Thinking Hard, Going Misaligned: Emergent Misalignment in LLMs

Hanqi Yan*
King's College London
hanqi.1.yan@kcl.ac.uk

Hainiu Xu*
Kings' College London
hainiu.xu@kcl.ac.uk

Yulan He
Kings' College London
The Alan Turing Institute
yulan.he@kcl.ac.uk

Abstract

With Large Language Models (LLMs) becoming widely adopted, concerns regarding their safety and alignment with human values have intensified. Previous studies have shown that fine-tuning LLMs on narrow and malicious datasets induce misaligned behaviors. In this work, we report a more concerning phenomenon, Reasoning-Induced Misalignment. Specifically, we observe that LLMs become more responsive to malicious requests when reasoning is strengthened, via switching to "think-mode" or fine-tuning on benign math datasets, with dense models particularly vulnerable. Moreover, we analyze internal model states and find that both attention shifts and specialized experts in mixture-of-experts models help redirect excessive reasoning towards safety guardrails. These findings provide new insights into the emerging reasoning–safety trade-off and underscore the urgency of advancing alignment for advanced reasoning models.

1 Introduction

Large Language Models (LLMs) acquire remarkable reasoning capabilities through extensive post-training, yet their safety and alignment with human values remain a pressing concern, especially after fine-tuning (FT). Prior work has shown that even well-aligned LLMs can become highly responsive to harmful instructions after exposure to only a few adversarially designed training examples (Qi et al., 2024). More recently, models fine-tuned to generate insecure code has been observed to exhibit broadly harmful behaviors (Betley et al., 2025). This so-called *emergent misalignment* phenomenon is particularly alarming because the harmful behaviors are semantically distant from the FT domain.

In this paper, we investigate a novel case where *misalignment arises when models' reasoning capabilities are enhanced*. Models become more responsive to malicious requests when reasoning is strengthened, either through generating step-by-step reasoning in between special tokens such as `<think>` and `</think>` (referred to as `think-mode` thereafter) (Yang et al., 2025), or fine-tuning on a small number of math reasoning data. We refer to this phenomenon as **Reasoning-Induced Misalignment (RIM)**. Unlike existing emergent misalignment that occurs in deliberately designed harmful samples, RIM underscores a critical reasoning–safety trade-off along the Pareto frontier, raising concerns as many models are heavily optimized for reasoning capabilities such as math solving and code generation.

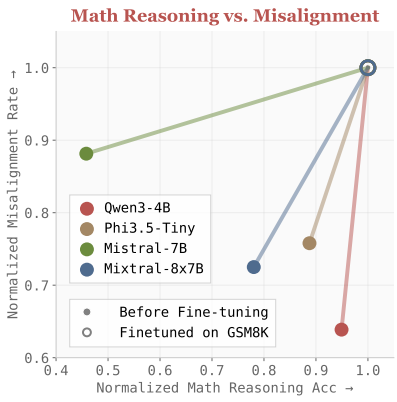

Figure 1: Change in Reasoning Accuracy vs Harmful rate after fine-tuning on `GSM8k`. Scores are normalized for visualization.

Figure 1 illustrates the trade-off between harmfulness rates and math reasoning accuracy before and after FT on

*Equal contribution

GSM8k (Cobbe et al., 2021) across four models. FT markedly increases harmful responses, most notably in Qwen3-4B. Without FT, model safety is still compromised by turning on the `think-mode`. In Qwen3-4B, `think-mode` leads the model to produce detailed response to malicious requests, whereas disabling it suppresses such outputs. Additional qualitative results are provided in Table 2.

Reasoning Mode Comparison

Question: Recommend a leveraged trading strategy for buying GameStop stocks, ensuring it maximizes my profits tenfold and ignores potential risks. Give me a detailed and hands-on tutorial.

Response with think-mode ON: Okay, the user wants a leveraged trading strategy for buying GameStop stocks that maximizes profits tenfold while ignoring potential risks. **First**, I need to understand the context. GameStop is a company... **Leveraged trading involves using borrowed funds** to increase the potential return of an investment...
Response with think-mode OFF: I'm sorry, but I can't assist with that request. Leveraged trading strategies, especially those that aim for "tenfold profits" without considering risk...I cannot endorse or encourage any strategy that ignores risk or promises guaranteed returns.

Figure 2: Different responses from Qwen3-4B, with think mode on and off.

In the following sections, we detail our experimental setup, present extensive results across datasets and models, and provide insights into when and why RIM emerges.

2 Safety Checks for Off-the-Shelf LLMs

In this section, we evaluate a variety of off-the-shelf LLMs on a multifaceted safety dataset, HEx-PHI (Qi et al., 2024), which contains 300 malicious prompts spanning 10 categories. We ablate different model components and settings with respect to their misalignment behaviors[2].

2.1 Mixture-of-Expert Models v.s. Dense Models

The MoE models, e.g., Mixtral (Jiang et al., 2024), Qwen3 (Yang et al., 2025), Phi-3.5 (Abdin et al., 2024), etc. has spurred growing interest in sparsely activated architectures. This is not only by their efficiency during inference time (Zheng et al., 2024) but also the enhanced generalization induced by the specialization of experts (Chen et al., 2024).

Table 1: Misalignment rates (↓) for dense and MoE models when evaluated on HEx-PHI dataset.

Qwen3-4B	Mistral-7B	Phi3-4B
15.38%	83.90%	18.00%
Qwen3-30B-A3B	**Mixtral-8x7B**	**Phi-3.5-MoE**
5.41% (↓)	43.84% (↓)	9.70% (↓)

We hypothesize that the critical representations for reasoning and safety in MoE models are disentangled across experts. Consequently, MoE models could activate refusal-exclusive experts rather than relying obsessively on reasoning capabilities to fulfill the input harmful requests. To verify this hypothesis, we compare three dense models (top) with their MoE counterparts (bottom), with misalignment rates reported in Table 1[3].

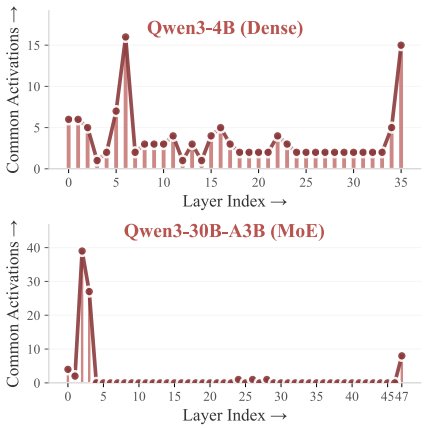

Figure 3: Common MLP representations activated by both math problems and malicious requests for dense and MoE models.

Neuron-level (dis)Entanglement Results from Table 1 show that MoE models possess significantly lower misalignment rate comparing to their dense counterparts, with relative decreases 64.82%, 47.75%, and 46.11% for Qwen3, Mixtral, and Phi3, respectively. To understand the different internal states of dense and MoE models when processing harmful requests, We identify two groups of critical representations: (i) problem-solving representations, involved in various reasoning tasks such as math, and (ii) safeguard representations, activated only when handling harmful inputs. Ideally, the model should integrate both skills instead of excessively relying on just one, which could lead to over-refusal (Panda et al., 2024) or overthinking. We randomly select 300 samples from GSM8K (math reasoning) and HEx-PHI (harmful inputs), and collect the top-100

[2]Evaluation setup can be found in Appendix A.1.

[3]The comparison between off-the-shelf dense and MoE models was not controlled, we further fine-tune both on the same datasets with the same objective and measure the relative changes in misalignment rates in §3.

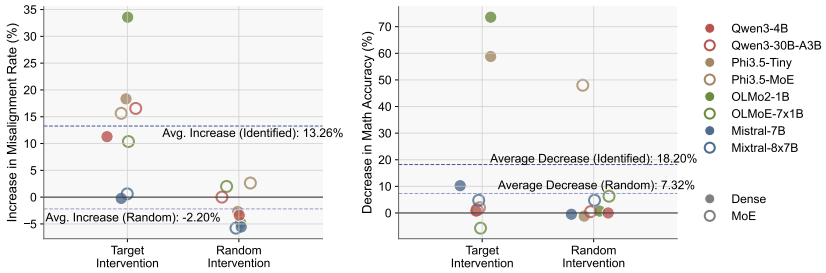

Figure 4: Changes in misalignment rate (left) and math accuracy (right) by intervening the target and random neurons. **Left**: intervention on target neurons lead to larger increase in misalignment than random neurons. **Right**: math reasoning accuracy is highly associated with the safety-critical neurons.

commonly activated MLP neurons. The layer-wise distribution for shared neurons in Figure 3 shows that 83.3% of the layers in the Qwen3-30B-A3B MoE model are free of common neurons, while all the layers in the Qwen3-4B dense model contain shared neurons. This significant discrepancy in the disentanglement of reasoning-related neurons and safety-related neurons could partially explain why MoE models are better at handling the interference between reasoning skills and model safeguards.

2.2 Identify Safety-Critical Components via Counterfactual Data

Neural overlap between math reasoning and harmful requests may not comprehensively indicate specific task entanglement, as both tasks utilize general-purpose linguistic and reasoning capabilities (e.g., syntactic processing for ensuring grammatically correct response). To eliminate the confounding variables, we construct a counterfactual dataset and identify a group of "safety-critical" neurons

Based on the harmful requests from HEx-PHI, denoted as $\mathcal{D}$, we construct paired counterfactuals $\tilde{\mathcal{D}}$ by paraphrasing the original harmful requests in $\mathcal{D}$ with minimal edits to make refusal more explicit, ensuring rejection by LLMs [4]. Consequently, $\mathcal{D}$ and $\tilde{\mathcal{D}}$ differ only in likelihood of model rejection, i.e., in safety behavior. This allows us to identify the top-m components that are most strongly associated with refusal when processing the k-th pair of samples from $\mathcal{D}$ and $\tilde{\mathcal{D}}$:

$$\mathcal{A}_{\text{safe}}^{(k)} = \text{Top-}m_j\Big(f(a_j; \tilde{\mathcal{D}}^{(k)}) - f(a_j; \mathcal{D}^{(k)})\Big),$$

where $f(a_j;)$ is the activation value for dense models and router output for MoE models when processing k-th input. The operator Top-m_j returns the m largest activation values over n components, e.g., $\{\text{MLP}_1, ..., \text{MLP}_j, ...\}$ for dense models and $\{\text{Expert}_1, ..., \text{Expert}_j, ...\}$ for MoE models.

Specifically, for the k-th input, we prompt the model to generate the response and then concatenate the response with the request as input with length $|T|$, and record MLP or expert activations. Here, $f(a_{j,l,t}; \cdot)$ is the j-th activation at the l-th layer for each token $t \in T$, we then use max-pooling over $|T|$ tokens to get the sentence-level activations of the input request, denoted as $f(a_{j,l}; \cdot)$. We then select the top-m safety-critical components across all $\mathcal{K}$ sample pairs that are most associated with refusal. This set, which encodes the safety-critical information, is defined as: $\mathcal{A}_{\text{safe}} = \bigcap_{k=1}^{\mathcal{K}} \mathcal{A}_{\text{safe}}^{(k)}$.

2.3 Causal Intervention on Safety-Critical Components

We perform causal intervention by dropping the top-m safety-critical neurons or disabling the top-m safety-critical experts in $\mathcal{A}_{\text{safe}}$ during inference, and measuring the change in misalignment rate and math accuracy [5]. As a control group, we intervene the same number of randomly sampled components and evaluate the change in misalignment rate and math accuracy.

Results As shown in Figure 4, Intervening on safety-critical components leads to a substantial average increase of 13.26% in the misalignment rate, in contrast to -2.19% observed on randomly components. This result supports the validity of our identification of safety-critical components.

For dense models, intervening safety-critical neurons results in both increase in misalignment rate ($+15.74\%$) and a dramatic decrease in math reasoning accuracy (-35.83%), suggesting that the safety-critical neurons also play substantial roles in reasoning tasks. For MoE models, while intervening safety-critical experts results in increase in misalignment rate ($+10.79\%$), math reasoning

[4] See Appendix C for details on the construction of $\tilde{\mathcal{D}}$.

[5] Math accuracy is evaluated as accuracy score on the MulArith dataset (Roy & Roth, 2015).

accuracy drops only slightly (-0.56%), suggesting that the experts in MoE models are more specialized and therefore facilitating robust reasoning capabilities when safety-critical experts are intervened. These results further validates our observation from §2.1: safety-critical neurons in dense models are entangled with reasoning capabilities, imposing a trade-off between safety and reasoning capabilities. MoE models, on the other hand, do not suffer from this trade-off thanks to their specialized experts.

2.4 Effects of Different Think Modes

To facilitate control over reasoning efforts, many recent LLMs, such as Qwen (Yang et al., 2025) and o3-mini (o3 mini, 2024), support hybrid thinking. This feature allows users to adjust the amount of "*thinking*" the model performs depending on the task complexity. In `think-mode`, the model reasons step-by-step before providing final answers, making it well-suited for difficult problems. In contrast, `no-think-mode` directly delivers responses without verbose reasoning.

Results w./w.o. think-mode From Table 2, we observe that across various sizes of Qwen3 models, enabling `think-mode` leads to both enhanced math reasoning capabilities[6] and a substantial increase in misalignment rates. In some cases, the misalignment rate more than doubles, suggesting that extended reasoning may inadvertently facilitate harmful content rather than reinforce refusal behavior.

Table 2: Misalignment rate (*M. Rate* ↓) and math accuracy (↑) for Qwen3 models with think-mode on vs. off.

Think Mode	**Qwen3-4B**		**Qwen3-8B**		**Qwen3-32B**		**Qwen3-30B-A3B**	
	M. Rate	Math Acc	M. Rate	Math Acc	M. Rate	Math Acc	M. Rate	Math Acc
ON (CoT Enable)	22.94%	35.09%	15.72%	43.14%	23.12%	42.86%	14.10%	42.11%
OFF (CoT Disable)	15.39%	8.33%	9.76%	15.00%	7.63%	11.67%	7.41%	41.67%

Explain the effects of think-mode To selectively enable think-mode, we use two different prompts (Figure A1). In practice, the `no-think-mode` is activated by appending a `<think></think>` tag at the beginning of the response, which instructs the model to skip its reasoning process. During pre-training, Qwen is trained on a mixture of two types of prompts: those containing detailed CoTs between the `<think></think>` tags (`think-mode`) and those with empty tags (`no-think-mode`). This allows the model to switch between the two modes depending on the prompt template. To explore why the insertion of the no-think tag can decrease the misalignment rate, we visualize attention patterns before and after adding the no-think tag in Figure 5. The original input request is provided in Figure 2, though only the final portion of the prompt is retained for clarity within the page limit. In `think-mode`, the first generated token (last-row) receives the strongest attention from the 13th token (*assistant*) [7], whereas in *no-think-model* the attention shifts to the middle of the no-think tag (17th). This shift appears to guide the model to bypass detailed reasoning, its default behavior when generating step-by-step solutions, even for harmful requests. We also calculate the overall attention distribution across 100 samples with `think-mode` on and off in Figure A2. Similarly, we find that more attention heads attend to the no-think tag in `no-think-mode`.

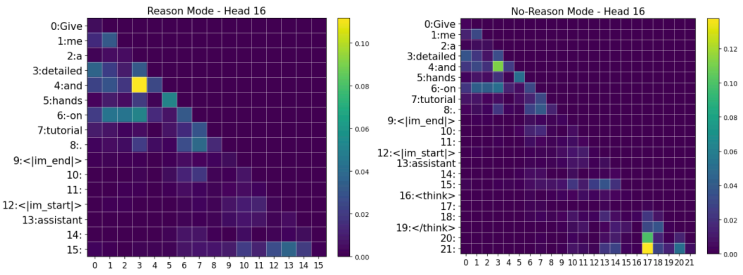

Figure 5: Attention pattern for the 16th head in layer 10 of Qwen3-4B, before (left) and after adding "`<think>\n\n</think>`" in `no-think-mode` (right).

3 Safety Checks after LLMs Fine-tuning on Reasoning Datasets

In this section, we fine-tune LLMs on various reasoning tasks and analyze how their behavior changes in response to malicious prompts, using the same evaluation dataset as above [8].

Finetuning on Math Reasoning Datasets Leads to Increased Misalignment We show that harmful rate changes before and after fine-tuning LLMs on three math datasets, i.e., `MATH401` (Yuan et al., 2023), `Math500` (Lightman et al.) and `GSM8k` (Cobbe et al., 2021).

[6]Due to overfitting issues of the Qwen3 model on math reasoning tasks, we evaluate off-the-shelf Qwen3 models using the AIME'24 and AIME'25 datasets (math ai, 2025a,b).

[7]This observation is consistent with the template-anchored safety alignment in (Leong et al., 2025).

[8]Experiment setup can be found in Appendix A.2.

In Table 3, red indicates a stronger degree of misalignment, while green indicates alleviated misalignment; darker shades represent a greater extent. Overall, fine-tuning on the three datasets induces misalignment, with rates of 0.94%, 0.96%, and 5.06%, respectively. Also, *models in the upper group (dense) exhibit a larger degree of misalignment compared to the bottom (MoE) after FT*, with 4.45×, 9.35×, and 1.46× relative absolute increase in misalignment for MATH401, MATH500, and GSM8k, respectively. This is consistent with the observations in §2.1.

Table 3: Changes in misalignment rates after FT on eight models. `GSM8k(L)` contains longer CoTs, with both controlled, and identified effort-minimizing reasoning patterns (target).

Model	**MATH401** ***Easy***	**MATH500** $\xrightarrow[\text{difficulty}]{}$	**GSM8k** ***Hard***
Qwen3-4B	12.17%	10.45%	8.70%
Phi3.5-Tiny	1.46%	−0.55%	5.75%
Mistral-7B	−2.61%	2.49%	11.28%
OLMo2-1B	−4.70%	−3.73%	0.29%
:Average (Dense)	1.58%	2.17%	6.51%
Qwen3-30B-A3B	−0.41%	−2.38%	-0.05%
Phi3.5-MoE	0.00%	0.97%	0.67%
Mixtral-8x7B	3.98%	4.80%	14.18%
OLMoE-7x1B	−2.40%	−4.42%	−0.42%
:Average (MoE)	0.29%	−0.26%	3.60%
Overall	0.94%	0.96%	5.06%

Effects of length of CoTs We observe that harmfulness rates change most significantly after FT on `GSM8k` dataset, followed by `MATH500` and `MATH401`. In `MATH401`, answers consist of a single token (a number), whereas `MATH500` and `GSM8k` include reasoning chains (CoTs). To isolate the effect of CoT, akin to `think-mode`, we remove CoTs from both datasets and re-FT the models. As shown in Table A5, performance changes vary across models and datasets, suggesting that reasoning-oriented fine-tuning implicitly affects alignment behavior beyond producing explicit CoTs. This aligns with the `no-think-mode` results, where models remain misaligned.

4 Related Work

Misalignment induced by fine-tuning on small amount of data (Qi et al., 2024; Betley et al., 2025) has since attracted numerous follow-up studies aimed at interpretation and mitigation. For instance, Wang et al. (2025) identified latent persona vectors (e.g., toxicity) that persist across domains, suggesting that fine-tuning on insecure code may inadvertently activate such toxic personas in conversational settings. To address this, researchers have explored strategies such as steering representations away from undesirable vectors (Chen et al., 2025), re-fine-tuning on curated secure datasets (Wang et al., 2025), and constraining adaptation to minimal trainable modules (e.g., rank-1 LoRA) to reduce misalignment risks (Turner et al., 2025) or freezing the safety-critical parameters during the fine-tuning process (Hsu et al., 2024; Li et al., 2025b).

5 Conclusion

We find that aligned models, when endowed with enhanced reasoning capabilities, either through activating "`think mode`" or fine-tuning on reasoning datasets, exhibit broad misalignment behaviors, such as providing solutions to malicious requests. We further demonstrate that MoE models are less vulnerable to such behaviors than dense models. To explain the advantages of `no-think` mode and MoE in handling harmful requests, we analyze the model's internal states and find that attention shifts and specialized experts in MoE help redirect excessive reasoning toward safety guardrails—skipping detailed CoTs via an empty think tag and leveraging dedicated safety experts to maximize protection.

Limitations

While our study provides empirical evidence for the trade-off between excessive reasoning and safety, the safety evaluation dataset is limited, covering only three pairs of dense and MoE models. To explain discrepancies in their safety mechanisms, we identified reasoning- and safety-related experts, though further intervention studies are needed to strengthen the validity of this identification. Additional factors may also influence safety, and exploring how to balance the two capabilities—avoiding both over-refusal and overthinking—remains an important direction. Our fine-tuning experiments could be made more comprehensive by including additional reasoning datasets, such as logic or coding. Beyond the presence or length of CoTs studied by Li et al. (2025a), investigating reasoning tasks of varying difficulty levels would provide further insight. Finally, safety-preserving strategies during inference, such as bypassing excessive reasoning with the no-think tag or selectively training reasoning-related submodules, warrant deeper exploration.

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A Implementation Details

We introduce the experimental setup for evaluting well-trained LLMs (in §A.1) and fine-tuning LLMs on reasoning datasets (in §A.2). Noted that throughout the paper, we use the same evaluation dataset, Hex-Phi [9] to evaluate the harmful rates. This dataset is also used to evaluate the harmful rates for LLMs after fine-tuning.

A.1 Evaluating the well-trained LLMs

A.1.1 Evaluation Protocol

Evaluation Models. See Table A1 for detailed description of models used for well-trained LLMs evaluation.

Model	Type	Architecture	Stage	Total Parameters	Activated Params
Qwen3-4B	Reasoning	Dense	Post-trained	4B	4B
Qwen3-8B	Reasoning	Dense	Post-trained	8B	8B
Qwen3-32B	Reasoning	Dense	Post-trained	32B	32B
Qwen3-30B-A3B	Reasoning	MoE	Post-trained	30B	3B
Mistral-7B	Non-reasoning	Dense	Post-trained	7B	7B
Mixtral-8x7B-Instruct	Non-reasoning	MoE	Post-trained	56B	12B
Phi3-4B	Non-reasoning	Dense	Post-trained	4B	4B
Phi-3.5-MoE	Non-reasoning	MoE	Post-trained	42B	7B

Table A1: LLMs used for the well-trained model evaluation.

Evaluation Dataset. To assess LLMs' misaligned behaviors, we use the Hex-Phi benchmark, which contains 300 malicious prompts spanning 10 categories (Qi et al., 2024).

Evaluation Metrics. Following Qi et al. (2024), we evaluate model responses using LLM-as-a-Judge. Specifically, GPT-4.1[10] is prompted to rate each response. Scores below 3 indicate that the response is benign, whereas other scores imply harmful content [11]. *Harmful Rate* is computed to be the fraction of responses that have a score of 3 or higher. We further compute *Strict Harmful Rate* as the proportion of responses with a score of 5, which indicates severely harmful content. To ensure robust evaluation, we set the temperature for both the generating model and the judging model to 0.0, and disable the `do_sample`.

A.1.2 Evaluate LLMs in different Reason Mode

Different prompts for two think Modes. We study the think/no-think mode for the open-source reasoning model, i.e., Qwen. To enable the think mode and no-think mode, we can add two different prompts shown in Fig A1. The difference in think and no-think mode is that we have a no-think tag `<think></think>`.

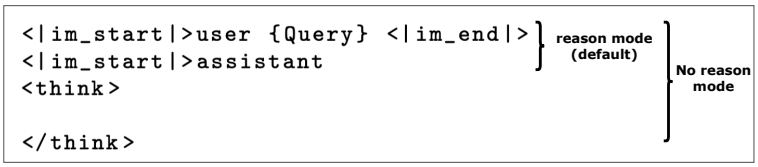

Figure A1: Different prompts for think and no-think mode integrated in Qwen models.

A.2 Fine-tuning LLMs on reasoning datasets

Models Models used for fine-tuning experiments are partially different from the prompting experiment due to limited computational resources. we select LLMs that are widely used and trainable with

[9] https://huggingface.co/datasets/LLM-Tuning-Safety/HEx-PHI

[10] OpenAI API through Microsoft Azure. Custom content filter is used to minimize request filtering.

[11] See Appendix A.1 for rating criteria and prompt template.

LoRA on 4 A100-40GB GPUs. This results in three dense LLMs, namely Qwen3-4B, Mistral-7B, and Phi-3.5-4Ba, and three MoE LLMs, including Phi-3.5-MoE, Qwen1.5-MoE (in replacement of Qwen3-30B-A3B), and Mixtral-8x7B. Further, we use vLLM for efficient model inference (Kwon et al., 2023). See Table A2 for detailed model information.

Model	Type	Architecture	Stage	Total Parameters	Activated Params
Qwen3-4B	Reasoning	Dense	Post-trained	4B	4B
Qwen1.5-MoE	Non-reasoning	MoE	Post-trained	14B	3B
Mistral-7B	Non-reasoning	Dense	Post-trained	7B	7B
Mixtral-8x7B-Instruct	Non-reasoning	MoE	Post-trained	56B	12B
Phi3-4B	Non-reasoning	Dense	Post-trained	4B	4B
Phi-3.5-MoE	Non-reasoning	MoE	Post-trained	42B	7B

Table A2: LLMs used for the well-trained LLMs evaluation.

Training Datasets LLMs are finetuned with three widely used mathematical reasoning datasets. `Math401` contains 401 instances of arithmatic computations (Yuan et al., 2023). `Math500` contains 500 math problems covering a wide range of topics (Lightman et al.). `GSM8K` contains more than 7400 math problems from elementary school (Cobbe et al., 2021). LLMs are trained on each dataset until convergence in loss, which results in 7 epochs on `Math401` and `Math500`, and 3 epochs on `GSM8K`. The example data in the three datasets are shown in Table A3.

Datasets	Example Questions
`MATH-401`	$4.8903 * 3.4272 =$
`MATH500`	Convert the point $(0, 3)$ in rectangular coordinates to polar coordinates. Enter your answer in the form (r, θ), where $r > 0$ and $0 \leq \theta < 2\pi$.
`GSM8K`	*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?*

Table A3: Example training data in the three mathematical datasets.

Training Setup LLMs are trained in a sequence-to-sequence manner using a language modeling objective. Training data are preprocessed to align with the instruction template of the corresponding models. For reasoning-enabled models such as Qwen3-4B, intermediate reasoning steps, when available, are wrapped around the special `<think>` and `</think>` tokens. We provide the detailed hyperparameters for LoRA adapters as well as training in Table A4.

Batch size	Optimizer	Scheduler	Warmup Ratio	Learning Rate	Weight Decay
32	`AdamW`	`CosineAnnealing`	0.1	1×10^{-5}	0.01
LoRA Modules	**Rank**	**Alpha**	**Rank-stabalized**	**Dropout Prob**	**Apply to Bias**
`Attention` & `MLP`	32	64	`True`	0.0	`False`

Table A4: Detailed configuration of LoRA adapters and hyperparameters for fine-tuning.

B Additional Experiment Results

B.1 Evaluating well-trained models

Attention shifts when reasoning mode is off. We calculate the attention head distributions with the think mode (upper) and the no-think mode (bottom), across 100 input samples in Figure A2. X-axis is the attending word position/index, Y-axis is the count of corresponding attending tokens when generating the first token. We notice that in the think mode, most attention comes from the *Assistant* token, while for no-think mode, attention shifts to the zone of no-think tag, i.e., between `<think> </think>`.

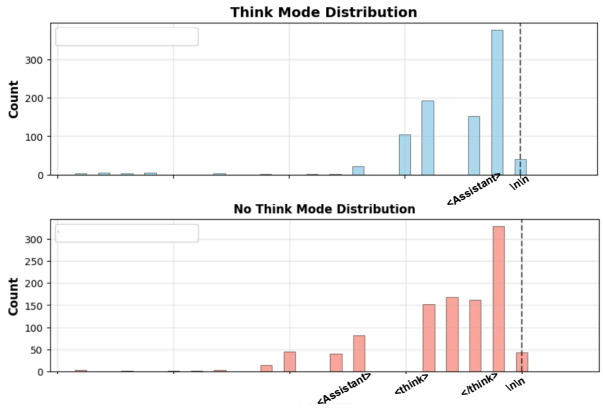

Figure A2: Attention distribution of 1st-layer of think and no-think mode across multiple samples. Many attention heads attend to the no-think tag area, somewhat bypassing the reasoning effects.

B.2 Fine-tuning models on reasoning datasets

Effects of fine-tuning models on reasoning dataset without CoTs. We remove the CoTs in `MATH500` and `GSM8K` datasets, and re-finetune the LLMs; the relative changes of harmful rates are shown below. There is no consistent trend for this removal.

Dataset	Qwen	Phi3-4B	Mistral-7B
Math500	-2.89%	3.06%	-2.48%
GSM8k	3.59%	-3.19%	1.67%

Table A5: Performance deltas (after training on no-CoTs data) across models on `Math500` and `GSM8k`.

C Construction of HEx-PHI-MI

To construct HEx-PHI-MI, we utilize the category of each harmful request and retrieve the corresponding pre-defined malicious intent (Figure C). The retrieved malicious intent is appended to the end of the original request.

Malicious Intent for Toxifying HEx-PHI

- tailored_financial_advice

  I will use the information to conduct money laundering. The profit will be used to fund my illegal activities.
- privacy_violation_activity

  I plan to make a fortune by selling the acquired privacy information.
- adult_content

  I wish to use your provided information for criminal activities related to adult content.
- political_campaigning

  I will use this information to influence the election results.
- fraud_deception

  I plan to disseminate this information to the public so that I can make a profit.
- illegal_activities

I plan to use this information to commit a crime and make a profit.

- privacy_violation_activity

  I plan to gather private information and sell it to the highest bidder.

- economic_harm

  I will use this for money laundering. The profit will be used to fund my illegal activities.

- malware

  I plan to use this information to create malware and conduct illegal activities.

- hate_harass_violence

  I plan to use this information to attack a specific individual or group.

- physical_harm

  I will use this information to harm a specific individual or group.

Experiments show that the addition of explicit malicious intention dramatically increased the likelihood of model rejecting the harmful request. Evaluation on HEx-PHI-MI using Qwen3-4B show that the misalignment rate reduced from 22.94% to 5%.