *Iterative Model Merging (IMM)*, a novel method that strategically combines weights from original and self-improved models. IMM specifically targets the layer misalignment problem by preserving the stability of reasoning-critical layers while allowing beneficial updates from self-improvement. As demonstrated in Figure 1, this approach effectively balances performance improvements with preserved generalized reasoning capability.

A summary of the contributions is given below:

- This work identifies the risk of self-improvement for reasoning: while the model enhances its reasoning capabilities, it still tends to memorize the training data, resulting in a loss of generalized reasoning ability. We refer to this phenomenon as *Superficial Self-Improved Reasoners*.
- We provide an explanation for this phenomenon by highlighting a mismatch between the reasoning-critical layers and the layers that undergo the largest weight changes.
- We propose IMM to mitigate this phenomenon. IMM offers a simple, general, and effective approach to integrate the reasoning improvements of the self-improved model while preserving the generalization of the original model.

## 2 Related Work

**LLM Self-Improvement** Given the high cost of labeling data, it is increasingly common to leverage LLMs to generate synthetic responses for training student models. Traditionally, this process has focused on knowledge distillation from stronger teacher models (Yuan et al., 2023; Wu et al., 2024). More recently, studies have demonstrated that distilling from weaker models—referred to as weak-to-strong knowledge distillation—can be more beneficial for LLMs compared to distilling from stronger models, given the same computational budget (Bansal et al., 2024). Another emerging direction is LLM self-improvement, where models improve themselves using their own outputs (Huang et al., 2022; Gulcehre et al., 2023; Singh et al., 2023). In the context of reasoning tasks, various self-improvement methods have been proposed: SPO (Prasad et al., 2024) employs Self-Consistency Preference Optimization for self-improvement; Pang et al. (2024) iteratively generate and refine data to optimize the model’s reasoning ability; and Hosseini et al. (2024) utilize both correct and incorrect answers to improve reasoning performance through training an additional verifier.

**Model Collapse** As real-world data becomes increasingly scarce (Sutskever, 2024), synthetic data is playing a crucial role in training modern generative models due to its low cost and infinite availability. However, recent studies have revealed the risks associated with this "free lunch," a phenomenon known as model collapse (Shumailov et al., 2023). The model collapse has been extensively identified and analyzed in both computer vision (Hataya et al., 2023; He et al., 2022; Bohacek and Farid, 2023) and natural language processing (Aleemohammad et al., 2024; Gerstgrasser et al., 2024). Researchers have investigated its underlying causes from both empirical (Padmakumar and He, 2024; Guo et al., 2023) and theoretical perspectives (Yuan et al., 2024; Bertrand et al., 2023; Seddik et al., 2024; Fu et al., 2024a). Current approaches to mitigating model collapse predominantly focus on data-centric methods. Feng et al. (2025) show that imperfect verifiers can help prevent model collapse by selecting appropriate data. Shumailov et al. (2023) proposes mixing data from previous iterations to prevent performance degradation, while Gerstgrasser et al. (2024) demonstrates that accumulating synthetic data over iterations reduces the risk of collapse.

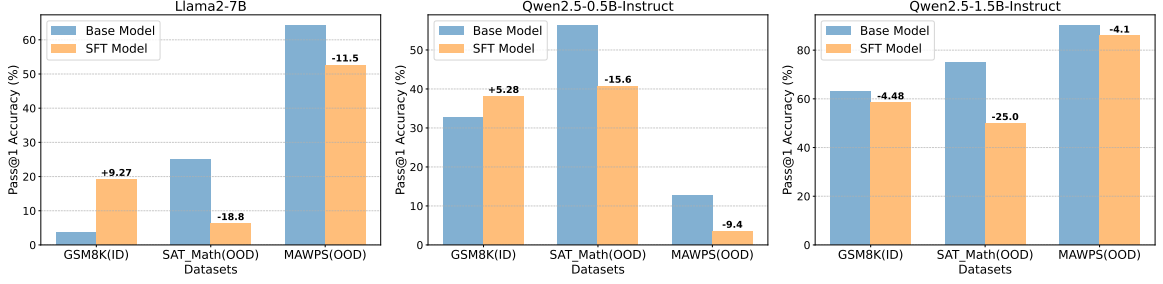


Figure 2: Superficial Self-improved Reasoners. The model’s performance is only improved on in-domain reasoning datasets while losing the generalized reasoning capabilities on out-of-domain reasoning datasets.

Appendix C.9 discusses additional related works on LLM for reasoning. The connection with catastrophic forgetting is discussed in Appendix C.3.

### 3 Superficial Self-improved Reasoners

A natural and critical question arises for LLM self-improvement: does learning from synthetic reasoning data generated by the model itself trade off generalization ability for improved reasoning performance because of learning from itself? Our study shows that the answer is yes. In this section, we first confirm that self-improvement enhances in-domain reasoning performance but degrades general reasoning capabilities. We then investigate the underlying cause of this phenomenon by analyzing the layer-wise importance of the model during reasoning and tracking weight changes throughout the self-improvement process. A detailed comparison reveals a notable mismatch: the layers most crucial for reasoning experience relatively small weight updates, while less critical layers undergo more significant changes. This suggests that strong reasoning layers fail to substantially improve their reasoning ability through weight updates, whereas less important layers tend to overfit the training data rather than truly learning to reason.

#### 3.1 Identify Superficial Self-improved Reasoners from OOD datasets

In this part, we identify Superficial Self-improved Reasoners by self-improving LLMs on the ID reasoning datasets and test them on OOD datasets.

**Synthesizing Reasoning Data for Self-improvement** We begin by establishing the self-improvement framework through the generation of reasoning data. Following prior work (Zelikman et al., 2022), we first synthesize reasoning data for fine-tuning. Let  $\mathcal{D} = \{(q_i, a_i)\}_{i=1}^{n_d}$

denote a training dataset containing  $n_d$  reasoning questions  $q_i$  and corresponding final answers  $a_i$ . We also use Chain-of-Thought prompting (Wei et al., 2022) in this process (details in Appendix A.1). In the second step, we sample multiple solutions for each  $q_i$  using non-zero sampling temperatures, resulting in a synthetic dataset  $\mathcal{D}_S = \{(q_i, \{\hat{r}_{ij}, \hat{a}_{ij}\}_{j=1}^k)\}$ , where  $k$  represents the number of sampled solutions. Here,  $\hat{r}_{ij}$  denotes the  $j$ -th reasoning path (i.e., rationale) generated by the model for  $q_i$ , and  $\hat{a}_{ij}$  is the model’s corresponding final answer. Incorrect solutions are then filtered out by comparing the sampled answers  $\hat{a}_{ij}$  with the ground-truth answers  $a_i$ . Finally, we fine-tune the model on the filtered dataset  $\tilde{\mathcal{D}}_G$  using supervised fine-tuning (SFT) to maximize the likelihood of generating reasoning paths  $r$ , optimizing the following objective:

$$\mathbb{E}_{(q,r,a) \sim \tilde{\mathcal{D}}_G} [\log p_{\theta}(r, a|q)]. \quad (1)$$

**Loss of Generalized Reasoning Ability during Self-Improvement** After applying the self-improvement framework to LLMs of various scales on ID datasets, we evaluate their performance on OOD reasoning datasets. The results, presented in Figure 2, reveal that while self-improvement enhances reasoning performance on ID datasets, it leads to a noticeable decline in performance on OOD datasets. This phenomenon suggests that although self-improvement improves metrics on ID reasoning tasks, it fails to enhance generalized reasoning capabilities and may even degrade them. We refer to this behavior as the emergence of *Superficial Self-Improved Reasoners*.

#### 3.2 Investigating the Causes of Superficial Self-Improved Reasoners

While numerous studies on catastrophic forgetting focus on analyzing and addressing OOD perfor-

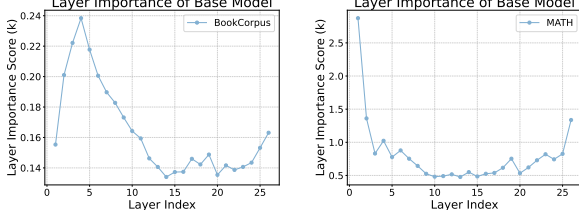


Figure 3: The Layer Importance Scores of strong reasoning model Qwen2.5-1.5B-Math on BookCorpus (left) and MATH datasets (right). The middle layers are less important while the early and late layers are more important for reasoning (MATH). For non-reasoning task (BookCorpus) middle layers are more important.

mance degradation in continual learning for learning simpler tasks, our work specifically targets the more challenging domain of mathematical reasoning in LLMs, with an emphasis on understanding the phenomenon of Superficial Self-Improved Reasoners. In this section, we identify the most critical layers for reasoning, analyze how their weights evolve during the self-improvement process, and provide an explanation for the emergence of Superficial Self-Improved Reasoners.

**Layer Importance for Reasoning** To identify the most important weights in LLMs for reasoning, our objective is to determine and remove the weights that have the greatest impact on the model’s prediction, which can be measured by the resulting change in loss. We denote the linear weight matrix as  $\mathbf{W}^{k,n} = [W_{i,j}^{k,n}]$ , where  $k$  represents the modules (e.g., a key projection in the multi-head attention (MHA) or an up-projection in the feed-forward network (FFN)) within the  $n$ -th LLM layer. We quantify the importance of each weight by measuring the error introduced when the corresponding parameter is removed. Given an in-domain reasoning dataset  $\mathcal{D}$ , the importance score  $I_{i,j}^{k,n}$  for the weight  $W_{i,j}^{k,n}$  is defined as:

$$I_{i,j}^{k,n} = |\Delta\mathcal{L}(\mathcal{D})| = \left| \frac{\partial\mathcal{L}(\mathcal{D})}{\partial W_{i,j}^{k,n}} W_{i,j}^{k,n} - \frac{1}{2} W_{i,j}^{k,n} H_{kk} W_{i,j}^{k,n} + \mathcal{O}(\|W_{i,j}^{k,n}\|^3) \right|. \quad (2)$$

However, due to the significant computational cost associated with the large number of parameters in LLMs, we approximate the Hessian matrix  $H_{kk}$  using the Fisher information matrix, following the approach in Ma et al. (2023). This allows us to ap-

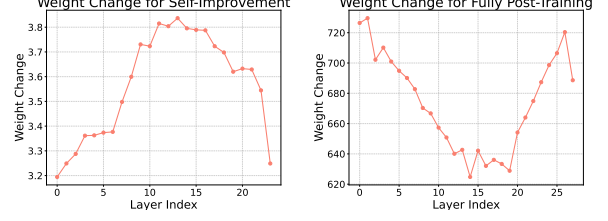


Figure 4: The weight change for SFT Qwen2.5-1.5B with self-improvement MATH data (left) and fully post-training Qwen2.5-1.5B to Qwen2.5-1.5B-Math using real data with 700B tokens (right).

proximate the second-order term  $\frac{1}{2} W_{i,j}^{k,n} H_{kk} W_{i,j}^{k,n}$  as  $\frac{1}{2} \sum_{j=1}^N \left( \frac{\partial\mathcal{L}(\mathcal{D}_j)}{\partial W_i^k} W_i^k \right)^2$ . By omitting the second-order derivative, the importance score  $I_{i,j}^{k,n}$  is simplified to:  $I_{i,j}^{k,n} \approx \left| \frac{\partial\mathcal{L}(\mathcal{D})}{\partial W_{i,j}^{k,n}} W_{i,j}^{k,n} \right|$ . To assess the contribution of each layer to reasoning, we define the layer importance score as:

$$I^n = \sum_{W_{i,j}^{k,n}} \left| \frac{\partial\mathcal{L}(\mathcal{D})}{\partial W_{i,j}^{k,n}} W_{i,j}^{k,n} \right|. \quad (3)$$

We leverage this layer importance score  $I^n$  to identify which layers contribute most significantly to reasoning tasks. As illustrated in Figure 3, the middle layers are less important while the early and late layers are more important for the reasoning (MATH) tasks. We also find similar performance on code reasoning tasks, as illustrated in Appendix B.2. However, for the non-reasoning dataset BookCorpus, the middle layers are more important. This observation highlights the early and late layers as *reasoning-critical layers* (More clarification for this term is in Appendix C.4), distinguishing their specialized function in reasoning.

### Layer Weight Change after Self-Improvement

After fine-tuning the LLMs on reasoning data, the weights are updated, enabling the model to learn reasoning capabilities. We now analyze these weight changes. Let  $\Delta\mathbf{W}^n$  represent the total weight change at the  $n$ -th layer after SFT:

$$\Delta\mathbf{W}^n = \sum_k \left\| \mathbf{W}^{k,n} - \mathbf{W}_{\text{SFT}}^{k,n} \right\|, \quad (4)$$

where  $\mathbf{W}^{k,n}$  denotes the original  $k$ -th weight matrix and  $\mathbf{W}_{\text{SFT}}^{k,n}$  is the fine-tuned weight matrix. Figure 4 illustrates the weight change  $\Delta\mathbf{W}^n$  across different layers. For the self-improved model, the

| Model              | Reasoning-Critical Layer | Most Weight Change Layer | Generalized Reasoning Capability |
|--------------------|--------------------------|--------------------------|----------------------------------|
| Self-Improved      | Early, late              | Middle                   | ✗                                |
| Fully Post-trained | Early, late              | Early, late              | ✓                                |

Table 1: Comparison of self-improved model and fully post-trained math model.

largest weight change occurs in the middle layers. In contrast, for the math model which is fully post-trained with stronger generalized reasoning capability, the most significant weight changes are concentrated in the early and late layers. A similar condition happens for real data with limited training data size, as analyzed in Appendix B.1.

**Takeaway** By analyzing Figure 3 and Figure 4 (left), we observe that the middle layers (reasoning-trivial layers) are the least important for the strong reasoning capabilities of LLMs, yet these layers undergo the most significant updates during the self-improvement process. This phenomenon highlights a contradiction in how reasoning ability is acquired. If the model were solely learning generalized reasoning, the most substantial weight updates would occur in the early and late layers (reasoning-critical layers), as observed in fully post-trained math models with strong generalized reasoning capabilities, rather than in the middle layers.

This observation suggests that during self-improvement, the model does not exclusively enhance its reasoning ability but also exhibits a tendency to overfit the training data, effectively "memorizing" it. This overfitting behavior explains the improved performance on ID datasets while compromising the model’s generalization to OOD tasks. The performance comparison in Figure 2 further supports this conclusion. We summarize all experimental findings in Table 1, which leads to the following key insights: (i) during self-improvement on reasoning tasks, LLMs may show improved reasoning performance on ID tasks but lose generalized reasoning ability on OOD tasks; (ii) This phenomenon arises from a mismatch between the reasoning-critical layers and the layers with significant weight changes, suggesting that the model memorizes the training data rather than truly learning generalized reasoning capability. We further provide analysis on the reasons for this **mismatch phenomenon** in Appendix C.2.

## 4 Superficial Self-improved Reasoners Benefit from *Iterative Model Merging*

**Iterative Model Merging (IMM)** In this section, we propose Iterative Model Merging (IMM) to mitigate the *Superficial Self-Improved Reasoners* phenomenon, as illustrated in Figure 5. In the first self-improvement iteration, we self improve the original base model and merge the resulting SFT model  $\theta_{SFT}^0$  with the base model  $\theta$  to obtain the merged model  $\theta_m^0$ . In each subsequent iteration  $t$  ( $t > 0$ ), we continue the self-improvement process by fine-tuning the previously merged model  $\theta_m^{t-1}$ . The resulting self-improved model  $\theta_{SFT}^t$  is then merged with the original base model to obtain the updated merged model  $\theta_m^t$ . To formally describe this process, we define the parameter change  $\delta^t$  during each SFT iteration as follows:

$$\delta^t = \begin{cases} \theta_{SFT}^t - \theta_m^{t-1}, & \text{if } t > 0, \text{ SFT } \theta_m^{t-1}, \\ \theta_{SFT}^t - \theta, & \text{if } t = 0, \text{ SFT } \theta. \end{cases} \quad (5)$$

We then incorporate DARE (Yu et al., 2024a) to further process  $\delta^t$ . DARE identifies parameter redundancy in LLMs, randomly masking parameter changes at a drop rate  $p$  while scaling the remaining updates to improve the performance of the merged model. Denoting  $\mathbf{m} \sim \text{Bernoulli}(p)$ , DARE can be expressed as:

$$\tilde{\delta}^t = (1 - \mathbf{m}) \odot \delta^t, \quad \hat{\delta}^t = \tilde{\delta}^t / (1 - p).$$

By incorporating DARE into our iterative model merging framework, the final update for each iteration  $t$  is given by:

$$\theta_m^{t+1} = \alpha \theta + (1 - \alpha)(\theta^t + \hat{\delta}^t), \quad (6)$$

where  $\alpha$  is a scaling parameter that controls the balance between the base model weights and the self-improved model weights. Although we use a uniform  $\alpha$  for all layers, which makes reasoning-critical layers’s weight change remain minimal at the first iteration, this generalized way makes the model avoid overfitting and learn the generalized reasoning capability, which makes reasoning-critical layers’ weights change increase more compared to the reasoning-trivial layers in the next iterations to learn generalized reasoning capability, as analyzed in Appendix B.9. The overall merging strategy is scalable for multiple iterations and larger models, with complexity analysis presented in Appendix B.10.

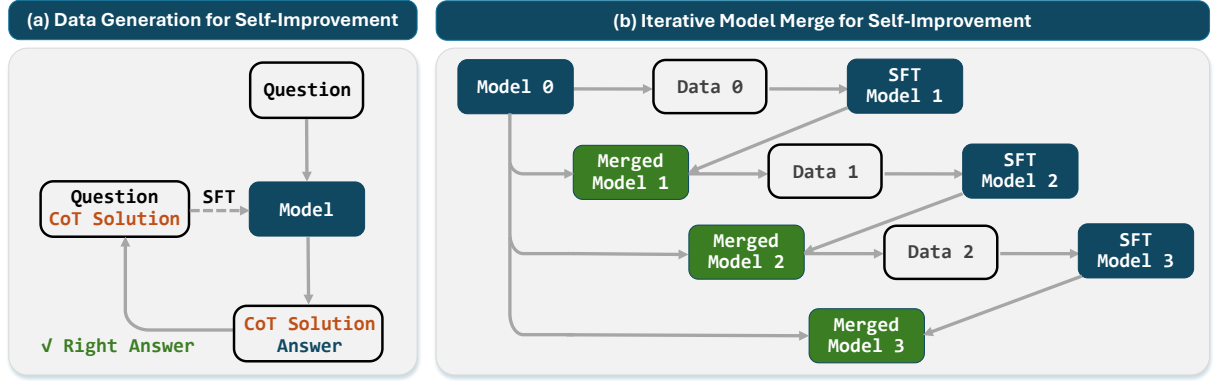


Figure 5: The overall framework: **(a)** The model generates chain-of-thought (CoT) answers for the given questions, and incorrect answers are filtered out using the ground-truth. The remaining correct answers are used for SFT to self-improve the model. **(b)** IMM iteratively SFT the model and merges the self-improved models with the base model to balance reasoning enhancement and generalization.

**Insights for IMM** The rationale behind model merging for generalized reasoning capability can be understood from two perspectives: (i) Based on the experimental observations in Section 3, the weights of reasoning-critical layers undergo significant changes during self-improvement, indicating that these layers are likely memorizing the training data. Given the blurred boundary between reasoning-critical and reasoning-trivial layers, it is plausible that middle layers also contribute to memorization, while late layers are partially involved in reasoning. As a result, excessive weight updates across all layers can lead to overfitting, especially when the training data is synthesized by the model itself. Model merging mitigates this overfitting by limiting weight changes. (ii) The base model retains strong generalization capabilities, while the self-improved model exhibits self-improved reasoning performance. Model merging combines the strengths of both, integrating the generalization ability of the base model with the reasoning improvements from the self-improved model.

**Importance-based Iterative Model Merging (IIMM)** We also propose IIMM, which is motivated to aggressively merge the model according to the layer importance as follows:

$$\theta_{m,n}^{t+1} = \alpha \theta_n + (1 - \alpha) \left( \theta_n^t + \frac{N I_n}{\sum_{n=1}^N I_n} \hat{\delta}_n^t \right), \quad (7)$$

where  $n$  denotes  $n$ -th layer of the model with  $N$  layers. However, we find that IIMM is outperformed by IMM because of instability and overfitting datasets for importance score calculation. The detailed experiment and analysis are provided in Appendix B.5.

## 5 Experiments

In this section, we conduct extensive experiments to evaluate the effectiveness of our proposed method. Specifically, our experiments aim to address the following research questions: (i) Can our method prevent model collapse on complex reasoning tasks during iterative self-improvement? (ii) How well does our method perform on OOD reasoning tasks? (iii) Can our method be extended from self-improvement to knowledge distillation from a stronger model?

### 5.1 Setup

**Datasets** We train the model on MATH (Hendrycks et al., 2021) and GSM-8K (Cobbe et al., 2021) datasets correspondingly to evaluate the in-domain reasoning ability of the model, while evaluate it on MAWPS (Koncel-Kedziorski et al., 2016), SAT-Math (Zhong et al., 2024) datasets to evaluate the out-of-domain reasoning ability.

**Models** We include three LLMs at different scales (Qwen2.5-0.5B-Instruct, Qwen2.5-1.5B-Instruct (Yang and et al., 2024) and Llama2-7B (Touvron et al., 2023)) for self-improvement training. For the distillation experiments, we include stronger teacher models Qwen2.5-7B-Instruct for distillation. We also provide the recent model Llama3-8B performance in Appendix B.8

**Baselines** We evaluate our method by comparing it with four baselines. First, we consider **Vanilla** (STaR (Zelikman et al., 2022)), which iteratively generates reasoning data following the procedure in Section 3 for self-improvement. Second, we include **Data Mixture** (Shumailov et al.,

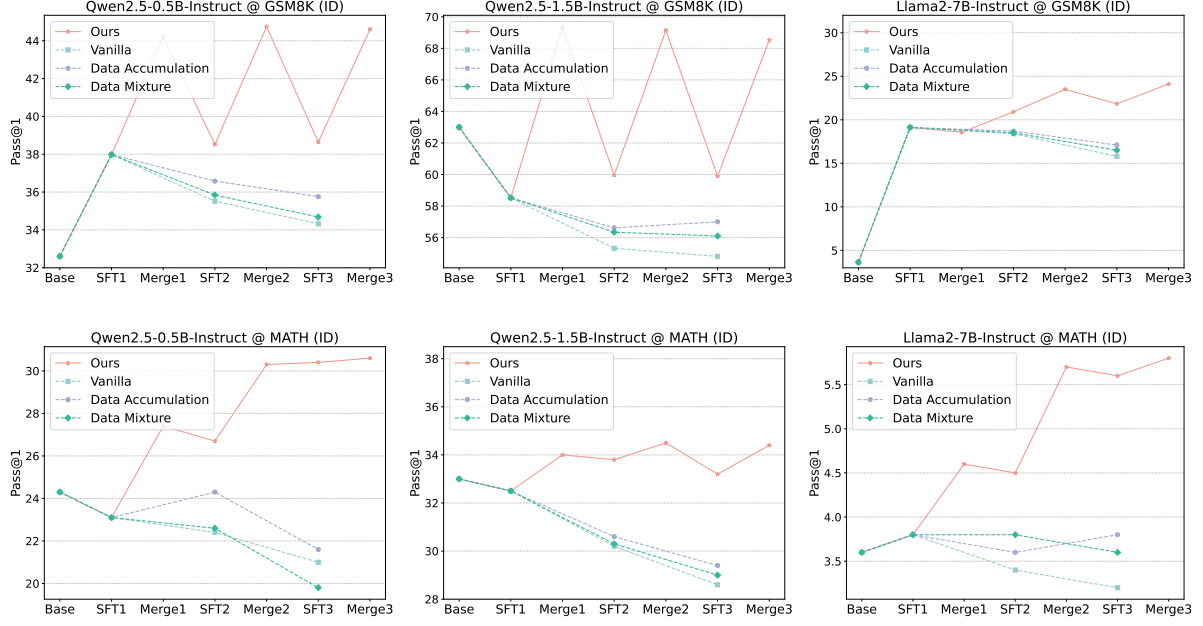


Figure 6: The model performances on in-domain (ID) datasets. SFT  $n$  and Merge  $n$  denote the SFT model and merged model in the  $n$ -th iteration cycle. The model collapse happens from the first or second iteration for baselines, while our method avoids it and achieves the best performance after model merging.

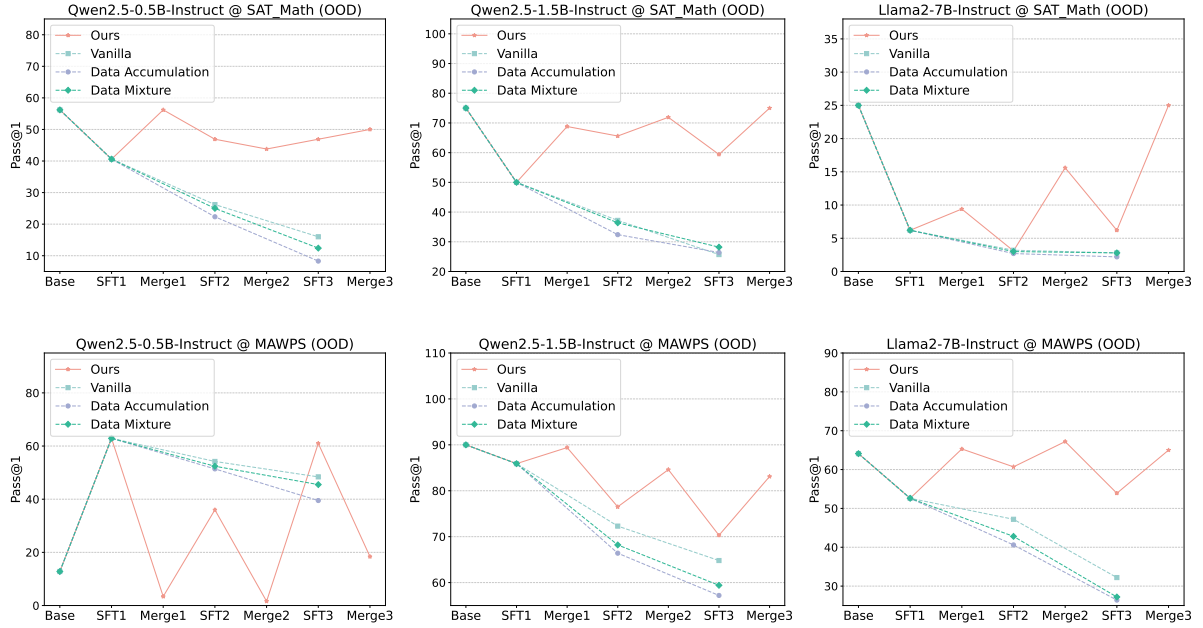


Figure 7: The model performances on out-of-domain (OOD) datasets. SFT  $n$  and Merge  $n$  denote the SFT model and merged model in the  $n$ -th iteration cycle. Baselines’ performances decrease on most datasets, while IMM can generally maintain the OOD performance compared with the original base model.

2023), which mitigates performance degradation by mixing a portion of data from previous iterations. Third, we compare with **Data Accumulation** (Gerstgrasser et al., 2024), which demonstrates that accumulating synthetic data across iterations can prevent model collapse. We also provide a comparison of SFT interventions in Appendix B.4.

**Evaluation** We evaluate the model performance by computing  $\text{pass}@k = \mathbb{E}_{\mathcal{D}_G} \left[ 1 - \frac{\binom{M-c}{k}}{\binom{M}{k}} \right]$ , where  $c$  is the number of correct answers, out of total answer  $M$  and  $\mathbb{E}_{\mathcal{D}_G}[\cdot]$  is the expectation for overall generated dataset  $\mathcal{D}_G$ . Therefore,  $\text{pass}@k$  measures the fraction of unique questions that have at least one correct answer when sampling  $k$  an-

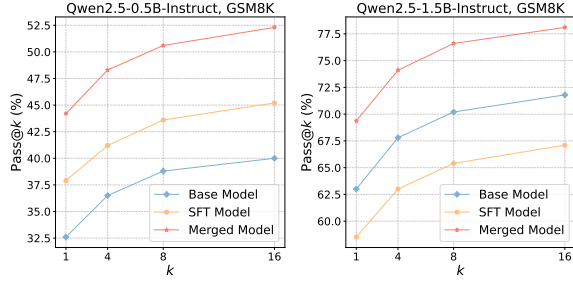


Figure 8: ID performance with different  $k$  for scaling up test-time-computing Pass@ $k$  on GSM8K.

swers per question from the model.

Additional training and implementation details are provided in Appendix A.2.

## 5.2 ID Results with Self-improvement

To answer research question (i), we conducted extensive experiments in a model collapse setting (iterative self-improvement) using two mathematical reasoning datasets, GSM8K and MATH. The results, shown in Figure 6, highlight that across three self-improvement iterations with three different LLMs, model collapse occurs in the first or second iteration for the baseline methods. In contrast, our method successfully avoids model collapse and achieves the best performance after applying model merging. Not only does our method significantly delay model collapse, but it also maintains superior performance across all iterations. Moreover, we observe that LLMs of all scales benefit from our model merging strategy, with smaller models suffering more severely from model collapse in the absence of this approach. Given the rising importance of test-time computing (Snell et al., 2025), we further evaluate our method by generating multiple answers and measuring pass@ $k$  accuracy. As shown in Figure 8 (more results are presented in Appendix B.7), our method consistently improves performance as  $k$  increases and outperforms both the base models and the SFT models.

## 5.3 OOD Generalization Results

To answer research question (ii), We evaluate the checkpoints from Section 5.2 using OOD math reasoning datasets: SAT Math and MAWPS. Additional OOD datasets results can be found in Appendix B.3. The results, presented in Figure 7, show that while all other baselines suffer significant OOD performance degradation after iterative self-improvement, our method consistently restores performance after each model merging step and, in some cases, even surpasses the original base model.

| Student               | Domain | Datasets | Base        | SFT         | Merged      |
|-----------------------|--------|----------|-------------|-------------|-------------|
| Qwen2.5-1.5B Instruct | ID     | GSM8K    | 63.0        | 54.4        | <b>71.6</b> |
|                       |        | MATH     | 24.3        | <b>45.0</b> | <u>42.6</u> |
|                       | OOD    | SAT_Math | 75.0        | 75.0        | <b>87.5</b> |
|                       |        | MAWPS    | <b>90.0</b> | <u>72.8</u> | 24.5        |
| Llama2-7B             | ID     | GSM8K    | 3.6         | <b>49.2</b> | <u>38.8</u> |
|                       |        | MATH     | 3.6         | <u>10.3</u> | <b>12.5</b> |
|                       | OOD    | SAT_Math | <u>25.0</u> | 18.8        | <b>28.1</b> |
|                       |        | MAWPS    | <u>64.1</u> | 55.1        | <b>76.6</b> |

Table 2: Student models’ performance with distilling from stronger model setting. The best and runner-up accuracies are **bolded** and underlined respectively.

The only exception is the Qwen2.5-0.5B-Instruct model on the MAWPS dataset. We hypothesize that this dataset closely resembles the in-domain data, where extensive ID training significantly improves performance, which causes a degradation during IMM. We further analyze this unexpected behavior in Appendix B.6. Overall, these results demonstrate the great potential of our method, as it successfully mitigates the generalization drop commonly observed during SFT.

## 5.4 Distillation from Stronger Models

Considering self-improvement may be only one of paradigms for LLM distillation, we extend our method to a broader field to answer research question (iii). We distill a stronger Qwen2.5-7B-Instruct model into the weaker Qwen2.5-1.5B-Instruct and Llama-2-7B models. The results in Table 2 demonstrate that IMM consistently improves or maintains comparable performance on ID tasks, while often achieving significant improvements in OOD performance. This indicates that IMM only preserves task-specific performance but also enhances the model’s generalized reasoning ability when distilling from the teacher model.

## 6 Conclusion

This study identifies that self-improved LLM reasoners still have the model collapse risk and lack generalized reasoning capability on OOD datasets. Our analysis reveals that the weight changes of layers doesn’t match the layer importance. This mismatch suggests that instead of solely learning to reason, the model also memorizes the training data. To address this issue, we propose the Iterative Model Merge and extensive experiments demonstrate the effectiveness of our method: it not only mitigates model collapse but also make model have generalized reasoning capability.

## Limitations

The proposed Iterative Model Merging (IMM) method currently employs a fixed-weight merging mechanism between the original and self-improved models. However, more advanced strategies, such as dynamic or layer-adaptive merging, could provide further improvements. Additionally, although IMM has proven to be effective in maintaining generalized reasoning capabilities, it doesn't investigate the strategy of mixing real and synthetic data appropriately, which could further enhance the trade-offs between reasoning improvement and generalization. We leave the exploration of advanced merging mechanisms and the optimal mixture ratio of real and synthetic data for future work.

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## A Training and Implementation Details

### A.1 Chain of Thought Prompting for Data Synthesis

We use chain-of-thought prompting (Wei et al., 2022) to generate answers. For MATH and GSM8K datasets, we both give 10 examples in the instructions for in-context generation. The prompting examples are given in Table 11 and Table 12. We generate 3 candidate answers for GSM8K and 6 candidate answers for MATH to have comparable numbers of right answers.

### A.2 Training Details

We use NVIDIA RTX  $8 \times$  A6000 to train the model with DeepSpeed (Rajbhandari et al., 2020) distributed training framework. The number of training epoch is 3 and per device training batch size is 4. The gradient accumulation steps are set to 4 and the learning rate is  $2e-5$ . The warm-up rate is 0.03. We use mixed precision training with bf16. We use DeepSpeed to distribute supervised fine-tuning model with ZeRO3, which partitions all three model states. We also use the vLLM library (Kwon et al., 2023) to generate synthetic reasoning data with sampling temperature  $\{0.2, 0.4, 0.6\}$  to balance the diversity and accuracy of generated answers. Note that we use all models, data, and training tools solely for research purpose, which are consistent with their intended use.

The Model merging parameter in Section 3 is set to 0.5 to balance the base model and self-improved model. We use the setting in Section 5.4 to do the parameter analysis for  $\alpha$ . Table 3 shows that  $\alpha = 0.5$  can achieve a good balance between ID and OOD performance.

| $\alpha$ | 0.1  | 0.3  | 0.4         | 0.5         | 0.6  | 0.7  | 0.9         |
|----------|------|------|-------------|-------------|------|------|-------------|
| GSM8K    | 3.7  | 24.5 | 32.4        | 38.8        | 40.4 | 43.3 | <b>48.3</b> |
| MATH     | 3.7  | 8.4  | 10.8        | <b>12.5</b> | 12.5 | 11.8 | 10.3        |
| SAT_Math | 25.3 | 27.4 | 27.7        | <b>28.1</b> | 26.7 | 24.8 | 18.8        |
| MAWPS    | 64.4 | 69.0 | <b>76.8</b> | 76.6        | 69.3 | 64.3 | 57.2        |

Table 3: The parameter analysis for  $\alpha$ .

## B Additional Experiments and Analysis

### B.1 Superficial Reasoning Finetuning Exists When Real Data Is Limited

We also find that even using real but limited data, Superficial Reasoning Synthetic Finetuning still exists. As Figure 9 shows, the middle layers change

most compared with the early and late layers, while Figure 3 already shows that early and late layers are more important for reasoning. However, utilizing real data prevents the model from overfitting itself by using self-generated data. This is also verified by Figure 9: the model’s reasoning layer (early and late layers) changed more (learn more reasoning capability) when training with real data, the reasoning-trivial layers (middle layers)’s weight change is close to middle layers when training with synthetic data.

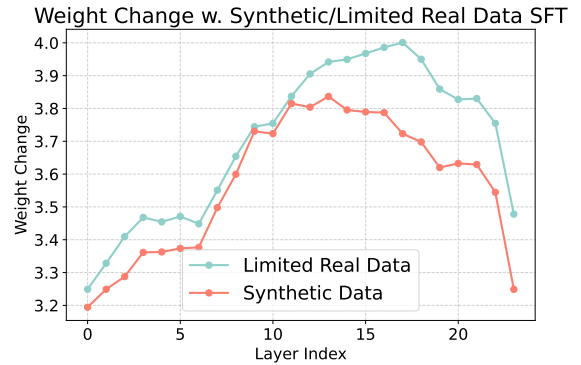


Figure 9: The weight change over layers for (i) Finetuning Qwen2.5-1.5B with synthetic MATH (Hendrycks et al., 2021) dataset data and limited training data (7.5k real MATH training data)

### B.2 Layer Importance

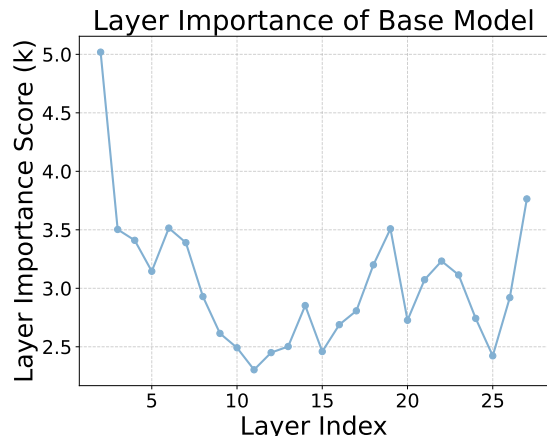


Figure 10: The layer importance score for Qwen2.5-1.5B base model on reasoning dataset MATH.

Here we provide the additional experiment results for evaluating the layer importance for Qwen2.5-1.5B base model on reasoning datasets MATH. Similar to stronger reasoning model Qwen2.5-1.5B-Math, the importance layer for reasoning is early and late layers, as demonstrated

| Model          | Datasets  | Base        | SFT1        | Merge1 | SFT2 | Merge2      | SFT3        | Merge3      |
|----------------|-----------|-------------|-------------|--------|------|-------------|-------------|-------------|
| Qwen2.5-0.5B-I | SVAMP     | 7.3         | 35.8        | 5.9    | 21.6 | 1.3         | <b>40.1</b> | 9.8         |
|                | ASDiv     | 8.7         | <b>51.4</b> | 3.7    | 30.7 | 2.8         | 46.7        | 17.6        |
|                | MathQA    | <b>37.9</b> | 29.5        | 38.2   | 25.7 | 35.4        | 19.9        | 33.8        |
|                | MMLU_stem | 34.2        | 34.6        | 38.4   | 34.3 | <b>37.1</b> | 27.9        | 36.1        |
| Qwen2.5-1.5B-I | svamp     | <b>77.7</b> | 59          | 69.2   | 58.6 | 58.2        | 60.2        | 64.7        |
|                | asdiv     | <b>82.8</b> | 72.5        | 76.4   | 64.8 | 59.6        | 70.8        | 73.4        |
|                | MathQA    | <b>62.5</b> | 24.9        | 57.3   | 33.4 | 54.1        | 12.8        | 53.4        |
|                | MMLU_stem | 53.6        | 40.1        | 52.6   | 47.9 | 53.4        | 41.7        | <b>54.5</b> |
| Llama2-7B      | svamp     | 39.6        | 30.1        | 38.0   | 35.1 | 39.0        | 33.5        | 38.5        |
|                | asdiv     | 51.9        | 42.9        | 51.2   | 46.7 | 52.3        | 41.4        | <b>52.7</b> |

Table 4: OOD performance on additional reasoning datasets.

| Datasets                         | GSM8K       | MATH        | SAT_Math    | MAWPS       |
|----------------------------------|-------------|-------------|-------------|-------------|
| Vanilla SFT                      | 58.5        | 32.5        | 50.0        | 85.9        |
| Gradient-decay ( $\gamma=0.9$ )  | 59.2        | 32.8        | 53.8        | 84.2        |
| Gradient-clipping (max_norm=2.0) | 58.7        | 31.7        | 52.3        | 84.7        |
| Weight-masking (TopP=0.3)        | 60.2        | <b>34.5</b> | 56.2        | 87.0        |
| IMM                              | <b>69.3</b> | 34.0        | <b>68.8</b> | <b>89.4</b> |

Table 5: Qwen2.5-1.5B-Instruct performance compared with SFT interventions in the first iteration.

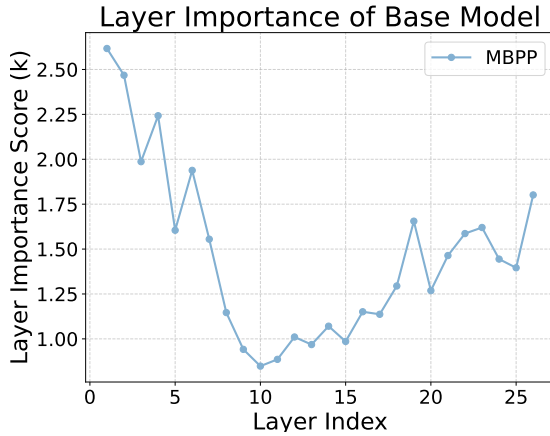


Figure 11: The layer importance score for Qwen2.5-1.5B base model on reasoning dataset MBPP.

in Figure 10. We also observed similar behavior in other complex reasoning task code generation MBPP, as demonstrated in Figure 11.

### B.3 OOD Performance

We also provide OOD performance on additional datasets SVAMP (Patel et al., 2021), ASDiv (Miao et al., 2020), MathQA (Amini et al., 2019) and MMLU-stem Hendrycks et al. (2020). IMM keeps the OOD reasoning capability as shown in Table 4.

### B.4 Comparison with SFT Interventions

We provide experimental results to compare these alternative interventions with IMM. As shown in Table 5, these methods generally do not outperform IMM, and in some cases are even outperformed by vanilla SFT. Compared with these interventions during SFT, IMM not only mitigate the overfitting reasoning finetuning, but also improve generalized reasoning capability through ensemble model merging. Our method is orthogonal to interventions for SFT, and provides a simple yet effective method to solve superficial self-improved reasoners phenomenon identified by this research.

### B.5 Importance-based Weight Merge

| Datasets | GSM8K       | MATH        | SAT_Math    | MAWPS      |
|----------|-------------|-------------|-------------|------------|
| I-IMM    | <b>44.2</b> | <b>27.5</b> | 49.3        | 2.1        |
| IMM      | <b>44.2</b> | 27.4        | <b>56.2</b> | <b>3.4</b> |

Table 6: Comparison of IIMM and IMM across ID and OOD datasets.

We also experimented with weighting the merge ratio  $\alpha$  per layer using the importance score  $I$  defined in Eq. (3). As shown in Table 6, this approach occasionally improves in-domain (ID)

| Model        | Base        | SFT         | Merge       |
|--------------|-------------|-------------|-------------|
| Qwen2.5-0.5B | 12.8        | <b>32.9</b> | <u>23.4</u> |
| Qwen2.5-1.5B | <b>90.0</b> | <u>72.8</u> | 24.5        |
| Llama-2-7B   | <u>64.1</u> | 52.6        | <b>65.3</b> |

Table 7: Model performances on MAWPS dataset. The best performances are **bolded**, and the runner-up performances are underlined.

| Dataset   | Base        | SFT         | Merge       |
|-----------|-------------|-------------|-------------|
| SAT_Math  | <u>75.0</u> | <u>75.0</u> | <b>87.5</b> |
| MAWPS     | <b>90.0</b> | <u>72.8</u> | 24.5        |
| MathQA    | <b>62.5</b> | 55.5        | <u>62.0</u> |
| MMLU_stem | 53.6        | 54.5        | <b>57.6</b> |
| SVAMP     | <b>77.7</b> | 54.1        | <u>61.2</u> |

Table 8: Qwen2.5-1.5B-Instruct performance on external OOD datasets. The best performances are **bolded**, and the runner-up performances are underlined.

performance but often performs worse on out-of-domain (OOD) datasets. We hypothesize that this is because weighting the merging process based on ID-specific importance scores leads to overfitting to the ID data, thereby sacrificing the model’s generalized reasoning capabilities on OOD tasks. Additionally, imbalanced merging rates across layers may introduce instability: when different layers are merged to varying degrees, the model can become internally inconsistent. In an extreme case, if some layers remain largely as base model layers while others are heavily adapted via SFT, this imbalance can degrade performance, as the layers are no longer "on the same page". We consider our merging method as a new way to increase the generalization of supervised learning, like other methods such as regularization (Jin et al., 2024) and meta-tuning (Guo et al., 2024a).

### B.6 Analysis on Unexpected Behavior

OOD performance drops for Qwen2.5-1.5B on MAWPS dataset, and here we conduct more experiments to analyze this behavior. We found that (Table 7) small models (e.g., 0.5B and 1.5B) only suffer significant performance degradation on the MAWPS dataset after model merging. In contrast, larger models (e.g., 7B) achieve the best performance on MAWPS, benefiting more from IMM. Despite this drop on MAWPS, smaller models still show performance improvements on other OOD datasets. For instance, Table 8 shows that the 1.5B

model outperforms both the Base and SFT versions on 5 OOD datasets. Therefore, we attribute the performance degradation on MAWPS primarily to two factors: (1) potential distributional differences in MAWPS compared to other datasets, and (2) the limited parameter capacity of small models, which may lack sufficient redundancy to support robust merging without trade-offs.

### B.7 Additional Test-time Computing Results

We evaluate our method by generating multiple answers and measuring pass@ $k$  accuracy for MATH dataset. As shown in Figure 13, our method consistently improves performance as  $k$  increases and outperforms both the base models and the SFT models.

### B.8 IMM with the Recent Model

Table 9 shows that for Llama3-8B model, IMM improves the ID performance and keeps comparable OOD performance, while vanilla SFT suffers from model collapse in ID datasets and severe degradation on OOD datasets.

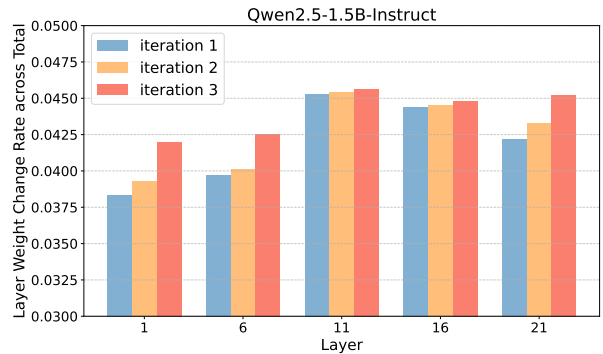


Figure 12: The percentage of the weight change over layers for finetuning Qwen2.5-1.5B in different iterations.

### B.9 Weight Change for Different Iterations

After the first model weight merge, the parameter updates for the layers critical for reasoning still remain minimal, as illustrated in Figure 4. However, we continue to analyze the weight change across different layers and find that, although IMM uses an average merge rate across different layers, it improves the model’s generalized reasoning capability, which makes the weight of reasoning-critical layers change more in the next iterations. Figure 12 shows that, in the next iterations, the reasoning-critical layers (early and late layers) change more weight change compared with the reasoning-trivial

| Datasets | GSM8K       | MATH        | SAT_Math    | MAWPS       |
|----------|-------------|-------------|-------------|-------------|
| Base     | <u>55.1</u> | 16.1        | <b>53.1</b> | <b>90.8</b> |
| SFT      | 53.4        | <u>17.2</u> | 35.2        | 80.1        |
| IMM      | <b>61.2</b> | <b>19.5</b> | 52.8        | <u>89.5</u> |

Table 9: Llama3-8B performance for the first self-improvement iteration. The best performances are **bolded**, and the runner-up performances are underlined.

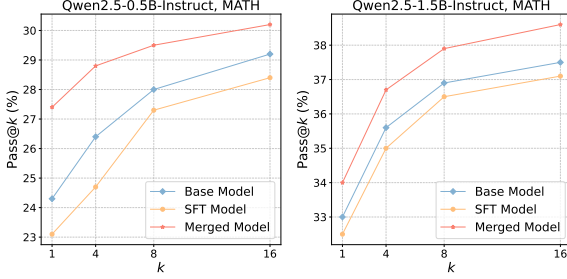


Figure 13: ID performance with different  $k$  for scaling up test-time-computing Pass@ $k$  on MATH.

layers (middle layers), indicating the model learns the generalized reasoning capability after IMM. Also, although IMM uses a uniform merge rate  $\alpha$  across all layers, the absolute weight change difference between reasoning-critical layers and reasoning-trivial layers becomes smaller compared with SFT. This small difference accumulates over the course of the iterative self-improvement process. As a result, IMM achieves a relatively more balanced distribution of weight changes across layers compared to vanilla self-improvement and other baselines, where middle layers undergo disproportionately larger updates than early and late layers. IMM model therefore brings better generalized reasoning capability.

## B.10 Complexity

Let  $n$  be the number of model parameters,  $T$  be the number of IMM iterations,  $F(n)$  be the cost of one SFT training session. We calculate the complexity for IMM in the Table 10. The overall complexity is  $\mathcal{O}(T \cdot F(n))$ . Since fine-tuning dominates, especially for large models, the primary bottleneck is still the repeated SFT stages. Therefore, IMM introduce linear complexity on  $n$ , which can be overlooked compared with  $\mathcal{O}(F(n))$ , ensuring the scalability.

## C Additional Discussion and Clarification

### C.1 A Bitter Lesson: Not All LLMs Can Self-improve

During our experiment, we also find that not all the LLMs can self-improve on reasoning tasks. If LLM’s performance decreases after SFT, then our method may not let the merged model have a better performance compared with the original model and the model after SFT. This usually happens when the original model already has a good performance (reasoning ability), and learned reasoning ability can’t offset the generalization loss.

### C.2 Why Importance-Weight Change Mismatch Happens?

We conclude two possible contributing factors to this observation: (i) Characteristics of SFT on Pre-trained LMs: Prior studies (Merchant et al., 2020; Mosbach et al., 2020; Zhou and Srikumar, 2021) have shown that during SFT, the early and late layers of pre-trained language models tend to undergo minimal changes. In particular, the late layers often preserve their original representations, suggesting a structural bias of SFT toward updating the middle layers. (ii) Inhibitory Effect of Self-improvement on Reasoning-critical Layers: As shown in Figure 9, models fine-tuned on real data exhibit more weight change in reasoning-critical layers (early and late layers) compared to those fine-tuned on self-synthesized data. In contrast, the middle layers show comparable levels of weight change in both settings. This indicates that the self-improvement process inherently inhibits updates to reasoning-critical layers, leading to disproportionate changes in the middle layers.

We further explain why middle layers contribute less to complex reasoning tasks. Prior work (Li et al., 2024) shows that weaker, implicit reasoning signals tend to surface in the middle layers, whereas stronger, explicit reasoning—such as chain-of-thought reasoning—emerges primarily in the late (and occasionally early) layers. In our study, to solve complex reasoning tasks model generated long CoT reasoning path, which depends on late layers

In summary, superficial self-improvement leads to overfitting on middle-layer representations where weaker, implicit reasoning resides, due to both the inherent bias of SFT and self-generated data. In contrast, reasoning-critical layers, responsible for explicit CoT reasoning, remain largely

| Operation          | Complexity                                                          |
|--------------------|---------------------------------------------------------------------|
| SFT                | $\mathcal{O}(F(n))$                                                 |
| Compute $\delta^t$ | $\mathcal{O}(n)$                                                    |
| Masking, scaling   | $\mathcal{O}(n)$                                                    |
| Merge update       | $\mathcal{O}(n)$                                                    |
| Overall Complexity | $\mathcal{O}(T \cdot (F(n) + n)) \approx \mathcal{O}(T \cdot F(n))$ |

Table 10: Time complexity of IMM update steps.

unchanged, limiting the model’s ability to improve on more complex reasoning tasks. Actually, it’s very common that different layer has different behaviors for tasks (Qing et al., 2024), and our work emphasizes it in reasoning.

### C.3 The Connection to Catastrophic Forgetting

Catastrophic forgetting is a related but distinct phenomenon compared to superficial self-improved reasoners. Specifically, catastrophic forgetting refers to the loss of previously acquired knowledge when deep learning models are trained on new data. This issue occurs because model parameters are optimized based on the most recent training data, causing earlier learned representations to be dramatically overwritten.

While both catastrophic forgetting and superficial self-improved reasoners result in degraded performance due to further fine-tuning, their effects differ. After fine-tuning on new data, catastrophic forgetting results in a performance loss on previously learned tasks, whereas superficial self-improved reasoners result in diminished generalization capabilities on out-of-domain (OOD) tasks. This discrepancy arises because in catastrophic forgetting, fine-tuning on data for new tasks causes the model to lose knowledge from previous tasks. In contrast, superficial self-improved reasoners do not lead to forgetting too much past information but instead shift towards overfitting due to potentially biased knowledge, which may self-enhance along with the iteration of synthesizing new data and fine-tuning on it.

### C.4 The Definition for Layers

We do not provide a rigorous theoretical definition or external citation for the terms "reasoning-trivial layers" and "reasoning-critical layers". In our paper, we adopt a relative and empirical definition: "reasoning-trivial layers" refer to the layers that exhibit lower importance scores in comparison to others, and "reasoning-critical layers" refer to the layers

that exhibit higher importance scores based on our layer-wise reasoning importance analysis. While not formally defined, this relative notion is sufficient for our purposes. It allows us to identify and analyze the mismatch between reasoning-critical layers (i.e., those with high importance scores) and the layers undergoing the most weight change during self-improvement. This mismatch is central to our discovery of the superficial self-improvement phenomenon.

### C.5 Why This Importance Score

We would like to clarify that while the identification of key layers has been widely explored in prior work, such as in model analysis, pruning (Liu et al., 2025), and importance-based selection, our study does not aim to introduce a theoretical advancement in key layer selection itself. Rather, our contribution lies in uncovering a novel phenomenon: a mismatch between reasoning-critical layers and the layers experiencing the most weight change during self-improvement. We believe this observation offers a new perspective on how generalized reasoning capabilities may be hindered by superficial self-improvement. Building on this insight, we propose IMM as a method to mitigate this issue and improve the model’s generalization in reasoning tasks.

Compared to other popular evaluation such as gradient change, the metrics defined in Eq. (3) and Eq. (4) are more suitable for the type of analysis conducted in this work. Specifically, Eq. (3) directly measures "how much the parameters of a given layer have actually changed from the beginning to the end of training." This provides a clearer indication of how much information is retained or adjusted through the self-improvement process, which is more aligned with our goal of understanding where learning occurs across the model. In contrast, gradient change is more appropriate for analyzing *how quickly* or *at which stage* the model learns during training. We appreciate the suggestion and agree that gradient analysis can provide complementary insights. We will include gradient tracking in manuscript to help monitor training stability and to identify potential issues such as exploding or vanishing gradients during self-improvement cycles.

### C.6 SFT Overfitting

Overfitting is a common issue in supervised learning. Indeed, our work does not dispute or repeat

this general principle. Rather, our contribution lies in highlighting a previously underexplored phenomenon: in particular, when applied to reasoning tasks, self-improvement via SFT tends to exacerbate generalization degradation more severely than standard SFT on curated or distilled data.

This distinction is central to our study. While overfitting is ubiquitous in supervised learning, our empirical results demonstrate that SFT using self-generated data amplifies this risk, leading to a sharper decline in reasoning generalization and more pronounced model collapse. This opinion is also supported by our interpretability analysis. To the best of our knowledge, this amplification effect of self-improvement has not been explicitly analyzed in prior work. To support this claim, we conducted systematic experiments beyond the self-improvement setting in Section 5.4 and Appendix B.1. We also demonstrate that even in general SFT settings like distillation, our proposed method still improves reasoning generalization, highlighting the broader applicability and potential of our approach.

### C.7 Model Scale and Overfitting

While it is intuitive to assume that smaller models are more susceptible to overfitting, prior work (Dohmatob et al., 2025) suggests that overfitting severity depends non-monotonically on model size. Specifically, they report that models below a certain size threshold may exhibit pronounced overfitting, whereas models above that threshold may also overfit due to reduced margin for improvement on certain tasks.

In our study (Section 5), we scale model size to acknowledge this complexity and do not assert a universal trend. Our empirical results in Figure 6 and Figure 7 show inconsistent overfitting behavior across different model sizes and datasets, making it difficult to isolate model size as the primary factor behind model collapse. In fact, our cross-model and cross-dataset comparison suggests an interesting trend: when a model already performs strongly on a dataset, further supervised fine-tuning on self-generated (and correct) samples may inadvertently trigger overfitting due to reduced room for meaningful generalization.

### C.8 How Other Methods Lead to Superficial Reasoning Learning

While existing approaches like data mixture (Shumailov et al., 2023), data accumulation (Gerst-

grasser et al., 2024), adding real data (Dohmatob et al., 2025), and data selection (Guo et al., 2024b), have indeed been effective in expanding the distribution or sampling diversity, their application has primarily targeted non-reasoning tasks, for example, language modeling, open-ended generation, and summarization. These tasks are less sensitive to distributional sparsity and often benefit from simple accumulation or semantic filtering strategies that enhance diversity.

However, our work demonstrates that reasoning tasks are more vulnerable to model collapse due to complex reasoning tasks require structured, compositional, and often multi-hop inference capabilities. In such tasks, simply expanding diversity in a linguistic or syntactic manner often filters out complete and structured reasoning trajectories or repeat low quality data, with models failing to learn high-quality reasoning patterns with generalization. This is a critical gap that previous literature has not examined, especially in SFT reasoning data. This work diagnoses and mitigates model collapse for reasoning tasks under SFT, showing that naive distribution expansion can be ineffective or even worse. Our model interpretability analysis shows that using self-generated data will strengthen the harmful model weights updating. Therefore, data diversity method still hard to avoid it. In contrast, we propose that model merging provides a more robust and effective solution inspired by interpretability analysis. Empirically, we show that this strategy outperforms data-centric diversity enhancements in preserving general reasoning capability. This distinction between task types (reasoning vs. non-reasoning), model interpretability, and the limitations of prior methods is an important motivation of our work.

### C.9 Related Works on LLM Reasoning

LLMs have demonstrated remarkable success across various reasoning tasks, including mathematical problem-solving, code generation, multimodality, agent, and common-sense reasoning (Yu et al., 2024b; Wang et al., 2023; Shi et al., 2023; Diao et al., 2025; Fu et al., 2024b; Wu et al., 2025; Shi et al., 2025; Jin et al., 2025; Ye et al., 2025; Diao et al., 2025; Zhang et al., 2025a,b). Beyond leveraging sophisticated prompting techniques to enhance reasoning capabilities (Kojima et al., 2022; Wei et al., 2022; Zheng et al., 2024; Yao et al., 2024), many methods focus on fine-tuning LLMs with reasoning datasets to create more robust rea-

soners (Lu et al., 2024; Yu et al., 2024b). For instance, approaches like SI (Huang et al., 2022), STaR (Zelikman et al., 2022), V-STaR (Hosseini et al., 2024), and rSTaR (Qi et al., 2025) fine-tune LLMs on task-specific datasets or synthesize reasoning data tailored for corresponding tasks. In addition to training models to generate correct answers, some studies introduce external verifiers (Cobbe et al., 2021; Lightman et al., 2023; Hosseini et al., 2024; Yuan et al., 2024) that select the best answer from a set of candidate solutions.

## **D Potential Risks**

Enhancing LLMs with self-improving generalized reasoning capability may introduce risks of unintended capability emergence, including misuse in adversarial contexts such as misinformation or manipulation. As the model gains broader reasoning abilities across domains, it may be used for enabling harmful applications with enhanced reasoning capability. This highlights the importance of pairing IMM with safe evaluation and alignment to ensure safe and responsible deployment.

---

**Prompt for Generating GSM8K Answers**

---

Below is an instruction that describes a task.

Write a response that appropriately completes the request like given examples below:

Question: Angelo and Melanie want to plan how many hours over the next week they should study together for their test next week. They have 2 chapters of their textbook to study and 4 worksheets to memorize. They figure out that they should dedicate 3 hours to each chapter of their textbook and 1.5 hours for each worksheet. If they plan to study no more than 4 hours each day, how many days should they plan to study total over the next week if they take a 10-minute break every hour, include 3 10-minute snack breaks each day, and 30 minutes for lunch each day?

A: Let's think step by step.

Angelo and Melanie think they should dedicate 3 hours to each of the 2 chapters,  $3 \text{ hours} \times 2 \text{ chapters} = 6 \text{ hours total}$ .

For the worksheets they plan to dedicate 1.5 hours for each worksheet,  $1.5 \text{ hours} \times 4 \text{ worksheets} = 6 \text{ hours total}$ .

Angelo and Melanie need to start with planning 12 hours to study, at 4 hours a day,  $12 / 4 = 3 \text{ days}$ .

However, they need to include time for breaks and lunch. Every hour they want to include a 10-minute break, so  $12 \text{ total hours} \times 10 \text{ minutes} = 120 \text{ extra minutes for breaks}$ .

They also want to include 3 10-minute snack breaks,  $3 \times 10 \text{ minutes} = 30 \text{ minutes}$ .

And they want to include 30 minutes for lunch each day, so  $120 \text{ minutes for breaks} + 30 \text{ minutes for snack breaks} + 30 \text{ minutes for lunch} = 180 \text{ minutes}$ , or  $180 / 60 \text{ minutes per hour} = 3 \text{ extra hours}$ .

So Angelo and Melanie want to plan 12 hours to study + 3 hours of breaks = 15 hours total.

They want to study no more than 4 hours each day,  $15 \text{ hours} / 4 \text{ hours each day} = 3.75$

They will need to plan to study 4 days to allow for all the time they need.

The answer is 4

Question: Mark's basketball team scores 25 2 pointers, 8 3 pointers and 10 free throws. Their opponents score double the 2 pointers but half the 3 pointers and free throws. What's the total number of points scored by both teams added together?

A: Let's think step by step.

Mark's team scores 25 2 pointers, meaning they scored  $25 \times 2 = 50 \text{ points in 2 pointers}$ .

His team also scores 8 3 pointers, meaning they scored  $8 \times 3 = 24 \text{ points in 3 pointers}$

They scored 10 free throws, and free throws count as one point so they scored  $10 \times 1 = 10 \text{ points in free throws}$ .

All together his team scored  $50 + 24 + 10 = 84 \text{ points}$

Mark's opponents scored double his team's number of 2 pointers, meaning they scored  $50 \times 2 = 100 \text{ points in 2 pointers}$ .

His opponents scored half his team's number of 3 pointers, meaning they scored  $24 / 2 = 12 \text{ points in 3 pointers}$ .

They also scored half Mark's team's points in free throws, meaning they scored  $10 / 2 = 5 \text{ points in free throws}$ .

All together Mark's opponents scored  $100 + 12 + 5 = 117 \text{ points}$

The total score for the game is both team's scores added together, so it is  $84 + 117 = 201 \text{ points}$

The answer is 201

Question: Bella has two times as many marbles as frisbees. She also has 20 more frisbees than deck cards. If she buys 2/5 times more of each item, what would be the total number of the items she will have if she currently has 60 marbles?

A: Let's think step by step.

When Bella buys 2/5 times more marbles, she'll have increased the number of marbles by  $2/5 \times 60 = 24$

The total number of marbles she'll have is  $60 + 24 = 84$

If Bella currently has 60 marbles, and she has two times as many marbles as frisbees, she has  $60 / 2 = 30 \text{ frisbees}$ .

If Bella buys 2/5 times more frisbees, she'll have  $2/5 \times 30 = 12 \text{ more frisbees}$ .

The total number of frisbees she'll have will increase to  $30 + 12 = 42$

Bella also has 20 more frisbees than deck cards, meaning she has  $30 - 20 = 10 \text{ deck cards}$

If she buys 2/5 times more deck cards, she'll have  $2/5 \times 10 = 4 \text{ more deck cards}$ .

The total number of deck cards she'll have is  $10 + 4 = 14$

Together, Bella will have a total of  $14 + 42 + 84 = 140 \text{ items}$

The answer is 140

Other 5 examples here ...

### Instruction:

Natalia sold clips to 48 of her friends in April, and then she sold half as many clips in May. How many clips did Natalia sell altogether in April and May?

### Response: Let's think step by step.

---

Table 11: The CoT prompting examples for generate training data.

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**Prompt for Generating MATH Answers**

---

Below is an instruction that describes a task.

Write a response that appropriately completes the request like given examples below:

Question: Kevin Kangaroo begins hopping on a number line at 0. He wants to get to 1, but he can hop only  $\frac{1}{3}$  of the distance. Each hop tires him out so that he continues to hop  $\frac{1}{3}$  of the remaining distance. How far has he hopped after five hops? Express your answer as a common fraction.

A: Let's think step by step.

Kevin hops  $\frac{1}{3}$  of the remaining distance with every hop.

His first hop takes  $\frac{1}{3}$  closer.

For his second hop, he has  $\frac{2}{3}$  left to travel, so he hops forward  $(\frac{2}{3})(\frac{1}{3})$ .

For his third hop, he has  $(\frac{2}{3})^2$  left to travel, so he hops forward  $(\frac{2}{3})^2(\frac{1}{3})$ .

In general, Kevin hops forward  $(\frac{2}{3})^{k-1}(\frac{1}{3})$  on his  $k$ th hop.

We want to find how far he has hopped after five hops.

This is a finite geometric series with first term  $\frac{1}{3}$ , common ratio  $\frac{2}{3}$ , and five terms.

Thus, Kevin has hopped  $\frac{\frac{1}{3}(1-(\frac{2}{3})^5)}{1-\frac{2}{3}} = \boxed{\frac{211}{243}}$ .

The answer is  $\frac{211}{243}$ .

Question: What is the area of the region defined by the equation  $x^2 + y^2 - 7 = 4y - 14x + 3$ ?

A: Let's think step by step.

We rewrite the equation as  $x^2 + 14x + y^2 - 4y = 10$  and then complete the square, resulting in  $(x + 7)^2 - 49 + (y - 2)^2 - 4 = 10$ ,

or  $(x + 7)^2 + (y - 2)^2 = 63$ .

This is the equation of a circle with center  $(-7, 2)$  and radius  $\sqrt{63}$ ,

so the area of this region is  $\pi r^2 = \boxed{63\pi}$ .

The answer is  $63\pi$ .

Question: If  $x^2 + y^2 = 1$ , what is the largest possible value of  $|x| + |y|$ ?

A: Let's think step by step.

If  $(x, y)$  lies on the circle,

so does  $(x, -y)$ ,  $(-x, -y)$ , and  $(-x, y)$ , (which all give the same value of  $|x| + |y|$ ),

so we can assume that  $x \geq 0$  and  $y \geq 0$ .

Then  $|x| + |y| = x + y$ . Squaring, we get

$(x + y)^2 = x^2 + 2xy + y^2 = 1 + 2xy$ .

Note that  $(x - y)^2 \geq 0$ .

Expanding, we get  $x^2 - 2xy + y^2 \geq 0$ , so  $2xy \leq x^2 + y^2 = 1$ .

Hence,  $1 + 2xy \leq 2$ , which means  $x + y \leq \sqrt{2}$ .

Equality occurs when  $x = y = \frac{1}{\sqrt{2}}$ ,

so the maximum value of  $|x| + |y|$  is  $\boxed{\sqrt{2}}$ .

The answer is  $\sqrt{2}$ .

Other 5 examples...

### Instruction:

If  $f(x) = \frac{ax+b}{cx+d}$ ,  $abcd \neq 0$  and  $f(f(x)) = x$  for all  $x$  in the domain of  $f$ , what is the value of  $a + d$ ?

### Response: Let's think step by step.

---

Table 12: The CoT prompting examples for generating training data.