LEAN-STAR: LEARNING TO INTERLEAVE THINKING AND PROVING

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Paper under double-blind review

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

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029 030 031 032 033 034 035 036 Theorem proving is a fundamental aspect of mathematics, and mathematical reasoning is an important part of artificial intelligence [\(Newell & Simon, 1956;](#page-11-0) [Zhou, 2023\)](#page-13-0). *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 [\(De Moura et al., 2015\)](#page-10-0). Automated theorem proving, if successful, can also help discover unknown errors in previous proofs^{[1](#page-0-0)}, 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 [\(Avigad, 2023;](#page-10-1) [First, 2023;](#page-10-2) [Buzzard,](#page-10-3) [2024;](#page-10-3) [of Sciences, 2023\)](#page-12-0).

037 038 039 040 041 042 043 044 Recently, language models have shown promising progress in formal theorem proving [\(Polu & Sutskever,](#page-12-1) [2020;](#page-12-1) [Rabe et al., 2020;](#page-12-2) [Wu et al., 2021;](#page-13-1) [Han et al., 2021;](#page-11-1) [Lample et al., 2022;](#page-11-2) [Yang et al., 2023;](#page-13-2) [Li et al.,](#page-11-3) [2024\)](#page-11-3). Existing approaches typically train a model solely based on the proofs in a formal language (code) such as Lean [\(De Moura et al., 2015\)](#page-10-0), Isabelle [\(Nipkow et al., 2002\)](#page-11-4), or Coq [\(Coq, 1996\)](#page-10-4). Our key observation is that such approaches ignore a wealth of *informal* information that may be useful for learning to prove theorems [\(Welleck et al., 2021;](#page-12-3) [2022\)](#page-12-4). 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 [\(Tao, 2023\)](#page-12-5).

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 [\(Zelikman et al., 2022\)](#page-13-3), we enable language models to interleave step-by-step rationales (i.e., thoughts) [\(Nye et al., 2021;](#page-11-5) [Wei et al., 2022\)](#page-12-6) with formal proving in a two-stage process. In an initial phase, we prompt a sufficiently capable language model, such as GPT-4 [\(Achiam et al., 2023\)](#page-10-5), and generate retrospective thoughts based on a dataset of human-written proofs, such as Mathlib, the largest collection of human-written proofs in Lean [\(mathlib Community, 2020\)](#page-11-6). Subsequently, we fine-tune a thought-augmented tactic predictor [\(Bohme & Nipkow, 2010;](#page-10-6) [Blanchette et al.,](#page-10-7) [2016;](#page-10-7) [Gloeckle et al., 2023;](#page-11-7) [Czajka & Kaliszyk, 2018\)](#page-10-8) 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 [\(Anthony et al., 2017;](#page-10-9) [Singh et al., 2023\)](#page-12-7), 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 [\(Szegedy, 2020;](#page-12-8) [Wang et al., 2020;](#page-12-9) [Wu et al., 2022\)](#page-13-4) or translate informal proofs into formal proofs [\(Agrawal et al., 2022;](#page-10-10) [Jiang et al., 2022;](#page-11-8) [Azerbayev et al., 2023a;](#page-10-11) [Zhou et al., 2024a;](#page-13-5) [Huang et al., 2024\)](#page-11-9). 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 [\(mathlib Community, 2020\)](#page-11-6), 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 [\(Ying et al., 2024\)](#page-13-6) 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 [\(Zheng](#page-13-7) [et al., 2021\)](#page-13-7). 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 [\(Polu & Sutskever, 2020\)](#page-12-1), which trains a language model on (proof **094 095 096 097 098 099 100 101 102 103 104 105 106 107** 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 [\(Han et al., 2022\)](#page-11-10), novel proof search methods [\(Lample et al., 2022;](#page-11-2) [Wang et al., 2023b\)](#page-12-10), further training through curriculum learning [\(Polu et al.,](#page-12-11) [2022\)](#page-12-11), retrieval augmentation [\(Yang et al., 2023\)](#page-13-2), or practical tools [\(Welleck & Saha, 2023\)](#page-12-12). Others use prompted models to generate tactics [\(Azerbayev et al., 2023b;](#page-10-12) [Thakur et al., 2023\)](#page-12-13), or fine-tune models to generate a full proof [\(First et al., 2023\)](#page-11-11). A second *auto-formalization* [\(Wu et al., 2022\)](#page-13-4) thread incorporates informal mathematics into formal theorem proving. Draft-Sketch-Prove [\(Jiang et al., 2022\)](#page-11-8) 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 [\(Bohme & Nipkow, 2010\)](#page-10-6). Draft-Sketch-Prove and related methods [\(Wang et al., 2023a;](#page-12-14) [Zhao](#page-13-8) [et al., 2024;](#page-13-8) [Zhou et al., 2024b\)](#page-13-9) 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.

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109 110 111 112 113 114 115 116 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 [\(Nye et al.,](#page-11-5) [2021;](#page-11-5) [Wei et al., 2022;](#page-12-6) [Chen et al., 2022\)](#page-10-13). 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 [\(Brown et al., 2020\)](#page-10-14). 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.

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118 119 120 121 122 123 124 125 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.](#page-12-11) [\(2022\)](#page-12-11) showed that a simple RL algorithm, expert iteration, paired with curriculum learning can improve a formal theorem proving model. Self-Taught Reasoner (STaR) [\(Zelikman et al., 2022\)](#page-13-3) 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.](#page-12-7) [\(2023\)](#page-12-7) 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 [\(Polu et al., 2022\)](#page-12-11)). Our work builds on these ideas, providing the first study of bootstrapped thought-augmented proving.

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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\)](#page-2-0). Then we present Lean-STaR's data-generation ([§3.2.1,](#page-3-0) [§3.2.2\)](#page-3-1) and reinforcement learning $(\S3.2.3)$ phases. Finally, we present our evaluation protocols $(\S3.3)$.

3.1 PRELIMINARIES

135 136 137 138 139 140 *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 [\(De Moura et al.,](#page-10-0) [2015\)](#page-10-0), a popular interactive theorem prover. An example formal proof in Lean and its explanation are shown in Appendix [C.](#page-15-0)

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 thoughtaugmented 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 [\(Polu & Sutskever, 2020\)](#page-12-1), 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 [\(Polu & Sutskever, 2020\)](#page-12-1). 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

188 189 next tactic can then be expressed as:

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

193 194 195 196 197 198 199 200 201 202 203 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 [\(Brown et al., 2020\)](#page-10-14). To develop a language model capable of generating thoughts and tactics $a_i, t_i | s_i$, we need an entirely new dataset $D_T = \{(s^i, t^i, a^i) : i = 1, \dots, N\}$. However, in Lean, we only have a dataset of $D_S = \{(s^i, a^i) : i = 1, \dots, N\}$ 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 model^{[2](#page-4-2)}, 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.](#page-18-0) The design principle of the prompt is to prevent the oracle model from generating hindsight-like thoughts.

204 205 206 207 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

210 211 212 213 214 215 216 217 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 $D = \{s^i : i = 1, \dots, M\}$, 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.

218 219 220 221 This method can be seen as an offline RL method [\(Singh et al., 2023\)](#page-12-7) in the theorem proving MDP. In this MDP, the cumulative reward $R((s_0, t_0, a_0), (s_1, t_1, a_1), \cdots, (s_n, t_n, a_n)) = 1$ if and only if the proof trajectory is successful. The total expected reward is

$$
J(M, D) = \sum_{i} \mathbb{E}_{(s_0, t_0, a_0), \cdots, (s_n, t_n, a_n) \sim \pi_M(\cdot | s^i)} R((s_0, t_0, a_0), \cdots, (s_n, t_n, a_n)),
$$

and Lean-STaR's expert iteration can be seen as optimizing this reward [\(Singh et al., 2023\)](#page-12-7).

3.3 EVALUATION

228 229 230 231 232 233 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.

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 2 For 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 [\(Polu & Sutskever, 2020;](#page-12-1) [Yang et al., 2023;](#page-13-2) [Azerbayev et al., 2023b;](#page-10-12) [Welleck & Saha, 2023\)](#page-12-12). 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 $a_{i,1}...$ 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 [\(Polu](#page-12-1) [& Sutskever, 2020;](#page-12-1) [Yang et al., 2023;](#page-13-2) [Welleck & Saha, 2023\)](#page-12-12), we assume the state with maximum negative

282 283 284 285 286 287 288 289 290 log-probabilities is the "best"s. Specifically, we select state s_i with maximum $\sum_{i=1}^{i-1}$ $\sum_{j=0}$ – $\log p(a_j, s_j)$, where $(s_0, a_0), \cdots, (s_{i-1}, a_{i-1})$ 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.](#page-16-0) We attribute this to using average log probabilities, which may not be a reliable quality indicator when the thought sequence t_i is generated.

291 292 293 294 295 296 297 298 299 300 301 302 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_i . Figure [4](#page-5-0) compares best-first search and our sampling method.

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4 EXPERIMENTS

306 307 308 309 310 311 312 313 We instantiate Lean-STaR using the best available open language model pre-trained on the Lean corpus (InternLM2-Math-base-7b [\(Ying et al., 2024\)](#page-13-6)), and follow standard practice in using Lean's Mathlib as the underlying training set (via the Lean Dojo dataset [\(Yang et al., 2023\)](#page-13-2)). We generate an initial set of thoughts for Mathlib using GPT-4, perform two rounds of expert iteration, then evaluate the model on miniF2F [\(Zheng](#page-13-7) [et al., 2021\)](#page-13-7) and leandojo [\(Yang et al., 2023\)](#page-13-2), 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.

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4.1 EXPERIMENTAL SETUP

317 318 319 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.

320 321 322 323 We randomly select 17, 256 different successful proof trajectories from *LeanDojo Benchmark 4 dataset* [\(Yang](#page-13-2) [et al., 2023\)](#page-13-2), and use GPT-4-0125 [\(OpenAI, 2023\)](#page-12-15) 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](#page-14-0) due to space.

324 325 326 327 328 We evaluate our method on the *MiniF2F* benchmark [\(Zheng et al., 2021\)](#page-13-7). We use a similar evaluation setting as previous works [\(Yang et al., 2023;](#page-13-2) [Welleck & Saha, 2023;](#page-12-12) [Ying et al., 2024\)](#page-13-6), 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\)](#page-4-1). We choose these settings to resemble the inference budget used in our baselines, which follow previous work [\(Welleck & Saha, 2023;](#page-12-12) [Azerbayev et al., 2023b;](#page-10-12) [Ying et al., 2024\)](#page-13-6). Namely, for best-first **329 330 331 332 333 334** 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.

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363 364 365 366 367 368 search baselines we use beam search to generate the next tactic with $S = 32$, $K = 1$ [\(Welleck & Saha, 2023;](#page-12-12) [Azerbayev et al., 2023b;](#page-10-12) [Ying et al., 2024\)](#page-13-6). We do not compare with methods designed for other formal languages such as [Jiang et al.](#page-11-8) [\(2022\)](#page-11-8); [Xin et al.](#page-13-10) [\(2023\)](#page-13-10) since language differences greatly influence the pass rate due to the different tactics and automation. We also do not compare with [Lample et al.](#page-11-2) [\(2022\)](#page-11-2) 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

372 373 374 375 Our main results are reported in Table [7.](#page-17-0) 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 [\(Ying](#page-13-6) [et al., 2024\)](#page-13-6) using best-first search and 30.7% in COPRA [\(Thakur et al., 2023\)](#page-12-13) using GPT-4. With a larger compute budget, Lean-STaR's performance improves further to 36.1%.

376 377 378 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.](#page-17-0)

396 397 398 399 400 401 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,](#page-17-0) 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.

403 404 405 406 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 [\(Polu et al., 2022;](#page-12-11) [Zelikman et al., 2022;](#page-13-3) [Singh et al., 2023\)](#page-12-7)). Refer to Appendix [A.1](#page-14-0) for details.

407 408 409 410 411 412 413 We perform two iterations of expert iteration, and present the results in Table [7,](#page-17-0) 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
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- **419 420** We instantiate Lean-STaR using a stronger language model (InternLM2-Math-plus-7b [\(Ying et al., 2024\)](#page-13-6)), which was released after the experiment above. We follow a similar setup to the previous experiment.

421 422 In this experiment, we used 140, 000 thoughts annotated by GPT-4o [\(OpenAI, 2023\)](#page-12-15) 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 $N = 50, K = 32, \& T = 0.7$.

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.

439 440 441 442 443 Our new results are reported in Table [2.](#page-8-0) 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 [\(Ying](#page-13-6) [et al., 2024\)](#page-13-6). 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](#page-9-0) 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

454 455 456 457 458 459 460 461 462 463 464 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 [\(Carter & Monks,](#page-10-15) [2013;](#page-10-15) [Kang et al., 2020;](#page-11-12) [Szegedy, 2020;](#page-12-8) [Avigad, 2023;](#page-10-1) [First, 2023;](#page-10-2) [of Sciences, 2023\)](#page-12-0).

465 466 467 468 469 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.

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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 [\(Polu et al., 2022;](#page-12-11) [Zelikman et al., 2022;](#page-13-3) [Singh et al.,](#page-12-7) [2023\)](#page-12-7)). 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](#page-8-1) and Appendix [E.](#page-17-1)

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 $N = 50 \& K = 32 \& T = 0.7$.

 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,](#page-15-1) taken from [\(Lample et al.,](#page-11-2) [2022\)](#page-11-2). 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 case ih: $n \leq m \land n + k \leq m + k \Rightarrow$ $n + (k + 1) \le m + (k + 1)$. 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 $n \leq m \Leftrightarrow n+1 \leq m+1$. 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.

 Figure 5: A example proof and its visualization of $n \le m \Rightarrow n + k \le m + k$ in Lean, taken from [\(Lample et al., 2022\)](#page-11-2). 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.

752 753 754 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.

777 778 779 780 781 782 783 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 [\(Hendrycks et al., 2021\)](#page-11-13). These problems can have different levels of difficulty and types. Table [5](#page-16-1) 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

786 787 788 789 Table [6](#page-17-2) 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

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799 800 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 $N = 50, K = 32$.

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

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843 844 845 As shown in Table [8,](#page-18-1) 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.)

846 847 848 849 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.

E.1 SEARCH AND SAMPLING BUDGET

Table [9](#page-18-2) 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.

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F RETROSPECTIVE RATIONALE GENERATION PROMPT OF GPT-4

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      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.
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       # Write down the reasoning that can result in the selection of the Given Tactic.
       # Write down the Given Tactic.
      You have four principles to do this.
       # Craft reasoning that is comprehensive yet concise, contained ideally within
          two sentences.
       # Begin reasoning with the objective of the Given Theorem, ensuring logical
          progression, rather than constructing it retrospectively from the Given
          Tactic.
       # Avoid mentioning the Given Tactic and specific statement names from the Given
           Tactic throughout your reasoning.
       # Position the conclusion of the tactic after presenting all reasons, ensuring
          that details regarding the Given Tactic are not introduced at the start of
          your reasoning.
       Your output should be strictly in the following format and should not contain
          extra content:
       ### PLANNING OF REASONING
      Given the above goal and the given the target tactic <Given Tactic>, I should
          produce a reasoning that only based on the goal, and conclude to the exact <
          Given Tactic>, but not in the hindsight format.
       ### REASONING
      <your reasoning to the Given Tactic>
       ### TACTIC
       <Given Tactic>
       # Given Theorem:
       ```lean4
 {theorem["state_before"]}
       ```
       # Given Tactic:
       ```lean4
 {theorem["tactic"]}
       ```
```
987 988 G EXAMPLES OF GENERATED LEAN PROOFS WITH THOUGHTS

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       theorem aime_1990_p4 (x : R) (h<sub>0</sub> : 0 < x) (h<sub>1</sub> : x ^ 2 - 10 * x - 29 \neq 0)
            (h_2 : x \land 2 - 10 * x - 45 \neq 0) (h_3 : x \land 2 - 10 * x - 69 \neq 0)(h<sub>4</sub> : 1 / (x ^ 2 - 10 * x - 29) + 1 / (x ^ 2 - 10 * x - 45) - 2 / (x ^ 2 -
           10 \times x - 69 = 0: x = 13 :=
           norm_num at h<sub>1</sub> h<sub>2</sub> h<sub>3</sub> -- Reasoning: To prove `x = 13`, we examine the
           conditions under which the given equation holds, specifically focusing on
           the non-equality of the expressions involving x \wedge 2 - 10 \times x - 29, x \wedge 2- 10 \times x - 45, and x \times 2 - 10 \times x - 69. Simplifying these expressions
           using properties of real numbers and algebra allows us to directly compare
           them with their respective values, ultimately identifying x = 13 as the
           unique solution that satisfies all constraints.
           field_simp at \star -- Reasoning: To prove \{(x = 13)\}\), we leverage the given
            equalities involving rational fractions of \langle x^2 - 10x - c \rangle for various
            constants (c\), where (0 < x) and each (x^2 - 10x - c) is non-zero.
           By algebraically manipulating these expressions, we aim to derive a
           relationship among \langle x \rangle and these constants, specifically focusing on
           \langle 13\rangle, under the given non-zero conditions for the quadratic expressions.
           ring nf at h<sub>4</sub> \vdash -- Reasoning: To establish the equality `x = 13` under the
           given conditions, we need to manipulate the algebraic expression given by
            h_4 to reveal its dependence on x, recognizing that the presence of xin the expressions may affect the equation's truth value. The application
           of algebraic transformations on both sides of the equation will facilitate
           the identification of `x`'s value, taking into consideration the inequality
           conditions provided (`h<sub>1</sub>`, `h<sub>2</sub>`, `h<sub>3</sub>`).
           nlinarith - Reasoning: To prove \langle (x = 13) \rangle, we must manipulate the
           equation given by \langle h_4 \rangle to isolate \langle x \rangle, using the algebraic properties
           of equality and the assumption \langle h_0 \rangle which states \langle 0 \times x \rangle. This requires
           careful rearrangement and application of algebraic identities to simplify
           and rearrange terms, facilitating the direct application of the properties
           of real numbers to reach the desired conclusion.
       theorem amc12a_2002_p6 (n : N) (h<sub>0</sub> : 0 < n)
            : ∃ m, m > n ∧ ∃ p, m * p ≤ m + p :=
           use n + 1, by linarith only [h_0] -- Reasoning: To demonstrate the
           existence of such an `m' and `p' that satisfy the given inequalities, we
           leverage the property of natural numbers that ensures an increase in `n`
           from `0` leads to the possibility of finding such `m` and `p`. This
           approach is supported by the fundamental property of natural numbers and
           their arithmetic operations, suggesting that for a given `n` greater than
           `0`, there exists a successor `m` and a number `p` that satisfy the
           conditions outlined.
            exact \langle 0, by \sinh \rangle -- Reasoning: To demonstrate that there exists an (n)\in \mathbb{N}\setminus\{p\} such that \{(n + 1) * p \leq r + 1 + p\}) holds for some \{(p \in \mathbb{N} \mid \mathbb{N} \leq r + 1 + p\})\), we recognize that setting \(p = 0\) satisfies the inequality by the
           properties of zero in arithmetic. This is because (n + 1 > 0) by
           assumption, ensuring the left-hand side is non-negative and the right-hand
           side simplifies to (n + 1), making the inequality trivially true.
```


