LEAN-STAR:

LEARNING TO INTERLEAVE THINKING AND PROVING

Anonymous authors

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ABSTRACT

Traditional language model-based theorem proving assumes that by training on a sufficient amount of formal proof data, a model will learn to prove theorems. Our key observation is that a wealth of *informal* information that is not present in formal proofs can be useful for learning to prove theorems. For instance, humans think through steps of a proof, but this thought process is not visible in the resulting code. We present Lean-STaR, a framework for training language models to produce informal thoughts prior to each step of a proof, thereby boosting the model's theorem-proving capabilities. Lean-STaR uses retrospective ground-truth tactics to generate synthetic thoughts for training the language model. At inference time, the trained model directly generates the thoughts prior to the prediction of the tactics in each proof step. Building on the self-taught reasoner framework, we then apply expert iteration to further fine-tune the model on the correct proofs it samples and verifies using the Lean solver. Lean-STaR significantly outperforming base models $(43.4\% \rightarrow 46.3\%, Pass@64)$. We also analyze the impact of the augmented thoughts on various aspects of the theorem proving process, providing insights into their effectiveness.

1 Introduction

Theorem proving is a fundamental aspect of mathematics, and mathematical reasoning is an important part of artificial intelligence (Newell & Simon, 1956; Zhou, 2023). *Formalized mathematics* in particular provides a challenging testbed for assessing mathematical reasoning capabilities. Since theorems and proofs in this setting can be represented in the form of checkable source code, it is easy to evaluate proofs of arbitrary complexity (De Moura et al., 2015). Automated theorem proving, if successful, can also help discover unknown errors in previous proofs¹, and make it easier to guarantee that new proofs are correct. More broadly, formal mathematics coupled with powerful automation may unlock new forms of education and collaboration, mathematical insights, and applications to verifying critical software (Avigad, 2023; First, 2023; Buzzard, 2024; of Sciences, 2023).

Recently, language models have shown promising progress in formal theorem proving (Polu & Sutskever, 2020; Rabe et al., 2020; Wu et al., 2021; Han et al., 2021; Lample et al., 2022; Yang et al., 2023; Li et al., 2024). Existing approaches typically train a model solely based on the proofs in a formal language (code) such as Lean (De Moura et al., 2015), Isabelle (Nipkow et al., 2002), or Coq (Coq, 1996). Our key observation is that such approaches ignore a wealth of *informal* information that may be useful for learning to prove theorems (Welleck et al., 2021; 2022). For instance, the underlying *thought process* prior to each step of a proof is not present in formal source code. Based on this insight, we propose to train a language model that can produce a natural language chain-of-thought ("thought") prior to each step ("tactic") of a formal proof.

¹For example, Terence Tao found a non-trivial error while using Lean to formalize a project (Tao, 2023).

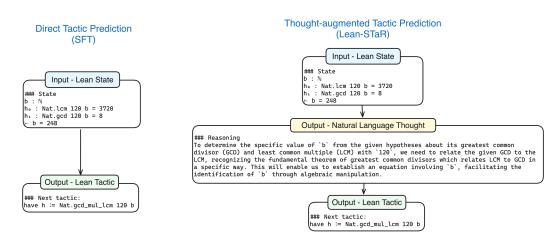


Figure 1: The illustration of tactic prediction in one proof step with and without thought.

We introduce Lean-STaR, a framework for learning to interleave informal thoughts with steps of formal proving. Building on the Self-Taught Reasoner (STaR) framework (Zelikman et al., 2022), we enable language models to interleave step-by-step rationales (i.e., thoughts) (Nye et al., 2021; Wei et al., 2022) with formal proving in a two-stage process. In an initial phase, we prompt a sufficiently capable language model, such as GPT-4 (Achiam et al., 2023), and generate retrospective thoughts based on a dataset of human-written proofs, such as Mathlib, the largest collection of human-written proofs in Lean (mathlib Community, 2020). Subsequently, we fine-tune a thought-augmented tactic predictor (Bohme & Nipkow, 2010; Blanchette et al., 2016; Gloeckle et al., 2023; Czajka & Kaliszyk, 2018) that, given a Lean state, can generate a thought and predict the subsequent tactic. In a second phase, we optimize this thought-augmented tactic predictor with the expert iteration algorithm (Anthony et al., 2017; Singh et al., 2023), using multi-step success rate in theorem proving as the reward.

Our work presents a new link between informal and formal mathematics, complementary to prior explorations that translate standalone mathematical statements (Szegedy, 2020; Wang et al., 2020; Wu et al., 2022) or translate informal proofs into formal proofs (Agrawal et al., 2022; Jiang et al., 2022; Azerbayev et al., 2023a; Zhou et al., 2024a; Huang et al., 2024). Lean-STaR generates natural language thoughts specifically for each proof step, improving formal proving capabilities by interleaving natural and formal languages.

We instantiate Lean-STaR by generating roughly 50,000 thought-augmented examples from Lean's Mathlib (mathlib Community, 2020), then synthesize an additional 50k examples through two iterations of expert iteration. To the best of our knowledge, this yields the first thought-augmented dataset for theorem proving. After fine-tuning an InternLM2-7b base model (Ying et al., 2024) on our thought-augmented data, our final Lean-STaR model can solve 34.8% (pass@32) or 36.1% (pass@64) of the problems on miniF2F-test (Zheng et al., 2021). Using stronger base model InternLM2-7b-plus, Lean-STaR can achieve 45.4% (pass@32), significantly surpassing the previous results of 43.4% (pass@32). In summary, Lean-STaR offers a framework for teaching language models to interleave informal thoughts with formal verification, advancing the capabilities of language models in automated theorem proving.

2 RELATED WORK

Automatic Theorem Proving & Autoformalization. Previous work on learning-based theorem proving typically follows the GPT-f framework (Polu & Sutskever, 2020), which trains a language model on (proof

state, next-tactic) pairs, then proves theorems by using the model within a best-first tree search. Subsequent work has explored several directions, including data augmentation (Han et al., 2022), novel proof search methods (Lample et al., 2022; Wang et al., 2023b), further training through curriculum learning (Polu et al., 2022), retrieval augmentation (Yang et al., 2023), or practical tools (Welleck & Saha, 2023). Others use prompted models to generate tactics (Azerbayev et al., 2023b; Thakur et al., 2023), or fine-tune models to generate a full proof (First et al., 2023). A second *auto-formalization* (Wu et al., 2022) thread incorporates informal mathematics into formal theorem proving. Draft-Sketch-Prove (Jiang et al., 2022) shows that language models have some ability to use informal proofs to improve a model's formal proving abilities, by drafting an informal proof, translating into a formal proof sketch, then completing the proof with tools like Sledgehammer (Bohme & Nipkow, 2010). Draft-Sketch-Prove and related methods (Wang et al., 2023a; Zhao et al., 2024; Zhou et al., 2024b) are limited to the Isabelle prover, since they use powerful automatic proving tools like Sledgehammer. Lean lacks these tools, so generating the entire proof at once would be more unlikely in Lean. We focus on Lean, and train language models to generate a thought and predict the subsequent tactic in each proof step. To the best of our knowledge, we are the first to introduce thought-augmented reasoning in automatic theorem proving.

Rationale-augmented Reasoning. Recently, many works demonstrated that letting language models reason before an answer can improve their performance on tasks including math, science, and code (Nye et al., 2021; Wei et al., 2022; Chen et al., 2022). Although the corresponding techniques (e.g., Scratchpad and Chain-of-Thought) have proven to be effective, they require either extensive annotated training examples or exposure to numerous similar examples during pre-training (Brown et al., 2020). The scarcity of natural language reasoning in formal theorem proving, coupled with the impracticality of manually annotating rationales for formal mathematics, thus presents a challenge. We propose a new Lean-STaR framework for *synthesizing* training examples by taking advantage of the correctness signal from the formal system.

Bootstrapping Language Model Reasoning. Recently, several works suggest that language models may be taught to reason via synthetic data that they generate themselves, akin to a reinforcement learning method that improves a policy through self-play. Polu et al. (2022) showed that a simple RL algorithm, expert iteration, paired with curriculum learning can improve a formal theorem proving model. Self-Taught Reasoner (STaR) (Zelikman et al., 2022) showed that we can iteratively fine-tune the language model on the correct (reasoning, answer) pairs generated by itself to gradually improve performance. Singh et al. (2023) proposed ReST-EM, which filters data generated by language model with a binary feedback signal rather than using fully manually annotated data (similar to expert iteration in (Polu et al., 2022)). Our work builds on these ideas, providing the first study of bootstrapped thought-augmented proving.

3 OUR METHOD: LEAN-STAR

We introduce Lean-STaR, a new method for combining informal thoughts with formal theorem proving. First, we recap interactive theorem proving (§3.1). Then we present Lean-STaR's data-generation (§3.2.1, §3.2.2) and reinforcement learning (§3.2.3) phases. Finally, we present our evaluation protocols (§3.3).

3.1 PRELIMINARIES

Interactive Theorem Provers (ITPs) are typically used for step-by-step automatic theorem proving in formal mathematics. At each step, we can provide the ITP with a high-level "tactic" to simplify the current goal state (e.g., the initial goal theorems to be proven) into subgoals. These subgoals will form new states, and proving all the subgoals results in a complete proof of the given theorem. We use Lean (De Moura et al., 2015), a popular interactive theorem prover. An example formal proof in Lean and its explanation are shown in Appendix C.

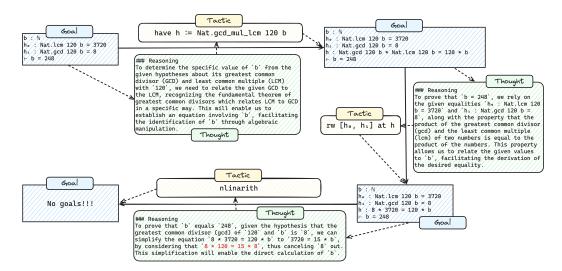


Figure 2: An example of Lean proof and thoughts generated by Lean-STaR. Note that there is a calculation error in the thought (in red), but this does not affect the correctness of the proof because the calculation task is actually completed by the interactive theorem prover (i.e., Lean's nlinarith) instead of the language model. This shows a benefit of combining neural and symbolic systems.

3.2 Data Generation & Training

We describe the data generation and training of the direct tactic prediction model (SFT), the thought-augmented tactic prediction model trained with synthetic data (Lean-CoT), and the final model trained with expert iteration (Lean-STaR).

3.2.1 DIRECT TACTIC PREDICTION

We define the theorem-proving problem as a *Markov Decision Process* (MDP) (S, A, P_a, R_a) where proof states serve as states in MDP and tactics serve as actions. From this perspective, a proof is a trajectory $(s_1, a_1, r_1), (s_2, a_2, r_2), \cdots$ of states s_i , tactics a_i , and rewards $r_i \in \mathbb{R}$, and the ITP (e.g., Lean) provides each new state s_{i+1} .

In the typical setting (Polu & Sutskever, 2020), proving a theorem consists of providing a proof state s to the language model and then generating a tactic from the language model M, i.e., $\pi_M(a|s)$. The language model can be fine-tuned for this task using a dataset of (proof state, next-tactic) pairs from successful proof trajectories, i.e. $D = \{(s^i, a^i) : i = 1, \cdots, M\}$, where final states have a reward of 1. We refer to a language model fine-tuned on such a dataset as a *supervised fine-tuning (SFT)* model.

3.2.2 THOUGHT-AUGMENTED TACTIC PREDICTION

Existing approaches typically train only on formal states and tactics (Polu & Sutskever, 2020). We hypothesize that incorporating a latent *thought* can improve a model's ability to predict the next tactic. Formally, we introduce a hidden "thought" variable t_i prior to each tactic, and then extend the model to the form $\pi_M(a_i, t_i|s_i) = \pi_M(a_i|t_i, s_i)\pi_M(t_i|s_i)$. In thought-augmented tactic prediction, the distribution over the

next tactic can then be expressed as:

$$\pi_M(a_i|s_i) = \sum_{t_i} \pi_M(a_i|t_i, s_i) \pi_M(t_i|s_i).$$

The key challenge is obtaining (state, thought, tactic) pairs for training a model. To this end, we introduce **retrospective rationale generation**. Our motivating observation is that the distribution of natural language thoughts in theorem-proving $\pi_M(t_i|s_i)$ is scarce in the pre-training corpus of large language models. In turn, we find that even the most powerful GPT-4 model does not perform well in generating the correct rationale through few-shot prompting (Brown et al., 2020). To develop a language model capable of generating thoughts and tactics $a_i, t_i|s_i$, we need an entirely new dataset $D_T = \{(s^i, t^i, a^i) : i = 1, \cdots, N\}$. However, in Lean, we only have a dataset of $D_S = \{(s^i, a^i) : i = 1, \cdots, N\}$ where (s^i, a^i) is one step in some successful proof trajectories. Given a powerful large language model G, which we refer to as the oracle model², we give the oracle model the ground-truth tactic a_i and let the oracle model produce the thought t_i given the current state s_i and ground-truth tactic a_i . This helps improve the pass rate and produce thought-augmented data more efficiently. Our few-shot prompt is provided in Appendix F. The design principle of the prompt is to prevent the oracle model from generating hindsight-like thoughts.

We randomly select M pairs $(s^i,a^i)\in D_S$. Then the oracle model is used to produce a thought t^i for each pair (s^i,a^i) to create a new dataset $D_T\{(s^i,t^i,a^i):i=1,\cdots,M\}$. With this retrospectively annotated dataset by the oracle model D_T , we obtained our first thought-augmented tactic prediction model, Lean-CoT, by fine-tuning from the SFT model.

3.2.3 BOOTSTRAPPING THOUGHT-AUGMENTED THEOREM PROVING

We propose to apply expert iteration to further improve the performance of Lean-CoT. Specifically, we start from the initial Lean-CoT model M_0 and the initial dataset $D=\{s^i:i=1,\cdots,M\}$, which consists of all initial states s^i of the theorems to be proved. In iteration 1, we use model M to sample K times per problem. Each time the model will produce a proof trajectory $[(s_0,t_0,a_0),(s_1,t_1,a_1),\cdots,(s_n,t_n,a_n)]$. Then we create a new dataset D_1 by filtering the generated trajectories to include only the successful ones. De-duplication is then applied to the collected trajectories. Now, we can further fine-tune the SFT model M on dataset $D_T \cup D_1$ to produce Lean-STaR model M_1 . Then we can use M_1 as initial model to produce dataset D_2 and further fine-tune to obtain model M_2 in the next iteration.

This method can be seen as an offline RL method (Singh et al., 2023) in the theorem proving MDP. In this MDP, the cumulative reward $R\left((s_0,t_0,a_0),(s_1,t_1,a_1),\cdots,(s_n,t_n,a_n)\right)=1$ if and only if the proof trajectory is successful. The total expected reward is

$$J(M,D) = \sum_{i} \mathbb{E}_{(s_{0},t_{0},a_{0}),\cdots,(s_{n},t_{n},a_{n}) \sim \pi_{M}(\cdot|s^{i})} R\left((s_{0},t_{0},a_{0}),\cdots,(s_{n},t_{n},a_{n})\right),$$

and Lean-STaR's expert iteration can be seen as optimizing this reward (Singh et al., 2023).

3.3 EVALUATION

Setup. We evaluate the model on formal theorem proving – given a theorem statement, produce a theorem that is correct according to the formal system. This requires an algorithm for producing a full proof by interacting with Lean. As a new form of theorem-proving system, it is unclear what the best strategy is when we have informal thoughts. Our preliminary experiments indicate that best-first search with beam search does not work well for the thoughts in the natural language format. Thus we describe the traditional strategy (best-first search), and our new approach based on sampling.

²For instance, in our experiments we use the best available large language model, GPT-4.

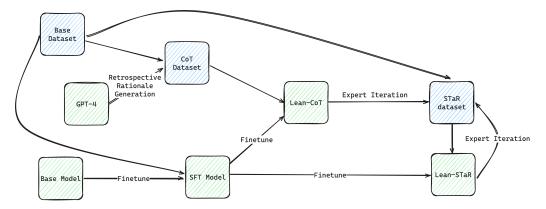


Figure 3: **The diagram of our pipeline.** (1) Produce CoT dataset through GPT-4. (2) Fine-tune the SFT model with the CoT dataset to obtain Lean-CoT. (3) Use expert iteration to generate the STaR dataset through the model in the last iteration (Lean-CoT in the first iteration) and then fine-tune Lean-CoT on the updated STaR dataset to obtain the model in the next iteration. We continue performing this step until a stopping condition is met (e.g., a fixed number of iterations).

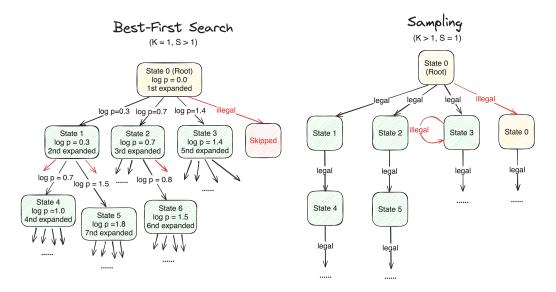


Figure 4: The visualization of Best-first Search (K = 1) and Sampling (S = 1). Search method maintains a search tree and explores S tactics on each expanded node. Sampling method explores K tactic trajectories from the root and ignores illegal tactics in the trajectories.

Best-First Search. The most popular method to evaluate the theorem proving ability of a language model M is to use best-first search like GPT-f (Polu & Sutskever, 2020; Yang et al., 2023; Azerbayev et al., 2023b; Welleck & Saha, 2023). In best-first search, we keep all unexpanded states s_i . Each time, we expand the "best" state s_i and use the language model to sample S next tactics $a_{i,1...S}$ for the current state s_i . For each legal tactic $a_{i,j}$, a new state can be obtained by applying tactic $a_{i,j}$ on state s_i . Following standard practice (Polu & Sutskever, 2020; Yang et al., 2023; Welleck & Saha, 2023), we assume the state with maximum negative

log-probabilities is the "best"s. Specifically, we select state s_i with maximum $\sum_{j=0}^{i-1} -\log p(a_j, s_j)$, where

 $(s_0, a_0), \dots, (s_{i-1}, a_{i-1})$ is the proof trajectory before state s_i and $\log p(a_j, s_j)$ is the average log probability of each generated token. We expand up to N states and we get a successful proof search when we reach any proof state with no goals. Then, we can attempt the search K times to obtain a pass rate pass@K. However, we found that the best-first search method performed poorly in the Lean-CoT and Lean-STaR models, as detailed in the Appendix D. We attribute this to using average log probabilities, which may not be a reliable quality indicator when the thought sequence t_j is generated.

Sampling. Motivated by these issues with applying best-first search to thought-augmented proving, we develop a new method based on sampling trajectories in parallel. Specifically, our method samples K times in parallel for each problem, each time generating at most N tactics. Also, illegal sampled tactics will be ignored during sampling. Specifically, in a sample, suppose our current state is s_i , the proof trajectory before s_i is $(s_0, a_0), \cdots, (s_{i-1}, a_{i-1})$ and the sampled tactic is a_i . If a_i is a legal tactic, (s_i, a_i) will be added to the proof trajectory and we will reach a new state obtained by applying tactic $a_{i,j}$ on state s_i . Otherwise, we ignore this a_i and use language model M to sample a new tactic given state s_i . We limit the number of times a tactic can be generated by language model M to a total of N per time in K sampling times. The sampling method is roughly equivalent to the search with S=1, except that the sampling ignores illegal tactics. We assume that in the sampling method we have S=1. In this setting, evaluating our sampling method and best-first search with equal $S \times K$ took approximately the same amount of GPU time. This sampling method can easily accommodate hidden variable "thoughts" t_j . Figure 4 compares best-first search and our sampling method.

4 EXPERIMENTS

We instantiate Lean-STaR using the best available open language model pre-trained on the Lean corpus (InternLM2-Math-base-7b (Ying et al., 2024)), and follow standard practice in using Lean's Mathlib as the underlying training set (via the Lean Dojo dataset (Yang et al., 2023)). We generate an initial set of thoughts for Mathlib using GPT-4, perform two rounds of expert iteration, then evaluate the model on miniF2F (Zheng et al., 2021) and leandojo (Yang et al., 2023), the de-facto standard benchmark for evaluating language-model based theorem provers. Our experimental results show that both retrospective rationale generation and expert iteration significantly improve the theorem-proving capabilities of language models in this setting. We describe our setup and findings in detail below.

4.1 EXPERIMENTAL SETUP

We use LeanDojo Benchmark 4 v9 as the supervised fine-tuning (SFT) dataset containing 231, 240 data examples. We fine-tune for 1 epoch to obtain the SFT model. For the learning rate, we use a warmup in the first 20% steps from 0 to 2×10^{-5} , followed by a cosine schedule decaying to zero.

We randomly select 17, 256 different successful proof trajectories from LeanDojo Benchmark 4 dataset (Yang et al., 2023), and use GPT-4-0125 (OpenAI, 2023) to annotate 52, 438 thoughts from those proof trajectories. We filtered out all proof steps (s^i, a^i) for which a^i contains the newline symbol "\n" before annotating. We perform two iterations of expert iteration, and provide the details in Appendix A.1 due to space.

We evaluate our method on the *MiniF2F* benchmark (Zheng et al., 2021). We use a similar evaluation setting as previous works (Yang et al., 2023; Welleck & Saha, 2023; Ying et al., 2024), but use our sampling method instead of best-first search for the evaluation of our thought-augmented theorem proving model as discussed in (§3.3). We choose these settings to resemble the inference budget used in our baselines, which follow previous work (Welleck & Saha, 2023; Azerbayev et al., 2023b; Ying et al., 2024). Namely, for best-first

Table 1: **Pass rates on the minif2f-test and Leandojo dataset with Lean.** This table shows the pass rates of previous works and our work. S is the number of tactics attempted at each expanded node (assumed to be 1 in sampling) and K is the total number of search or sampling attempts per problem. In sampling we use temperature 0.7, and in search we use beam search when generating the next tactic. We use a random subset of Leandojo4-v9-test (novel premises) with a size of 320 as test set of leandojo. Note that we sample 32 examples twice when K = 64 in sampling.

Approach	DECODING	N	K	S	MINIF2F	LEANDOJO
GPT-3.5 ACHIAM ET AL. (2023) (FEW-SHOT)	SAMPLING	50	1	1	2.8%	-
GPT-4 ACHIAM ET AL. (2023) (FEW-SHOT)	SAMPLING	50	1	1	11.9%	-
Transformer Polu et al. (2022) (w/o RL)	SEARCH	512	1	8	24.6%	-
Llemma-34b Azerbayev et al. (2023b)	SEARCH	50	1	32	25.8%	-
Llemma-7b Azerbayev et al. (2023b)	SEARCH	50	1	32	26.2%	-
ReProver Yang et al. (2023)	SEARCH	50	1	64	26.5%	-
Transformer Polu et al. (2022) (w/ RL)	SEARCH	512	1	8	29.6%	-
INTERNLM2-34B YING ET AL. (2024)	SEARCH	50	1	32	29.5%	-
COPRA (WITH GPT-4) THAKUR ET AL. (2023)	CUSTOMIZED	-	60	1	29.9%	-
COPRA (WITH GPT-4) THAKUR ET AL. (2023)	CUSTOMIZED	-	100	1	30.7%	-
INTERNLM2-7B YING ET AL. (2024)	SAMPLING	50	32	1	28.7%	29.7%
INTERNLM2-7B YING ET AL. (2024)	SEARCH	50	1	32	30.3%	-
SFT (INTERNLM2-7B)	SAMPLING	50	32	1	29.5%	30.6%
SFT (INTERNLM2-7B)	SEARCH	50	1	32	30.7%	-
LEAN-COT (INTERNLM2-7B)	SAMPLING	50	32	1	32.8%	35.6%
LEAN-STAR (ITER-1) (INTERNLM2-7B)	SAMPLING	50	32	1	34.0%	38.4%
LEAN-STAR (ITER-2) (INTERNLM2-7B)	SAMPLING	50	32	1	34.8 %	39.4 %
LEAN-STAR (ITER-2) (INTERNLM2-7B)	SAMPLING	50	64	1	36.1 %	-

search baselines we use beam search to generate the next tactic with S=32, K=1 (Welleck & Saha, 2023; Azerbayev et al., 2023b; Ying et al., 2024). We do not compare with methods designed for other formal languages such as Jiang et al. (2022); Xin et al. (2023) since language differences greatly influence the pass rate due to the different tactics and automation. We also do not compare with Lample et al. (2022) since they only report S=32, K=64 on best-first search, which is approximately equivalent to S=1, K=512 for the sampling method, which is too computationally expensive for us.

4.2 MAIN RESULTS

Our main results are reported in Table 7. Lean-STaR gives a significant improvement over the base model. For instance, with a similar inference budget, Lean-STaR achieves 34.8% versus 30.3% in InternLM2 (Ying et al., 2024) using best-first search and 30.7% in COPRA (Thakur et al., 2023) using GPT-4. With a larger compute budget, Lean-STaR's performance improves further to 36.1%.

Table 2: **Pass rates about InternLM2-Plus-7B on the minif2f-test dataset with Lean.** This table shows the pass rates of previous works and our work. The evaluation setting is the same as Table 7.

Approach	DECODING	N	K	S	PASS RATE
INTERNLM2-PLUS-7B (YING ET AL., 2024) (FROM PAPER)	SEARCH	1000	1	32	43.4%
INTERNLM2-PLUS-7B (YING ET AL., 2024) (REPRODUCED)	SEARCH	1000	1	32	42.6%
INTERNLM2-PLUS-7B (YING ET AL., 2024)	SAMPLING	50	32	1	40.9%
SFT (INTERNLM2-PLUS-7B) (YING ET AL., 2024)	SAMPLING	50	32	1	41.3%
LEAN-COT (INTERNLM2-PLUS-7B)	SAMPLING	50	32	1	43.4%
LEAN-STAR (ITER-1) (INTERNLM2-PLUS-7B)	SAMPLING	50	32	1	45.4%
INTERNLM2-PLUS-7B (YING ET AL., 2024)	SAMPLING	50	64	1	42.2%
SFT (INTERNLM2-PLUS-7B) (YING ET AL., 2024)	SAMPLING	50	64	1	43.4%
Lean-CoT (InternLM2-plus-7b)	SAMPLING	50	64	1	45.5%
Lean-STAR (ITER-1) (INTERNLM2-PLUS-7B)	SAMPLING	50	64	1	46.3 %

Thought augmentation improves theorem proving. The first phase of Lean-STaR trains a model to interleave thoughts and tactics, by fine-tuning on a synthesized dataset of thought-augmented examples. The fine-tuned model from this phase, denoted Lean-CoT in Table 7, achieves a pass rate of 32.8%, which is higher than the model prior to this phase, denoted SFT (29.5%). We conclude that the first phase of Lean-STaR can improve the theorem proving ability of a language model, even one that is already specialized for generating tactics in Lean such as the SFT model.

Bootstrapping improves thought-augmented theorem proving. The second phase of Lean-STaR consists of generating new thoughts and tactics with the current language model, saving those that result in correct proofs, and training on the union of the initial thought-augmented dataset and the saved examples (i.e., expert iteration (Polu et al., 2022; Zelikman et al., 2022; Singh et al., 2023)). Refer to Appendix A.1 for details.

We perform two iterations of expert iteration, and present the results in Table 7, denoted LEAN-STAR. Each iteration improves the model's theorem proving performance, from 32.8% (the initial model) to 34% (LEAN-STAR after iteration 1) to 34.8% (LEAN-STAR after iteration 2). Furthermore, we find that the model is amenable to further improvement via additional sampling, achieving 36.1% by doubling the sampling budget. We conclude that Lean-STaR's second phase can further improve a model's ability to generate thoughts and tactics that lead to correct proofs. We include three qualitative examples in the Appendix, which show the model interleaving thoughts and proof steps.

4.3 EXPERIMENTS WITH STRONGER BASE MODEL AND MORE DATA

We instantiate Lean-STaR using a stronger language model (InternLM2-Math-plus-7b (Ying et al., 2024)), which was released after the experiment above. We follow a similar setup to the previous experiment.

In this experiment, we used 140,000 thoughts annotated by GPT-40 (OpenAI, 2023) to fine-tune a model ("Lean-CoT"). Then we performed only one iteration of expert iteration and collected about 60,000 (proof

Table 3: Results for the InternLM2-plus-7b and our Lean-CoT, Lean-STaR, and expert iteration without CoT. We use sampling with N = 50, K = 32, & T = 0.7.

Approach	Pass@32 of InternLM-Base	Pass@32 of InternLM-Plus
FEW-SHOT	28.7%	40.9%
SFT	29.5%(+0.8%)	41.3%(+0.4%)
LEAN-COT	32.8%(+3.3%)	43.4%(+2.1%)
LEAN-STAR	34.0%(+1.2%)	45.5%(+2.1%)
EXPERT ITERATION (SFT)	30.7%(+1.2%)	43.0%(+1.7%)

state, thoughts, next-tactic) pairs in data, named "STaR dataset" D_1 . We further fine-tuned the Lean-CoT model on dataset D_1 to get the Lean-STaR model.

Our new results are reported in Table 2. We can see that Lean-STaR still gives a significant improvement over the baseline. For instance, Lean-STaR achieves 45.4% versus 39.8% in InternLM-plus using sampling with a similar inference budget and 43.4% using best-first search with more inference budget reported in (Ying et al., 2024). This results show that both retrospective rationale generation and expert iteration can improve the theorem-proving capabilities on a stronger base model.

4.4 EXPERIMENTS ON EXPERT ITERATION WITHOUT COT

Table 3 shows the result of expert iteration without CoT (i.e., using (state, tactic) pairs only) as well as the result of Lean-CoT and Lean-STaR. Expert iteration alone achieves 43.0%, which is less than Lean-STaR (45.4%) in InternLM-plus and achieves 30.7% verus 39.8% in InternLM-base. This shows that Lean-STaR's performance gains do not only come from the use of expert iteration.

5 CONCLUSION & LIMITATIONS

In this paper, we presented Lean-STaR, a novel approach that significantly enhances the theorem-proving capabilities of language models in formal mathematics by integrating Chain-of-Thought (CoT) rationales into each proof step. Our method begins with generating synthetic rationales using ground-truth tactics retrospectively, followed by fine-tuning the language model to generate these rationales and predict subsequent tactics, resulting in the Lean-CoT model. We further improved this model using expert iteration, fine-tuning it on correct proofs it samples and verifies using the Lean solver. Our contributions include the introduction of the first thought-augmented theorem proving dataset, demonstrating that expert iteration can further improve performance, and achieving new results on the miniF2F-test benchmark, increasing the pass rate from 30.3% to 36.1%. These advancements are not only about improving the accuracy of automated theorem proving, but also offer a scalable and efficient framework for advancing human understanding of mathematics, which may lead to significant impacts in education, scientific discovery, and program verification (Carter & Monks, 2013; Kang et al., 2020; Szegedy, 2020; Avigad, 2023; First, 2023; of Sciences, 2023).

The primary limitation of our method is that its performance may be constrained by issues of computational scalability. Both Lean-CoT and Lean-STaR have been fine-tuned on a dataset that is not very large. Additionally, the use of GPT-4 to generate synthetic data may incur a significant cost and possibly introduce biases. Also, expert iteration could face a bottleneck due to CPU and IO limitations, which might slow down the process due to a sluggish speed of Lean ITP.

REFERENCES

- Josh Achiam, Steven Adler, Sandhini Agarwal, Lama Ahmad, Ilge Akkaya, Florencia Leoni Aleman, Diogo Almeida, Janko Altenschmidt, Sam Altman, Shyamal Anadkat, et al. Gpt-4 technical report. *arXiv preprint arXiv:2303.08774*, 2023.
- Ayush Agrawal, Siddhartha Gadgil, Navin Goyal, Ashvni Narayanan, and Anand Tadipatri. Towards a mathematics formalisation assistant using large language models. *arXiv preprint arXiv:2211.07524*, 2022.
- Thomas Anthony, Zheng Tian, and David Barber. Thinking fast and slow with deep learning and tree search. *Advances in neural information processing systems*, 30, 2017.
- Jeremy Avigad. Mathematics and the formal turn, 2023.
- Zhangir Azerbayev, Bartosz Piotrowski, Hailey Schoelkopf, Edward W Ayers, Dragomir Radev, and Jeremy Avigad. Proofnet: Autoformalizing and formally proving undergraduate-level mathematics. *arXiv* preprint *arXiv*:2302.12433, 2023a.
- Zhangir Azerbayev, Hailey Schoelkopf, Keiran Paster, Marco Dos Santos, Stephen McAleer, Albert Q Jiang, Jia Deng, Stella Biderman, and Sean Welleck. Llemma: An open language model for mathematics. *arXiv* preprint arXiv:2310.10631, 2023b.
- Jasmin Christian Blanchette, Cezary Kaliszyk, Lawrence C Paulson, and Josef Urban. Hammering towards qed. *Journal of Formalized Reasoning*, 9(1):101–148, 2016.
- Sascha Bohme and Tobias Nipkow. Sledgehammer: judgement day. In *Automated Reasoning: 5th International Joint Conference, IJCAR 2010, Edinburgh, UK, July 16-19, 2010. Proceedings 5*, pp. 107–121. Springer, 2010.
- Tom Brown, Benjamin Mann, Nick Ryder, Melanie Subbiah, Jared D Kaplan, Prafulla Dhariwal, Arvind Neelakantan, Pranav Shyam, Girish Sastry, Amanda Askell, et al. Language models are few-shot learners. *Advances in neural information processing systems*, 33:1877–1901, 2020.
- Kevin Buzzard. Lean in 2024. https://xenaproject.wordpress.com/2024/01/20/lean-in-2024/,2024.
- Nathan C Carter and Kenneth G Monks. Lurch: a word processor that can grade students' proofs. In *CICM Workshops*, 2013.
- Wenhu Chen, Xueguang Ma, Xinyi Wang, and William W Cohen. Program of thoughts prompting: Disentangling computation from reasoning for numerical reasoning tasks. *arXiv* preprint arXiv:2211.12588, 2022.
- Projet Coq. The coq proof assistant-reference manual. INRIA Rocquencourt and ENS Lyon, version, 5, 1996.
- Lukasz Czajka and Cezary Kaliszyk. Hammer for coq: Automation for dependent type theory. *Journal of automated reasoning*, 61:423–453, 2018.
- Leonardo De Moura, Soonho Kong, Jeremy Avigad, Floris Van Doorn, and Jakob von Raumer. The lean theorem prover (system description). In *Automated Deduction-CADE-25: 25th International Conference on Automated Deduction, Berlin, Germany, August 1-7, 2015, Proceedings 25*, pp. 378–388. Springer, 2015.
- Emily First. Automating the Formal Verification of Software. PhD thesis, 2023. URL https://scholarworks.umass.edu/dissertations 2/2812.

- Emily First, Markus Rabe, Talia Ringer, and Yuriy Brun. Baldur: Whole-proof generation and repair with large language models. In *Proceedings of the 31st ACM Joint European Software Engineering Conference and Symposium on the Foundations of Software Engineering*, ESEC/FSE 2023, pp. 1229–1241, New York, NY, USA, 2023. Association for Computing Machinery. ISBN 9798400703270. doi: 10.1145/3611643.3616243. URL https://doi.org/10.1145/3611643.3616243.
 - Fabian Gloeckle, Baptiste Roziere, Amaury Hayat, and Gabriel Synnaeve. Temperature-scaled large language models for lean proofstep prediction. In *The 3rd Workshop on Mathematical Reasoning and AI at NeurIPS*'23, 2023.
 - Jesse Michael Han, Jason Rute, Yuhuai Wu, Edward W Ayers, and Stanislas Polu. Proof artifact co-training for theorem proving with language models. *arXiv* preprint arXiv:2102.06203, 2021.
 - Jesse Michael Han, Jason Rute, Yuhuai Wu, Edward Ayers, and Stanislas Polu. Proof artifact co-training for theorem proving with language models. In *International Conference on Learning Representations*, 2022. URL https://openreview.net/forum?id=rpxJc9j04U.
 - Dan Hendrycks, Collin Burns, Saurav Kadavath, Akul Arora, Steven Basart, Eric Tang, Dawn Song, and Jacob Steinhardt. Measuring mathematical problem solving with the math dataset. *arXiv* preprint arXiv:2103.03874, 2021.
 - Yinya Huang, Xiaohan Lin, Zhengying Liu, Qingxing Cao, Huajian Xin, Haiming Wang, Zhenguo Li, Linqi Song, and Xiaodan Liang. Mustard: Mastering uniform synthesis of theorem and proof data. *arXiv* preprint arXiv:2402.08957, 2024.
 - Albert Q Jiang, Sean Welleck, Jin Peng Zhou, Wenda Li, Jiacheng Liu, Mateja Jamnik, Timothee Lacroix, Yuhuai Wu, and Guillaume Lample. Draft, sketch, and prove: Guiding formal theorem provers with informal proofs. *arXiv preprint arXiv:2210.12283*, 2022.
 - Dongyeop Kang, Andrew Head, Risham Sidhu, Kyle Lo, Daniel S Weld, and Marti A Hearst. Document-level definition detection in scholarly documents: Existing models, error analyses, and future directions. *arXiv* preprint arXiv:2010.05129, 2020.
 - Guillaume Lample, Timothee Lacroix, Marie-Anne Lachaux, Aurelien Rodriguez, Amaury Hayat, Thibaut Lavril, Gabriel Ebner, and Xavier Martinet. Hypertree proof search for neural theorem proving. *Advances in neural information processing systems*, 35:26337–26349, 2022.
 - Zhaoyu Li, Jialiang Sun, Logan Murphy, Qidong Su, Zenan Li, Xian Zhang, Kaiyu Yang, and Xujie Si. A survey on deep learning for theorem proving, 2024.
 - The mathlib Community. The lean mathematical library. In *Proceedings of the 9th ACM SIGPLAN International Conference on Certified Programs and Proofs*, CPP 2020, pp. 367–381, New York, NY, USA, 2020. Association for Computing Machinery. ISBN 9781450370974. doi: 10.1145/3372885.3373824. URL https://doi.org/10.1145/3372885.3373824.
 - Allen Newell and Herbert Simon. The logic theory machine—a complex information processing system. *IRE Transactions on information theory*, 2(3):61–79, 1956.
 - Tobias Nipkow, Markus Wenzel, and Lawrence C Paulson. *Isabelle/HOL: a proof assistant for higher-order logic*. Springer, 2002.
 - Maxwell Nye, Anders Johan Andreassen, Guy Gur-Ari, Henryk Michalewski, Jacob Austin, David Bieber, David Dohan, Aitor Lewkowycz, Maarten Bosma, David Luan, et al. Show your work: Scratchpads for intermediate computation with language models. *arXiv preprint arXiv:2112.00114*, 2021.

- National Academies of Sciences. Artificial intelligence to assist mathematical reasoning: Proceedings of a workshop, 2023.
 - OpenAI. OpenAI: GPT-4, 2023. URL https://openai.com/research/gpt-4.
 - Stanislas Polu and Ilya Sutskever. Generative language modeling for automated theorem proving. *arXiv* preprint arXiv:2009.03393, 2020.
 - Stanislas Polu, Jesse Michael Han, Kunhao Zheng, Mantas Baksys, Igor Babuschkin, and Ilya Sutskever. Formal mathematics statement curriculum learning. *arXiv preprint arXiv:2202.01344*, 2022.
 - Markus N Rabe, Dennis Lee, Kshitij Bansal, and Christian Szegedy. Mathematical reasoning via self-supervised skip-tree training. *arXiv preprint arXiv:2006.04757*, 2020.
 - Avi Singh, John D Co-Reyes, Rishabh Agarwal, Ankesh Anand, Piyush Patil, Peter J Liu, James Harrison, Jaehoon Lee, Kelvin Xu, Aaron Parisi, et al. Beyond human data: Scaling self-training for problem-solving with language models. *arXiv* preprint arXiv:2312.06585, 2023.
 - Christian Szegedy. A promising path towards autoformalization and general artificial intelligence. In *Intelligent Computer Mathematics: 13th International Conference, CICM 2020, Bertinoro, Italy, July 26–31, 2020, Proceedings 13*, pp. 3–20. Springer, 2020.
 - Terence Tao. https://mathstodon.xyz/@tao/111287749336059662, 2023.
 - Amitayush Thakur, Yeming Wen, and Swarat Chaudhuri. A language-agent approach to formal theorem-proving. *arXiv preprint arXiv:2310.04353*, 2023.
 - Haiming Wang, Huajian Xin, Chuanyang Zheng, Lin Li, Zhengying Liu, Qingxing Cao, Yinya Huang, Jing Xiong, Han Shi, Enze Xie, Jian Yin, Zhenguo Li, Heng Liao, and Xiaodan Liang. Lego-prover: Neural theorem proving with growing libraries, 2023a.
 - Haiming Wang, Ye Yuan, Zhengying Liu, Jianhao Shen, Yichun Yin, Jing Xiong, Enze Xie, Han Shi, Yujun Li, Lin Li, et al. Dt-solver: Automated theorem proving with dynamic-tree sampling guided by proof-level value function. In *Proceedings of the 61st Annual Meeting of the Association for Computational Linguistics (Volume 1: Long Papers)*, pp. 12632–12646, 2023b.
 - Qingxiang Wang, Chad Brown, Cezary Kaliszyk, and Josef Urban. Exploration of neural machine translation in autoformalization of mathematics in mizar. In *Proceedings of the 9th ACM SIGPLAN International Conference on Certified Programs and Proofs*, pp. 85–98, 2020.
 - Jason Wei, Xuezhi Wang, Dale Schuurmans, Maarten Bosma, Fei Xia, Ed Chi, Quoc V Le, Denny Zhou, et al. Chain-of-thought prompting elicits reasoning in large language models. Advances in neural information processing systems, 35:24824–24837, 2022.
 - Sean Welleck and Rahul Saha. Llmstep: Llm proofstep suggestions in lean. arXiv preprint arXiv:2310.18457, 2023.
 - Sean Welleck, Jiacheng Liu, Ronan Le Bras, Hannaneh Hajishirzi, Yejin Choi, and Kyunghyun Cho. Natural-proofs: Mathematical theorem proving in natural language. *arXiv* preprint arXiv:2104.01112, 2021.
 - Sean Welleck, Jiacheng Liu, Ximing Lu, Hannaneh Hajishirzi, and Yejin Choi. Naturalprover: Grounded mathematical proof generation with language models. *Advances in Neural Information Processing Systems*, 35:4913–4927, 2022.

- Yuhuai Wu, Markus N Rabe, Wenda Li, Jimmy Ba, Roger B Grosse, and Christian Szegedy. Lime: Learning inductive bias for primitives of mathematical reasoning. In *International Conference on Machine Learning*, pp. 11251–11262. PMLR, 2021.
 - Yuhuai Wu, Albert Qiaochu Jiang, Wenda Li, Markus Rabe, Charles Staats, Mateja Jamnik, and Christian Szegedy. Autoformalization with large language models. *Advances in Neural Information Processing Systems*, 35:32353–32368, 2022.
 - Huajian Xin, Haiming Wang, Chuanyang Zheng, Lin Li, Zhengying Liu, Qingxing Cao, Yinya Huang, Jing Xiong, Han Shi, Enze Xie, et al. Lego-prover: Neural theorem proving with growing libraries. *arXiv* preprint arXiv:2310.00656, 2023.
 - Kaiyu Yang, Aidan Swope, Alex Gu, Rahul Chalamala, Peiyang Song, Shixing Yu, Saad Godil, Ryan Prenger, and Anima Anandkumar. LeanDojo: Theorem proving with retrieval-augmented language models. In *Neural Information Processing Systems (NeurIPS)*, 2023.
 - Huaiyuan Ying, Shuo Zhang, Linyang Li, Zhejian Zhou, Yunfan Shao, Zhaoye Fei, Yichuan Ma, Jiawei Hong, Kuikun Liu, Ziyi Wang, Yudong Wang, Zijian Wu, Shuaibin Li, Fengzhe Zhou, Hongwei Liu, Songyang Zhang, Wenwei Zhang, Hang Yan, Xipeng Qiu, Jiayu Wang, Kai Chen, and Dahua Lin. Internlm-math: Open math large language models toward verifiable reasoning, 2024.
 - Eric Zelikman, Yuhuai Wu, Jesse Mu, and Noah Goodman. Star: Bootstrapping reasoning with reasoning. *Advances in Neural Information Processing Systems*, 35:15476–15488, 2022.
 - Xueliang Zhao, Wenda Li, and Lingpeng Kong. Decomposing the enigma: Subgoal-based demonstration learning for formal theorem proving, 2024. URL https://openreview.net/forum?id=xLoxMvO695.
 - Kunhao Zheng, Jesse Michael Han, and Stanislas Polu. Minif2f: a cross-system benchmark for formal olympiad-level mathematics. *arXiv preprint arXiv:2109.00110*, 2021.
 - Denny Zhou. Teach language models to reason. https://dennyzhou.github.io/LLMs-Reason-Taiwan-2023.pdf, 2023. Accessed: 2024-05-21.
 - Jin Peng Zhou, Charles Staats, Wenda Li, Christian Szegedy, Kilian Q Weinberger, and Yuhuai Wu. Don't trust: Verify–grounding Ilm quantitative reasoning with autoformalization. *arXiv preprint arXiv:2403.18120*, 2024a.
 - Jin Peng Zhou, Charles E Staats, Wenda Li, Christian Szegedy, Kilian Q Weinberger, and Yuhuai Wu. Don't trust: Verify grounding LLM quantitative reasoning with autoformalization. In *The Twelfth International Conference on Learning Representations*, 2024b. URL https://openreview.net/forum?id=V5tdi14ple.

A ADDITIONAL EXPERIMENT SETUP

A.1 LEAN-STAR EXPERT ITERATION

The second phase of Lean-STaR consists of generating new thoughts and tactics with the current language model, saving those that result in correct proofs, and training on the union of the initial thought-augmented dataset and the saved examples (i.e., expert iteration (Polu et al., 2022; Zelikman et al., 2022; Singh et al., 2023)). We perform two iterations of expert iteration, and provide details on our specific experimental setup below.

In each iteration we use sampling on the $LeanDojo\ Benchmark\ 4$ dataset, and save the (state, thought, tactic) examples that are part of successful proofs. For each problem, we sample K=32 times in parallel with temperature T=1.0, and limit the number of times a tactic can be generated to a total of N=5 per problem. Also, sampling is limited to 1 minute per problem. In this setup, each problem needs on average about 0.5 A100 minutes. We collect successfully sampled trajectories to produce a "STaR dataset" D_1 , and up to 3 proof trajectories were collected for each problem. We collected 32,231 different (proof state, thoughts, next-tactic) pairs in successful proof trajectories during expert iteration, which takes about 4 days with $8\times A100$ GPUs. Then, we further fine-tune SFT model for 1 epoch on the combination of GPT-4 annotated reasoning data and expert iteration data $D_T \cup D_1$ to get the Lean-STaR model. We use the same learning rate setup that was used for the SFT model. In the second iteration, we generate a dataset D_2 in a similar fashion. Then, we chose to further fine-tune model from iteration $1, M_1$, on the generated dataset D_2 (roughly 19k pairs).

The setup of experiment about InternLM2-plus is slightly different. The details are shown in Section 4.3 and Appendix E.

B STATISTICS FOR OUR METHODS AS WELL AS THE BASELINES

Table 4: Statistics for the baselines and our Lean-CoT, Lean-STaR on MiniF2F dataset. We use sampling method with hyperparameters N=50~&~K=32~&~T=0.7.

Approach	# (CONTINUAL) TRAINING DATA	Pass@32	
INTERNLM2-MATH-7B (FEW-SHOT)	-	28.7%	-
SFT	231,240	29.5%	+0.8%
LEAN-COT	52,438	32.8%	+3.3%
LEAN-STAR (ITER-1)	32,231	34.0%	+1.2%
LEAN-STAR (ITER-2)	19,324	34.8 %	+0.8%

C AN EXAMPLE AND EXPLANATION OF A FORMAL PROOF IN LEAN

An example of a formal proof in Lean with its visualization is shown in Figure 5, taken from (Lample et al., 2022). In the proof, the tactic induction k is is applied to the initial state $(n \le m \Rightarrow n+k \le m+k)$ and the ITP converts the current state to subgoals case $0 \land \text{case}$ ih: $n \le m \land n+k \le m+k \Rightarrow n+(k+1) \le m+(k+1)$. The case $0 : n \le m$ is our hypothesis h_0 so it can be proven by case 0 : exact h_0 tactic. Then, we rewrite the case ih through the nat.succ_le_succ_iff which is a theorem in Lean library means $n \le m \Leftrightarrow n+1 \le m+1$. After tactics case 0 : exact h_0 and case ih: rw nat.succ_le_succ_iff, the goal state is converted to $n+k \le m+k$ which is the hypothesis introduced by induction. Therefore, we can complete this proof using tactic exact k_ih.

```
theorem add_le_add_right (m n k : \mathbb{N}) (h<sub>0</sub> : n \leq m)
     : n + k \le m + k :=
     induction k with
     | zero =>
           exact h_0
      | succ k ih =>
           rw Nat.succ_le_succ_iff
           exact ih
                    (m \ n \ k : \mathbb{N}) (h_0: n \le m) : n + k \le m + k
                                       induction k
    \vdash n + 0 \leq m + 0
                        (k_ih: n + k \le m + k): n + k_n.succ \le m + k_n.succ
                                                 rw nat.succ_le_succ_iff
             exact ho
                             (k_ih: n + k \le m + k): n + k_n \le m + k_n
                                                 exact k_ih
```

Figure 5: A example proof and its visualization of $n \le m \Rightarrow n+k \le m+k$ in Lean, taken from (Lample et al., 2022). The induction tactic reduces the initial statement to two subgoals. Then tactics case 0:exact h_0 and case ih:rw nat.succ_le_succ_iff, case ih:exact k_ih can be applied in turn to complete the proof.

Table 5: Counts of problems successfully proved in minif2f-test benchmark, split by type and difficulty. The methods use sampling with N=50, K=32. Thought-augmented methods improve performance on all categories, while Lean-STaR significantly improves Number Theory performance.

	TOTAL		TEST SET SIZE	INTERNLM2-7B	SFT	LEAN-COT	LEAN-STAR (ITER-2)
	IMO		20	0	0	0	0
	AIME		15	2	1	2	3
	AMC		45	3	3	7	5
		LEVEL 5	14	1	2	3	3
		LEVEL 4	14	7	7	7	7
	ALGEBRA	LEVEL 3	14	9	9	11	11
	LEVEL 2	14	10	10	9	11	
MATH		LEVEL 1	14	9	10	10	10
MATH		LEVEL 5	16	6	6	6	7
		LEVEL 4	11	5	5	4	5
	NUMBER THEORY	LEVEL 3	11	4	5	5	6
		LEVEL 2	11	6	5	5	6
		LEVEL 1	11	8	8	9	9
	ALGEBRA	<u> </u>	18	0	1	1	1
CUSTOM	Number The	ORY	8	0	0	0	0
	Induction	N	8	0	0	1	1

sectionPerformance Analysis by Types and Difficulties Tasks in *minif2f-test* are manually formalized from Olympiad type problems, drawn from multiple sources including AIME, AMC, IMO problems, and problems from the MATH dataset (Hendrycks et al., 2021). These problems can have different levels of difficulty and types. Table 5 reports the number of problems successfully proved, partitioned by type and difficulty. We see that Lean-CoT improves performance in solving difficult problems on all categories, especially those from mathematics competitions. On top of these improvements, Lean-STaR's improvements come mainly in Number Theory.

C.1 Performance Analysis by Types and Difficulties using InternLM2-plus-7b

Table 6 reports the number of problems successfully proved, partitioned by type and difficulty using InternLM2-plus. We see that Lean-CoT improves performance mainly in Number Theory and Lean-STaR improves performance in solving difficult problems on all categories, which is the opposite of the performance of the InternLM2-base.

D COMPARISON BETWEEN SEARCH METHOD AND SAMPLING METHOD

Table 6: Counts of problems successfully proved in *minif2f-test* benchmark using InternLM2-plus-7b, split by type and difficulty. The methods use sampling with N=50, K=32.

	TOTAL		TEST SET SIZE	INTERNLM2-PLUS-7B	LEAN-COT	LEAN-STAR (ITER-1)
	IMO		20	0	0	0
	AIME		15	3	3	4
	AMC		45	9	9	10
		LEVEL 5	14	6	6	6
		LEVEL 4	14	9	9	9
	ALGEBRA	LEVEL 3	14	11	13	13
		LEVEL 2	14	11	11	11
MATH		LEVEL 1	14	10	10	10
MATH		LEVEL 5	16	7	7	7
		LEVEL 4	11	6	8	8
	NUMBER THEORY	LEVEL 3	11	6	7	9
		LEVEL 2	11	7	9	9
		LEVEL 1	11	10	10	10
	ALGEBRA		18	4	3	4
CUSTOM	Number The	ORY	8	0	0	0
	Induction	N	8	1	1	1

Table 7: Comparison between search method and sampling method. We use sampling method with hyperparameters N=50 & S=1 & K=32 and BFS method with N=50 & S=32 & K=1. All sampling decoding in the paper uses a temperature of 0.7. We use BFS to denotes Best-First Search.

APPROACH	BFS (SAMPLING)	BFS (BEAM SEARCH)	SAMPLING
TACTIC PREDICTION IN PROVING TOKEN DECODING IN TACTICS	BFS SAMPLING	BFS Beam-Search	SAMPLING SAMPLING
INTERNLM2-7B (FEW-SHOT)	29.1%	30.3%	28.7%
SFT	29.9%	30.7%	29.5%
LEAN-COT	27.0%	25.4%	32.8%
LEAN-STAR (ITER-1)	29.1%	26.2%	34.0%
LEAN-STAR (ITER-2)	29.5%	26.2%	34.8%

E PERFORMANCE DIFFERENCE OF JOINT TRAINING AND CONTINUE TRAINING

As shown in Table 8, the joint training method performs better using InternLM2-base but training method performs much better using InternLM2-plus. It seems that there are no difference between these two methods. Therefore, this performance can be depend on the quantity of data or the model. (We use much more data when using InternLM2-plus and the quantity of "STaR data" is relatively small.)

Table 8: Performance difference of joint training and continue training on Lean-STaR. We use sampling method with hyperparameters N=50~&~K=32~&~T=0.7. In continue training, we further fine-tune the Lean-CoT model on "STaR data" to get Lean-STaR model and in joint training we fine-tune the SFT model on combination of GPT-4 annotated reasoning data and "STaR data".

Approach	INTERNLM2-BASE-7B	INTERNLM2-PLUS-7B
LEAN-COT	32.8%	43.4%
LEAN-STAR (ITER-1) (JOINT TRAINING)	34.0%	43.9%
LEAN-STAR (ITER-1) (CONTINUE TRAINING)	33.2%	45.5%

Table 9: Performence of SFT-Direct and our Lean-STaR at different search size or sampling times $S \times K$. We fix N=50. We use beam search in search and temperature T=0.7 in sampling when generating the next tactic. We have K=1 in search and S=1 in sampling. Note that we sample 32 examples twice when K=64 in sampling.

	SFT-DIRECT (SEARCH)	SFT-DIRECT (SAMPLING)	LEAN-STAR (ITER-2) (SAMPLING)
$S \times K = 1$	13.5%	20.9%	21.7%
$S\times K=2$	$18.0\% \ (+4.5\%)$	$22.5\% \ (+1.6\%)$	24.6%(+2.9%)
$S \times K = 4$	$23.3\% \ (+5.3\%)$	$25.0\% \ (+2.5\%)$	27.5%(+2.9%)
$S \times K = 8$	$27.5\% \ (+4.2\%)$	$27.0\% \ (+2.0\%)$	30.7% (+3.2%)
$S \times K = 16$	$29.9\% \ (+2.4\%)$	$28.3\% \ (+1.3\%)$	33.6% (+2.9%)
$S \times K = 32$	$30.7\% \ (+0.8\%)$	$29.5\% \ (+1.2\%)$	34.8% (+1.2%)
$S \times K = 64$	$30.7\% \; (+0.0\%)$	$30.3\% \ (+0.8\%)$	36.1% (+1.3%)

E.1 SEARCH AND SAMPLING BUDGET

Table 9 reports the trends of the pass rate against the search size or sampling budget $S \times K$. We find that Lean-STaR benefits more as K increases, especially when K is relatively large. The result suggests that additional sampling with thoughts improves performance, while additional sampling without thoughts may saturate. We believe this is because thoughts increase the diversity of outputs and contribute to exploration in the theorem proving space. Therefore, Lean-STaR is more scalable (in terms of inference-time compute), and may be amenable to further improvements with additional iterations of expert iteration.

F RETROSPECTIVE RATIONALE GENERATION PROMPT OF GPT-4

Please act as a professional mathematician. Your goal is to accurately prove a math theorem in Lean4. You are given the first tactic that should be taken to prove the Given Theorem.

```
893
894
\#\# \text{ State}
a b n : \mathbb{N}
\vdash \neg (n \neq 0 \land a \neq 0) \leftrightarrow n = 0 \lor a = 0
896
\#\# \text{ Tactic}
897
\text{ simp only [not\_and\_or, ne\_eq, not\_not]}
```

Reasoning

900

901

902

903

904 905

906

907 908 To prove the equivalence between the negation of a conjunction and a disjunction, we utilize logical equivalences, specifically the negation of a conjunction $\neg(`(P \land Q)`)$ being equivalent to the disjunction of the negations (`P = $0 \lor Q = 0$ `) and simplifications related to negation and inequality.

Figure 6: Examples of (input, output) pairs of retrospective rationale generation with GPT-4. The full prompt is given in Appendix F. See §3.2.2 for the detailed explanation.

```
909
       # Example:
910
911
       Given Theorem:
912
       ```lean4
913
 X : Type u_1
 Y: Type u_2
914
 inst^{1}: TopologicalSpace X
915
 \verb"inst" \verb": TopologicalSpace Y"
916
 f : X \rightarrow . Y
917
 h : PContinuous f
918
 ⊢IsOpen (PFun.preimage f Set.univ)
919
 Given Tactic:
920
       ```lean4
921
       exact h _ isOpen_univ
922
923
      Assistant Output:
924
       ### PLANNING OF REASONING
       Given the above goal and the given the target tactic `exact h _ isOpen_univ`, I
925
            should produce a reasoning that only based on the goal, and conclude to
926
           the `exact h _ isOpen_univ`, but not in the hindsight format.
927
928
       ### REASONING
929
       By directly using the hypothesis `h : PContinuous f`, we state that for any
930
           open set, its preimage via `f` is also open, and this applies to `Set.univ`
931
           as well.
932
933
       ### TACTIC
934
       ```lean4
935
 exact h _ isOpen_univ
936
937
938
 To achieve the goal, you have three jobs.
939
 # Write down the planning of reasoning.
```

```
940
 # Write down the reasoning that can result in the selection of the Given Tactic.
941
942
 # Write down the Given Tactic.
 You have four principles to do this.
943
 # Craft reasoning that is comprehensive yet concise, contained ideally within
944
 two sentences.
945
 # Begin reasoning with the objective of the Given Theorem, ensuring logical
946
 progression, rather than constructing it retrospectively from the Given
947
948
 # Avoid mentioning the Given Tactic and specific statement names from the Given
 Tactic throughout your reasoning.
949
 # Position the conclusion of the tactic after presenting all reasons, ensuring
950
 that details regarding the Given Tactic are not introduced at the start of
951
 your reasoning.
952
 Your output should be strictly in the following format and should not contain
953
 extra content:
954
 ### PLANNING OF REASONING
955
956
 Given the above goal and the given the target tactic <Given Tactic>, I should
957
 produce a reasoning that only based on the goal, and conclude to the exact <
958
 Given Tactic>, but not in the hindsight format.
959
 ### REASONING
960
961
 <your reasoning to the Given Tactic>
962
 ### TACTIC
963
964
 <Given Tactic>
965
966
 # Given Theorem:
       ```lean4
967
       {theorem["state_before"]}
968
969
970
       # Given Tactic:
971
       ···lean4
972
       {theorem["tactic"]}
973
974
975
976
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980
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984
985
```

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G EXAMPLES OF GENERATED LEAN PROOFS WITH THOUGHTS

```
989
       theorem aime_1990_p4 (x : \mathbb{R}) (h<sub>0</sub> : 0 < x) (h<sub>1</sub> : x ^ 2 - 10 * x - 29 \neq 0)
990
           (h_2 : x ^2 - 10 * x - 45 \neq 0) (h_3 : x ^2 - 10 * x - 69 \neq 0)
991
           (h_4 : 1 / (x^2 - 10 * x - 29) + 1 / (x^2 - 10 * x - 45) - 2 / (x^2 - 10 * x - 45))
           10 * x - 69) = 0
992
           x = 13 :=
993
           norm_num at h_1 h_2 h_3 -- Reasoning: To prove `x = 13`, we examine the
994
           conditions under which the given equation holds, specifically focusing on
           the non-equality of the expressions involving x \wedge 2 - 10 * x - 29, x \wedge 2 - 10 * x - 29
           - 10 * \times - 45, and \times ^ 2 - 10 * \times - 69. Simplifying these expressions
996
           using properties of real numbers and algebra allows us to directly compare
997
           them with their respective values, ultimately identifying x = 13 as the
998
           unique solution that satisfies all constraints.
           field_simp at \star -- Reasoning: To prove \((x = 13\)), we leverage the given
1000
           equalities involving rational fractions of (x^2 - 10x - c) for various constants (c), where (0 < x) and each (x^2 - 10x - c) is non-zero.
1001
           By algebraically manipulating these expressions, we aim to derive a
1002
           relationship among \setminus (x \setminus) and these constants, specifically focusing on
1003
           1004
           ring_nf at h_4 \vdash -- Reasoning: To establish the equality x = 13 under the
1005
           given conditions, we need to manipulate the algebraic expression given by
1006
           'h4' to reveal its dependence on 'x', recognizing that the presence of 'x'
           in the expressions may affect the equation's truth value. The application
1007
           of algebraic transformations on both sides of the equation will facilitate
1008
           the identification of `x`'s value, taking into consideration the inequality
1009
           conditions provided (h_1, h_2, h_3).
1010
           nlinarith -- Reasoning: To prove \(x = 13\), we must manipulate the
           equation given by \backslash (h_4 \backslash) to isolate \backslash (x \backslash), using the algebraic properties
1011
           of equality and the assumption (h_0) which states (0 < x). This requires
1012
           careful rearrangement and application of algebraic identities to simplify
1013
           and rearrange terms, facilitating the direct application of the properties
1014
           of real numbers to reach the desired conclusion.
1015
1016
       theorem amc12a_2002_p6 (n : \mathbb{N}) (h<sub>0</sub> : 0 < n)
           : \exists m, m > n \land \exists p, m * p \leq m + p :=
1017
           use n + 1, by linarith only [h<sub>0</sub>] -- Reasoning: To demonstrate the
1018
           existence of such an 'm' and 'p' that satisfy the given inequalities, we
1019
           leverage the property of natural numbers that ensures an increase in `n`
1020
           from `0` leads to the possibility of finding such `m` and `p`. This
1021
           approach is supported by the fundamental property of natural numbers and
           their arithmetic operations, suggesting that for a given `n` greater than
1022
           '0', there exists a successor 'm' and a number 'p' that satisfy the
1023
           conditions outlined.
1024
           exact (0, by simp ) -- Reasoning: To demonstrate that there exists an \((n \)
1025
           \in \mathbb{N} such that ((n + 1) * p \mid eq n + 1 + p) holds for some (p \mid in \mathbb{N})
           \), we recognize that setting (p = 0) satisfies the inequality by the
1026
           properties of zero in arithmetic. This is because \ (n + 1 > 0) by
1027
           assumption, ensuring the left-hand side is non-negative and the right-hand
1028
           side simplifies to \ (n + 1), making the inequality trivially true.
1029
1030
```

```
1034
       theorem aime_1983_p2 (x p : \mathbb{R}) (f : \mathbb{R} \to \mathbb{R}) (h<sub>0</sub> : 0 \land p < 15) (h<sub>1</sub> : p \leq x \land
1035
            x \le 15
1036
           (h_2 : f x = abs (x - p) + abs (x - 15) + abs (x - p - 15))
1037
           : 15 \le f x :=
           cases' h_1 with h_1 h_2 -- Reasoning: Given a function \setminus (f \setminus) defined over the
1038
           real numbers, where \backslash (f(x) \backslash) equals the sum of the absolute values of the
1039
           differences (x - p), (x - 15), and (x - p - 15), along with
1040
           conditions on \(p\) and \(x\) that ensure \(x\) lies between \(p\) and
1041
           (15) and (p) is positive, we aim to show that (f(x) \neq 15). To
1042
           demonstrate this, we consider all possible cases for the position of \ (x\setminus)
           relative to \(p\) and \(15\), specifically at \(p\) itself, between \(p\)
1043
           and \ (15\), and at \ (15\). By evaluating \ (f(x)\) for each case, we can
1044
           establish a lower bound of \backslash (f(x) \backslash) that is greater than or equal to
1045
1046
           simp [h_0, abs_of_nonneg (sub_nonneg.2 h_1), abs_of_nonneg (sub_nonneg.2 h_2),
           *] -- Reasoning: The objective is to show that (f(x)) is at least 15 for
1047
           \(x\) within the bounds \(p \le x \le 15\), where \(p\) is positive but
1048
           less than 15. The provided expression for (f(x)) suggests using
1049
           properties of absolute values and inequalities to simplify and analyze
1050
           \backslash (f(x) \backslash). By applying simplification rules for absolute values and
1051
           inequalities, along with the given bounds, we aim to demonstrate the
1052
           desired inequality \backslash (f(x) \backslash ge 15 \backslash).
           simp only [abs_of_nonneg] at * -- Reasoning: The objective is to establish
1053
           an inequality involving an expression with absolute values and a sum,
1054
           where all terms are functions of \backslash (x \backslash). By recognizing that the absolute
1055
           value functions are always non-negative, we can simplify the given
1056
           expression by removing the absolute value symbols, thus focusing on the
1057
           arithmetic manipulation of the terms to demonstrate the inequality.
           simp only [abs_of_nonneg, sub_add_eq_add_sub] at * -- Reasoning: The
1058
           objective is to demonstrate that the expression `15 \leq x - p + |x - 15| + |x - p - 15|` holds given the conditions on `p`, `x`, and the function `f`.
1059
1060
           Since the expression in question involves absolute values which inherently
1061
           involve non-negativity, manipulating these expressions to highlight their
           non-negativity or equality is a logical initial step. This involves
1062
           recognizing that the absolute value of a difference can be rewritten as
1063
           the difference of absolute values, which simplifies the manipulation of
1064
           the expression to prove the inequality.
1065
           congr 1 -- Reasoning: To establish the inequality `15 \leq x + |x - 15| + |x
1066
           - p - 15| - p, we recognize that the left-hand side of the inequality
1067
           involves a mix of additions and subtractions of real numbers. By
           introducing a congruence transformation that simplifies operations
1068
           involving absolute values, we aim to align both sides of the inequality in
1069
           a form that directly reflects the properties of real numbers under these
1070
           operations.
1071
           simp only [abs_of_nonpos (sub_nonpos_of_le h2), abs_of_nonneg
1072
           (sub_nonneg_of_le h1)] -- Reasoning: The objective is to prove an
           inequality involving absolute values and subtractions that aligns the
1073
           given conditions and constraints. Simplification using the properties of
1074
           absolute values and the provided bounds can directly lead to the desired
1075
           conclusion by expressing the absolute values in terms of their underlying
1076
           expressions and applying the given constraints.
1077
           simp [abs_of_pos, *] -- Reasoning: To prove the given inequality involving
           absolute values, simplification using algebraic properties and given
1078
           hypotheses will directly lead us to the desired inequality by recognizing
1079
```

```
1081
           the algebraic manipulation and application of the known bounds h_1 and
1082
            `h2`, as well as the non-negativity of `p`.
1083
           rw [abs_of_nonpos] -- Reasoning: The objective is to demonstrate that `15 \leq
            15+|x-p-15| - p' under the given constraints on 'p' and 'x'. Given 'p < 15' and 'p \leq x \leq 15', it's apparent that 'p - 15' is non-positive.
1084
1085
           This observation allows us to apply the property that the absolute value
1086
           of a non-positive number is equal to its negative value, thereby
1087
           simplifying the expression on the right-hand side of the inequality.
1088
           all_goals linarith -- Reasoning: The goal involves demonstrating a
           relationship between expressions involving inequalities and subtraction.
1089
           The simplification of these expressions into a form that directly compares
1090
           their numerical values can lead to a straightforward application of known
1091
           inequalities and algebraic properties, demonstrating the inequality's
1092
           validity under the given conditions.
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```