

# LLM-based Automated Theorem Proving Hinges on Scalable Synthetic Data Generation

Junyu Lai<sup>1</sup> Jiakun Zhang<sup>1</sup> Shuo Xu<sup>1</sup> Taolue Chen<sup>2</sup> Zihang Wang<sup>1</sup> Yao Yang<sup>1</sup>  
 Jiarui Zhang<sup>1</sup> Chun Cao<sup>1</sup> Jingwei Xu<sup>1\*</sup>

<sup>1</sup>State Key Laboratory for Novel Software Technology, Nanjing University, China

<sup>2</sup>School of Computing and Mathematical Sciences, Birkbeck, University of London, UK

{junyu\_lai, zjk, shuoxu, wangzihang, yangyao, jiarui\_zhang}@smail.nju.edu.cn  
 t.chen@bbk.ac.uk, {caochun, jingweix}@nju.edu.cn

## Abstract

Recent advancements in large language models (LLMs) have sparked considerable interest in automated theorem proving and a prominent line of research integrates stepwise LLM-based provers into tree search. In this paper, we introduce a novel proof-state exploration approach for training data synthesis, designed to produce diverse tactics across a wide range of intermediate proof states, thereby facilitating effective one-shot fine-tuning of LLM as the policy model. We also propose an adaptive beam size strategy, which effectively takes advantage of our data synthesis method and achieves a trade-off between exploration and exploitation during tree search. Evaluations on the MiniF2F and ProofNet benchmarks demonstrate that our method outperforms strong baselines under the stringent *Pass@1* metric, attaining an average pass rate of 60.74% on MiniF2F and 21.18% on ProofNet. These results underscore the impact of large-scale synthetic data in advancing automated theorem proving.

## 1 Introduction

Reasoning has emerged as a frontier in large language model (LLM) research. Numerous approaches have been proposed to enhance their reasoning capabilities [Yu et al., 2024, Giadikiaroglou et al., 2024], among which mathematical reasoning [Ahn et al., 2024] has received special attention from both academia and industry. The reasons are twofold: (1) it is widely considered as a strong indicator of LLM’s cognitive proficiency; and (2) it has a direct application in the emerging AI4Math area and great potential in software engineering [Li et al., 2024, Liu et al., 2024]. While extensive research has focused on solving mathematical problems given in natural language [Muennighoff et al., 2025, Xiang et al., 2025], we are mostly interested in proving theorems formulated in formal mathematical languages, because it represents a more fundamental challenge. To this end, we synergize interactive theorem provers (ITPs, aka proof assistant), represented by Lean [Moura and Ullrich, 2021], Isabelle [Paulson, 1994] and Rocq (previously known as Coq, [Barras et al., 1997]), and LLMs, effectively giving rise to a neuro-symbolic approach towards automated theorem proving (ATP).

In the literature, there are generally two classes of approaches which harness LLMs for ATP, commonly referred to as *tree search* methods and *whole-proof generation* methods [Ren et al., 2025]. The former repeatedly performs proof step generation, utilizing LLMs to prescribe a tactic to be applied to the current proof state. Overall, it is cast as a tree search process to generate the final proof. In contrast, the latter is performed in an end-to-end style, where LLMs are asked to produce an entire proof directly from the theorem, which is then verified by the proof assistant. Generally speaking, the

---

\*Corresponding author

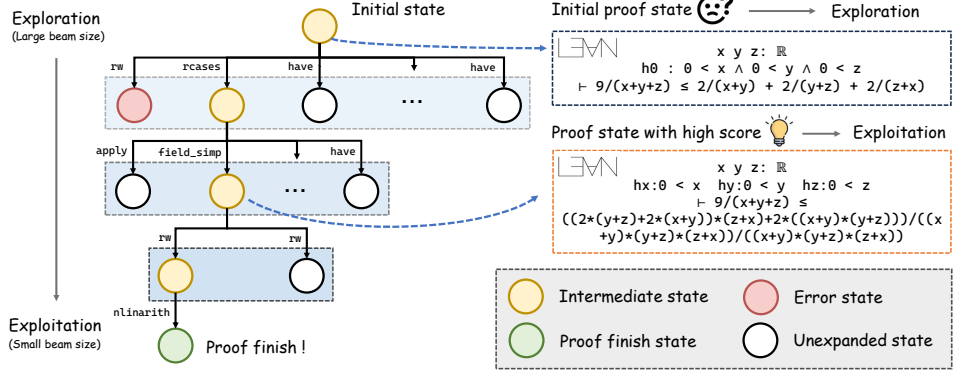


Figure 1: An illustration of the proposed tree search strategy. The example is derived from the MiniF2F benchmark, specifically the problem *algebra\_9onxpyzleqsum2onxpy*. For simplicity, only the tactics are retained in the depicted proof states, while the associated premises are omitted.

whole-proof methods are simpler, requiring less communication to coordinate between the LLM and the ITP. However, as the intermediate proof states are hidden, LLMs typically struggle to generate a long proof. In practice, these methods usually heavily rely on additional techniques, such as natural language comments to assist the proof [Lin et al., 2025, Xin et al., 2024a].

In our work, we adopt a tree search approach. This class of methods is advantageous in demanding relatively lower capability on the policy model, making it suitable for settings with smaller model sizes and limited computational resources. It also offers greater flexibility for incorporating customized, problem-specific strategies into the search process [Wang et al., 2024, An et al., 2024]. Furthermore, starting from a small number of seed problems, tree search enables extensive exploration of proof states, facilitating the synthesis of large volumes of new data for iterative training of the policy model, which is considerably challenging to achieve in whole-proof generation [Xin et al., 2024b]. We take Lean 4 as the base ITP due to its popularity in the community, although our methodology can be easily applied to other proof assistants.

Despite the advance in LLMs, they remain notably limited in formal mathematical reasoning [Yang et al., 2024a]. An fundamental cause is that LLMs are typically trained for general-purpose language understanding rather than for theorem proving, which requires substantial domain expertise in mathematics. To overcome this gap, post-training is indispensable, for which we focus on fine-tuning. A major challenge lies in the scarcity of high-quality training data for theorem proving. Proofs in ITPs are typically expressed as code in a domain-specific language (DSL) defined by the corresponding prover. Compared to widely used programming languages such as Python, proofs written in Lean are extremely limited in volume. For instance, standard Lean 4 libraries (e.g., Mathlib [mathlib Community, 2020]) provide less than 1GB data in total, insufficient for effectively fine-tuning LLMs. As a result, synthetic data generation has become a crucial component in adapting LLMs for ATP. Recent efforts have explored translating natural language mathematics into Lean 4 syntax using LLMs [Wu et al., 2022, Ying et al., 2024, Murphy et al., 2024], generating new problems by sampling from distributions (e.g., a fine-tuned policy model) learned over existing Lean 4 formalizations [Dong and Ma, 2025, Poesia et al., 2024, Xin et al., 2024b]. Another approach to improving model capability is Expert Iteration (EI) [Polu and Sutskever, 2020], which can be treated as a form of rejection sampling. Given a set of formalized mathematical problems, a model may fail to solve the more difficult instances but succeed on simpler ones. By collecting successful proofs from these solvable cases, a new dataset can be constructed to fine-tune the model, thereby gradually enhancing its capabilities. This method has been widely used in prior work [Polu and Sutskever, 2020, Polu et al., 2022, Wu et al., 2024, Xin et al., 2025]. However, EI suffers from significant inefficiency when applied in conjunction with tree search. In each iteration, the number of newly solvable problems is often limited, while performing full search over the entire dataset incurs substantial computational cost. This inefficiency makes EI impractical in settings with limited computational resources, highlighting the need for a more direct and resource-efficient data generation strategy.

In this paper, we propose a data synthesis method called *proof state exploration* for fine-tuning LLMs in ATP, along with a complementary *adaptive beam size strategy* for tree search during the proving process. Our data synthesis method begins with a set of formalized mathematical problems as seeds and leverages the existing policy model to explore related intermediate proof states via tree search. These intermediate states may correspond to goals that are logically equivalent to the original ones after a sequence of transformations, or to subgoals resulting from original problem decomposition. During the process, we explicitly decouple the generation of tactics from that of premises. Specifically, we adopt a constrained decoding algorithm [Hokamp and Liu, 2017] that restricts the model to sample from and de-duplicate within a curated set of commonly used tactics, followed by premise completion handled by the policy model. In addition, we introduce a heuristic pruning strategy to balance the trade-off between diversity in the generated outputs and computational efficiency during the exploration. This enables large-scale synthesis of intermediate proof states and transformation steps within tree search, thereby reducing the distribution gap between the training data and real-world proving scenarios. Moreover, our method does not rely on EI. Instead, our policy model is trained on data generated from a single, exhaustive exploration over existing formalized problems. This one-pass generation approach significantly reduces computational overhead while achieving competitive performance.

Although the LLM fine-tuned on this synthetic dataset can serve as a policy model capable of generating diverse tactics, it may not always prioritize proof completion during actual theorem proving. To mitigate this limitation, we propose a simple yet effective *adaptive beam size strategy* tailored to our data synthesis framework and integrated into the tree search process (cf. Figure 1). The strategy starts with a relatively large beam size to encourage broad exploration of the space of proof states. As the search proceeds, the beam size is gradually reduced, enabling the policy model to concentrate on high-scoring proof states. This dynamic adjustment improves the focus of the search and enhances the overall success rate of proof completion. Besides, we develop Dojo-BeamSearch-Visualization (DoBeVi) (cf. Appendix A.3) as the basic interaction tool between the model and the Lean 4 prover with a visualization module for tree search analysis.

*Evaluation.* We evaluate our method on two widely adopted benchmarks, MiniF2F and ProofNet, achieving average pass rates of 60.74% and 21.18%, respectively, under the constraints of *Pass@1* and a limited computational budget. These results outperform the current state-of-the-art methods based on tree search.

The main contributions of this paper are as follows.

- We propose a novel data synthesis method, *proof state exploration*, which enables large-scale generation of exploration data for fine-tune LLMs as policy models in ATP.
- We propose a simple but efficient *adaptive beam size strategy* that synergistically operates with the data synthesis method, effectively guiding the search process towards proof completion.
- We carry out extensive experiments demonstrating that our method can effectively balance exploration and exploitation during tree search, achieving state-of-the-art performance among existing tree search methods.

## 2 Background

*ITP and ATP.* In a nutshell, interactive theorem proving is a process to develop and verify formal proofs with the assistance of a computer, usually within a proof assistant (e.g., Lean, Isabelle, Rocq), and involves human guidance to structure and complete the proof. The general process is to formalize the theorem to be proven (i.e., the goal) in the language of the proof assistant first, and then repeatedly apply tactics to break the goal into subgoals. The tactic may involve case analysis, induction, rewriting, application of lemmas or axioms, etc. As such, the human user iteratively refines the proof to guide the prover, choosing which rules to apply and in what order. The prover checks that each inference step is valid according to the rules of the formal system. A major drawback is that this process requires heavy human expertise and thus largely lacks automation. LLM-based Automated Theorem Proving aims to find a proof automatically by simulating this process, effectively replacing the human user by an LLM.

*Tree Search LLM-based ATP.* As mentioned in the Section 1, we adopt a tree search approach towards LLM-based ATP. Generally speaking, tree search is a class of decision-making algorithms which

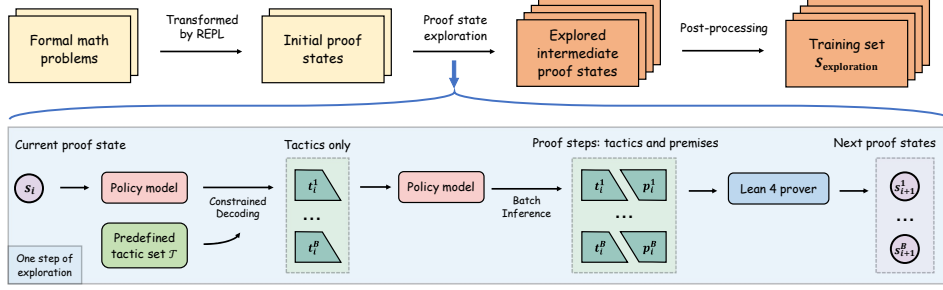


Figure 2: An illustration of the data synthesis pipeline.

consists of searching combinatorial spaces represented by trees, where nodes denote states and edges denote transitions (actions) from one state to another. In our setting, they enable an efficient navigation of the large and complex proof space.

At a high level, tree search LLM-based ATP can be cast as a reinforcement learning (RL) problem, where the state space comprises the proof states (aka proof terms). In general, proof states represent the current status of the proof at any given point in the interactive session between LLM and the proof assistant. Typically, they comprise the context (i.e., a list of assumptions, hypotheses and local variables), the current (sub)goals (i.e., the proposition needing to prove to complete the proof) and the number of subgoals to be proven. LLM acts as an actor, which, given the current proof state  $s_i$ , generates a tactic. In other words, LLM serves as the *policy model*. In theorem proving, tactics refer to commands, or instructions, that guide the process of constructing a proof. In RL terms, tactics can be regarded as an action  $a_i$ , based on which the proof assistant produces a new proof state  $s_{i+1}$ . This process continues until either the theorem is successfully proved or the maximum number of iterations is reached.

There are a plethora of search strategies, for instance, Monte Carlo tree search (MCTS) or best-first search (BFS). In BFS, each expansion step involves using the policy model to perform beam search decoding, generating a fixed number of top candidates (called the beam size). Typically, the process begins at the root node and iteratively expands the current node to produce potential child nodes. These candidates are then evaluated using a heuristic scoring function, and the node with the highest score is selected for the next expansion. The expansion-score-selection steps are repeated until a goal is reached or a termination condition is met. In our work, LLM, as the policy model, generates a set of tactics  $\{t_i^j\}_{j=1}^B$  for a proof state  $s_i$ , which are executed by the proof assistant one by one to obtain the corresponding set of next proof states  $\{s_{i+1}^j\}_{j=1}^B$ .

### 3 Methods

#### 3.1 Data synthesis by proof state exploration

In ITP, tactics play a central role. Normally, a tactic (e.g., `rw [add_assoc add_comm]`) consists of the tactic operator (e.g., `rw`) and the premises (e.g., `add_assoc` and `add_comm`). In this paper, to facilitate a finer-grained decomposition, what is commonly referred to as tactics are called *proof steps*, while *tactic* refers to the operator only. We propose to carry out *proof state exploration* to synthesize data. This is similar to tree search, but the crucial difference is that we prioritize the diversity of tactics. Our data synthesis method is described as Algorithm 1. (cf. Figure 2 as well).

**Motivated explanation.** The intuition is that proof assistants (e.g., Lean 4) normally provide a versatile range of tactics, which is considerably larger than, e.g., the set of reserved words in programming languages, and can even be defined by users. It is practically infeasible to adopt all of them in tree search. On the other hand, in practice, their actual use in theorem proving may not be as wild as, e.g., user-defined functions (which are virtually infinite, or at least cannot be enumerated exhaustively). Hence, as a trade-off, a reasonably curated set of commonly used tactics is sufficient to solve the vast majority of problems in practice. Besides that, for tree search, critically we need an “effective” set of (proof state, tactic) pairs. The observation is that in theorem proving, the same tactic

may have multiple meanings and can be used across various scenarios; for instance, the `apply` tactic may be used in five different scenarios.<sup>2</sup> Moreover, sometimes a tactic can be used in much broader cases; for instance, the tactic `rf1` can handle all *definitional equalities*. However, as the policy model, the LLM, like an inexperienced problem solver, may fail to realize that a tactic can actually be used when a proof state is encountered. Ideally, such domain-specific knowledge should be injected into LLMs via training, as they largely fall short of a certain level of abstraction capabilities so would be hard to learn via the standard tree search.

**The proposed proof state exploration method.** We intend to identify those tactics which occur rarely (with low probability) at a proof state. Just like a human problem solver normally has the “comfort zone” for certain methods when facing a problem, in tree search, the policy model likely picks up the tactic which has a higher probability. Quite often, this is sub-optimal or may represent a missed opportunity. Our proof state exploration may force the policy model to explore those tactics which it does not typically explore (i.e., force it to jump out of its comfort zone), by which a more diverse training set can be constructed.

To this end, we first identify the frequently used tactics. We scan the entire Mathlib to collect all defined tactics.<sup>3</sup> There are hundreds of them, most of which are rarely used. To filter these out, we need a representative dataset from which the frequency of each tactic can be collected. In our work, we use the STP dataset [Dong and Ma, 2025] from which a total of 173 distinct tactics are obtained. To further refine the set, we apply nucleus sampling with a threshold of  $\mathcal{P} = 0.999$  to filter out rarely used tactics, ultimately yielding a set  $\mathcal{T}$  of 60 commonly used tactics.

The design of the proof state exploration is guided by the above intuition and resembles the tree search. For each expansion step, we apply Constrained Decoding to force the LLM to output  $B$  different tactics (without premises) in  $\mathcal{T}$ . We set a large beam size (e.g.,  $B = 32$ ). After obtaining  $\{(s_i, t_i^j)\}_{j=1}^B$  with  $t_i^j \in \mathcal{T}$ , we feed these pairs back into the policy model to complete the premises, yielding a set  $\{(s_i, t_i^j, p_i^j)\}_{j=1}^B$  of proof steps from  $s_i$ . By applying each  $(t_i^j, p_i^j)$  to  $s_i$  using Lean 4 prover, we generate the corresponding set of next proof states  $s_{i+1}^j$ . Note that for exploration, even if *proof finish* state is encountered, the exploration continues until the entire budget is exhausted.

Potential issues for this proof state exploration include (1) as  $B$  is often large, obtaining deeper proof states (i.e., those “far away” from  $s_0$ ) can take a long time under limited computational resources; (2) in certain proof states, a large beam size can lead to the generation of meaningless proof steps. For example, the model may construct hypotheses that do not contribute to the progress of the proof.

To address these, we apply two heuristic strategies: (1) During each expansion, we prune the set by retaining only  $\alpha B$  branches, typically setting  $\alpha = 0.25$ . When pruning, we keep the top  $\beta$  branches with the highest joint probabilities and then randomly sample the remaining  $(\alpha B - \beta)$  branches uniformly from the rest. This balances exploration diversity and efficiency while preserving some of the policy model’s inherent tendency toward proof finish. (2) Some seeds are overly simple and do not require extensive exploration; too much exploration may even degrade the quality of the synthetic data. To control this, we use proof finish as a signal: if a distinct path achieving proof finish is found during an expansion, we reduce the expansion budget by a factor of  $\gamma = 0.9$ . This allows a simple seed to quickly terminate exploration after generating multiple distinct solutions, improving overall data synthesis efficiency.

After the proof state exploration, we obtain a dataset  $S_{\text{exploration}}$ . To produce the final dataset, we apply three post-processing steps: (1) De-duplication, to remove redundant samples; (2) Decontamination, where we use BLEU as a similarity metric to eliminate examples with high overlap with the evaluation benchmark; and (3) Rejection Sampling, where we discard all transitions that are invalid from the Lean 4 prover. The generated data is ultimately used to train policy LLM by performing Supervised Fine-Tuning on a base model using the full accumulated training data corpus.

### 3.2 Adaptive beam size strategy

The tree search approaches used for ATP are conceptually similar [Polu and Sutskever, 2020, Polu et al., 2022, Wu et al., 2024, Xin et al., 2025], differing mainly in (1) the policy model, (2) the scoring

<sup>2</sup>[https://www.ma.imperial.ac.uk/~buzzard/xena/formalising-mathematics-2024/Part\\_C/tactics/apply.html#](https://www.ma.imperial.ac.uk/~buzzard/xena/formalising-mathematics-2024/Part_C/tactics/apply.html#)

<sup>3</sup><https://github.com/haruhisa-enomoto/mathlib4-all-tactics>

---

**Algorithm 1:** Proof State Exploration Algorithm for Data synthesis.

---

```
Data:  $S = \{s_{0,n}\}_{n=1}^{|S|}$ ;          /*  $S$  is the original formalized datasets. */
Result:  $S_{\text{exploration}}$ 
 $S_{\text{exploration}} \leftarrow \emptyset$ ;
for  $s_{0,n} \in S$  do
     $s_0 \leftarrow s_{0,n}$ ;          /* ignore index  $n$  for simplicity */
     $q \leftarrow \emptyset$ ;
     $b \leftarrow 0$ ;          /*  $b$  is the consumed budget. */
     $q.\text{add}(s_0)$ ;
    while  $|q| > 0$  and  $b < \text{budget}$  do
         $s_i \leftarrow q.\text{get}()$ ;
         $\{t_i^j\}_{j=1}^B \leftarrow \text{policy\_model.constrained\_decoding}(s_i, \mathcal{T})$ ;
         $\{p_i^j\}_{j=1}^B \leftarrow \text{policy\_model.batch\_inference}(s_i, \{t_i^j\}_{j=1}^B)$ ;
        for  $j \in [1, B]$  do
             $s_{i+1} \leftarrow \text{lean\_prvoer}(s_i, t_i^j, p_i^j)$ ;
             $S_{\text{exploration}}.\text{add}((s_{i+1}, t_i^j, p_i^j, s_i))$ ;
            if  $s_{i+1}$  is a valid proof state then
                 $q.\text{add}(s_{i+1})$ ;
            end
        end
         $b.\text{add\_budget}()$ ;
    end
end
 $S_{\text{exploration}} \leftarrow \text{post\_processing}(S_{\text{exploration}})$ 
```

---

function, (3) the beam size, and (4) other budget-related parameters. In our tree search procedure, the policy model is trained using data collected by the proof state exploration, as in Section 3.1. For the score function, we take the sum of the LLM’s logarithmic joint probability over the beam (during beam search) and the parent node’s score as the current node’s score, that is:

$$\text{score}(s_{i+1}^j) = \log P_\theta(t_j|s_i) + \text{score}(s_i) \quad (1)$$

where  $P(t_j|s_i)$  is the model’s predicted probability of applying the tactic  $t_j$  at the state  $s_i$  and  $\theta$  denotes the policy models parameters.

In this work, we focus the pruning strategy on dynamically decaying the *beam size* during the tree search process. This design is motivated by the empirical finding that beam size has a particularly significant impact on overall performance compared to other factors in tree search. The details of the finding are presented in Section 4.3. The optimal beam size is difficult to determine in advance. The general observation is that, if the beam size is too small, the search may fail to discover proof states, missing potential opportunities; if the beam size is too large, the search may risk being trapped within one sub-tree rooted at a high-scoring intermediate node, resulting in futile expansions. Hence, it is necessary to adapt the beam size to better control the tree search.

We adopt a larger beam size at the early stages of tree search; as the search proceeds (i.e., the depth increases), we gradually reduce the beam size. This is largely aligned with the aforementioned observation. In particular, during the later stages of tree search, being trapped is particularly harmful as it may dump the search budget. By reducing the beam size, we effectively prune away less relevant branches and prevent the search from over-committing to one sub-tree too much. One may intuitively understand the design by taking an analogy of an IMO contestant. At the early stage, (s)he may want to widen the horizon by exploring different problem-solving strategies (e.g., reading books, surfing AoPS). However, when sitting in the competition (i.e., at a later stage), (s)he would better focus on relatively small strategies to attempt, prioritizing solving the problems successfully. To this end, we design an adaptive beam size function, namely,

$$\text{beam\_size} = B_{\min} + (B_{\max} - B_{\min}) \times \max(1 - \lambda M, 0) \quad (2)$$

where  $M = e/E$ , with  $e$  denoting the current expansion step and  $E$  representing the maximum number of expansions allowed by the budget. The parameter  $\lambda$  is a hyperparameter controlling the

decay rate of the beam size. The beam size gradually decreases from  $B_{\max}$  to  $B_{\min}$  as the search proceeds, thereby realizing the adaptive behavior described earlier. This search dynamic has also been confirmed empirically (cf. Figure 3 in Appendix).

## 4 Experiments

### 4.1 Evaluation settings

Below are the basic experimental settings (cf. Section A.4 for more details). All experiments were conducted on a server with 8 H800 GPUs; the code and model checkpoint are available<sup>4</sup>.

**Models.** We use Qwen2.5-Math-7B [Yang et al., 2024b] as the base model to train the policy model. During full fine-tuning, we use a batch size of 2,048 and a learning rate of  $2 \times 10^{-5}$ , training for one epoch. A cosine annealing schedule is employed for learning rate, reaching 10% of its initial value by the end of the epoch. Notably, the model training process does *not* incorporate EI.

**Datasets.** We use the STP dataset [Dong and Ma, 2025] as the seed and adopt BFS-Prover [Xin et al., 2025] as the policy model for *proof state exploration*. We first generate the synthetic dataset following the method in Section 3.1. Then, before the actual training begins, the dataset is further combined with human-authored data from Mathlib, followed by deduplication and decontamination. This results in a final training set comprising approximately 20 million proof transitions.

**Baselines.** We select two state-of-the-art models that also use tree search methods, InternLM2.5-StepProver [Wu et al., 2024] and BFS-Prover [Xin et al., 2025], as main baseline models, applying the same search budget in our experiments.

**Environments.** We develop DoBeVi (cf. Appendix A.3) as the basic interaction tool between the model and the Lean 4 prover (v4.10.0).

**Benchmarks, metrics and computation budgets.** We evaluate on two popular benchmarks, MiniF2F [Zheng et al., 2021] and ProofNet [Azerbaiyev et al., 2023a], using *Pass@1* as the metric. We follow the commonly adopted search budget in tree search methods:  $K \times B \times E$ , where  $K$  is the number of searches per theorem (i.e.,  $k$  in *Pass@k*);  $B$  is the beam size per expansion; and  $E$  is the maximum number of expansions allowed in a single search.

### 4.2 Main results

Table 1 presents the results of our model alongside baseline methods on MiniF2F and ProofNet. We fix  $K = 1$  and  $E = 600$  and adopt the beam sizes used in the original baseline papers. If a baseline has reported results under the same computational budget, we directly use those results; otherwise, we re-evaluate the baseline using our own tree search implementation under identical experimental settings, including additional search techniques detailed in Appendix A.4.

The results demonstrate that our method achieves better evaluation performance even under a relatively constrained computational budget without relying on EI. Moreover, under the fixed beam size setting, the optimal beam sizes for our policy model are found to be 8 on MiniF2F and 32 on ProofNet, respectively. By adopting our adaptive beam size strategy, we are able to further improve performance without searching for the best beam size settings.

### 4.3 Discussions

Unlike whole-proof generation methods, the performance of tree search methods is influenced by a variety of factors, in addition to the policy model. We found that the beam size is particularly critical, sometimes even comparable in importance to the policy model’s capability. As shown in Table 1, both our model and the baselines exhibit different optimal beam size choices across the MiniF2F and ProofNet benchmarks. We attribute this primarily to differences in training data distribution. Currently, most publicly available Lean 4 training datasets are derived from Lean-Workbook [Ying et al., 2024], whose distribution resembles the MATH subset of MiniF2F. Consequently, using a larger beam size in such settings tends to introduce redundant search branches, causing the search to

<sup>4</sup>The implementation code is accessible at [https://github.com/NJUDeepEngine/llm\\_based\\_atp](https://github.com/NJUDeepEngine/llm_based_atp). The policy model is accessible at [https://huggingface.co/NJUDeepEngine/llm\\_based\\_atp](https://huggingface.co/NJUDeepEngine/llm_based_atp)

Table 1: Overall evaluation results across MiniF2F-test and ProofNet-test. All baseline results evaluated by us are marked with an asterisk (\*), while the remaining results are directly imported from the original papers.

Method	Model Size	Budget	MiniF2F-test	ProofNet-test
Llemma [Azerbaiyev et al., 2023b]	7B	$1 \times 32 \times 100$	26.23%	-
ReProver [Yang et al., 2023]	229M	$K=1$	26.50%	13.80%
Lean-STaR [Lin et al., 2024]	7B	$64 \times 1 \times 50$	46.30%	-
InternLM2.5-StepProver[Wu et al., 2024]	7B	$1 \times 32 \times 600$	$47.3\% \pm 1.1\%$	$19.89\% \pm 0.68\%$ *
BFS-Prover[Xin et al., 2025]	7B	$1 \times 2 \times 600$	$55.49\% \pm 0.61\%$ *	$12.37\% \pm 1.44\%$ *
Ours (fixed beam size)	7B	$1 \times 4 \times 600$	$56.56\% \pm 1.13\%$	$13.01\% \pm 0.79\%$
		$1 \times 8 \times 600$	<b><math>59.51\% \pm 0.79\%</math></b>	$17.53\% \pm 0.26\%$
		$1 \times 16 \times 600$	$59.02\% \pm 1.13\%$	$19.35\% \pm 0.96\%$
		$1 \times 32 \times 600$	$57.05\% \pm 0.4\%$	<b><math>20.75\% \pm 0.94\%</math></b>
Ours (adaptive beam size)	7B	$K = 1, E = 600$	<b><math>60.74\% \pm 0.88\%</math></b>	<b><math>21.18\% \pm 0.55\%</math></b>

waste the budget without improving results. In contrast, for benchmarks such as ProofNet, which contain more out-of-distribution samples, increasing the beam size is necessary, which allows the model to explore a broader set tactics in the hope of reaching intermediate proof states similar to those encountered during training.

In tree search, a smaller beam size naturally makes the entire tree taller and thinner, resulting in longer average search depths (cf. Appendix A.7). Moreover, if the first expansion results are suboptimal, the subsequent search process may not reach proof finish at all. Therefore, when restricted to *Pass@1*, a beam size of 2 leads to larger variance, often requiring an increase in  $K$  within the budget to reduce the impact of randomness. This small beam size scenario is suitable when, during tree search, the policy model encounters a state similar to one it has learned before and can confidently select a proof step which likely leads to proof finish. Conversely, a larger beam size makes the tree structure shallower and wider, reducing the average search depth but potentially introducing many useless proof steps into the tree, lowering the search efficiency.

In addition, we adopt a standard formulation for the scoring function, which evaluates the tactic  $t_j$  rather than the new state  $s_{i+1}^j$ . As shown in Equation 1, the effectiveness of this scoring function primarily stems from the fact that a higher value of  $P(t_j | s_i)$  indicates that the policy model is more likely to have encountered proof states similar to  $s_i$  during training. As a result, it can, to some extent, prioritize proof steps that are more helpful for completing the proof. However, we argue that this scoring function still suffers from significant issues. For a detailed discussion and several unsuccessful attempts, please refer to Appendix A.5.

## 5 Related Work

**Automated theorem proving.** ATP has been a classic research area which is historically dominated by symbolic approaches [Pastre, 1993, Schürmann and Pfenning, 1998, Leino, 2013]. In recent years, the rise of LLMs has spurred renewed interest. One representative work is GPT-f [Polu and Sutskever, 2020], which uses the Expert Iteration approach to train the LLM for next proof step generation based on the current state, combined with tree search methods to prove theorems. Subsequent tree search methods have followed similar ideas, e.g., Polu et al. [2022], Lample et al. [2022], Lin et al. [2024]. Additionally, some work improves tree search tailored in ATP. For example, Wu et al. [2024] uses the DPO algorithm to train an auxiliary value network to evaluate intermediate proof states, avoiding the issue of directly using raw beam search probabilities as scoring signals.

In contrast, whole-proof generation methods [Xin et al., 2024a, Lin et al., 2025, Zhang et al., 2025, Wang et al., 2025a] aim to produce an entire proof in a single forward pass from the initial goal. While these methods do not leverage intermediate proof states, they are typically more efficient and allow for multiple rollouts to increase the likelihood of success. A notable example is DeepSeek-Prover-V1.5 [Xin et al., 2024a], which enhances performance by inserting natural language chain-of-thought (CoT) commentary into Lean 4 proofs during inference. Additionally, MA-LoT [Wang et al., 2025b] introduces a multi-agent architecture where separate models are responsible for analyzing and revising incorrect proofs, enabling iterative refinement toward a correct solution.



**Data synthesis for theorem proving.** One of the major bottlenecks in LLM-based automated theorem proving remains the lack of high-quality training data, particularly for Lean 4, a relatively new language with limited existing formalized data. Existing data generation methods can be broadly categorized into two groups.

The first category leverages LLMs to generate Lean 4 problems by building on the abundance of natural language mathematics. These approaches are generally referred to as *autoformalization*. However, current efforts primarily focus on autoformalizing problem *statements*, with less attention given to the autoformalization of proof processes [Wang et al., 2025a, Lu et al., 2024].

The second category bootstraps from a small set of existing Lean 4 problems to generate new ones through iterative synthesis. These methods typically involve a two-model framework: one model generates new conjectures, and the other attempts to prove them, enabling co-evolution of data and model capabilities. For instance, STP [Dong and Ma, 2025] uses problems from the Lean-Workbook dataset [Ying et al., 2024] as seeds. A conjecturer proposes conjectures related to the original problems, while a prover attempts to validate them—allowing both the training set and the model to be refined through this iterative process.

## 6 Limitations

**Limited adaptivity in beam size selection.** As discussed in Section 4.3, beam size is a critical factor in the effectiveness of tree search. While our proposed strategy provides a simple and effective means of dynamically adjusting the beam size, a more principled solution would involve training a dedicated model that, given a current proof state, predicts the optimal beam size for the policy model to use. Ideally, such a model would offer fully adaptive control during search. However, in practice, we found this approach challenging to implement. The primary difficulty lies in collecting sufficient high-quality training data for learning beam size prediction. Moreover, it is difficult for such a model to operate independently of the policy model, since the optimal beam size can be highly dependent on the specific behavior of the underlying policy model. As a result, we opted for a simple adaptive beam size decay strategy that complements our data synthesis framework. Exploring how to build more sophisticated, model-agnostic beam selection mechanisms, potentially via auxiliary learning signals or joint training, remains an open direction for future work.

**Potentially suboptimal scoring function.** Most current tree search methods based on best-first search apply the scoring function directly to the tactic or action, rather than to the resulting proof state. We argue that a more general and expressive scoring function should evaluate the entire transformation path from the root state  $s_0$  to the current state  $s_i$ , i.e.,

$$\text{score}(s_i) = f((s_0, t_0, s_1), (s_1, t_1, s_2), \dots, (s_{i-1}, t_{i-1}, s_i)).$$

Since this formulation may be too complex to implement in practice, we adopt a simplified approximation inspired by first-order Markov processes, assuming  $\text{score}(s_i) = f(s_{i-1}, t_{i-1}, s_i)$ . This structure provides two key advantages: (1) it allows for immediate pruning of low-quality transformations during search, saving computational budget; and (2) it supports path-level quality estimation via aggregation, e.g., by computing  $\sum_{n=1}^j \text{score}(s_n)$  or  $\prod_{n=1}^j \text{score}(s_n)$  across the trajectory. Nevertheless, further exploration is needed to design more expressive, yet computationally feasible, scoring functions that better capture long-range dependencies in proof trajectories.

**Dependence on the seed dataset.** A fundamental limitation of our data generation framework is its dependence on the seed dataset. The synthesized data is effectively constrained to the local neighborhood of the seed problems in the sample space. As a result, if the target problem lies far from the seed set in terms of distribution or difficulty, our method may struggle to generate useful intermediate states or transformations. In other words, under our current formulation, producing examples that are significantly more difficult than those in the seed set remains an open challenge.

## 7 Conclusions

In this paper, we have presented a data synthesis method and an adaptive tree search pruning strategy for automated theorem proving in Lean 4. Our proposed approach enables large-scale generation of

intermediate proof states and transformation steps without relying on ground-truth solutions, while maintaining diversity in the synthetic data. Combining with the adaptive beam size strategy, our method effectively balances exploration and exploitation throughout the tree search process. Together with the developed DoBeVi Lean 4 interaction tool, we expect our contributions will support and inspire further research within the ATP community, which is burgeoning but under development.

## References

- Fei Yu, Hongbo Zhang, Prayag Tiwari, and Benyou Wang. Natural language reasoning, a survey. *ACM Computing Surveys*, 56(12):1–39, 2024.
- Panagiotis Giadikiaroglou, Maria Lymperaiou, Giorgos Filandrianos, and Giorgos Stamou. Puzzle solving using reasoning of large language models: A survey. *arXiv preprint arXiv:2402.11291*, 2024.
- Janice Ahn, Rishu Verma, Renze Lou, Di Liu, Rui Zhang, and Wenpeng Yin. Large language models for mathematical reasoning: Progresses and challenges. *arXiv preprint arXiv:2402.00157*, 2024.
- Jia Li, Edward Beeching, Lewis Tunstall, Ben Lipkin, Roman Soletskyi, Shengyi Huang, Kashif Rasul, Longhui Yu, Albert Q Jiang, Ziju Shen, et al. Numinamath: The largest public dataset in ai4maths with 860k pairs of competition math problems and solutions. *Hugging Face repository*, 13:9, 2024.
- Junwei Liu, Kaixin Wang, Yixuan Chen, Xin Peng, Zhenpeng Chen, Lingming Zhang, and Yiling Lou. Large language model-based agents for software engineering: A survey. *arXiv preprint arXiv:2409.02977*, 2024.
- Niklas Muennighoff, Zitong Yang, Weijia Shi, Xiang Lisa Li, Li Fei-Fei, Hannaneh Hajishirzi, Luke Zettlemoyer, Percy Liang, Emmanuel Candès, and Tatsunori Hashimoto. s1: Simple test-time scaling. *arXiv preprint arXiv:2501.19393*, 2025.
- Violet Xiang, Charlie Snell, Kanishk Gandhi, Alon Albalak, Anikait Singh, Chase Blagden, Duy Phung, Rafael Rafailov, Nathan Lile, Dakota Mahan, et al. Towards system 2 reasoning in llms: Learning how to think with meta chain-of-thought. *arXiv preprint arXiv:2501.04682*, 2025.
- Leonardo de Moura and Sebastian Ullrich. The lean 4 theorem prover and programming language. In *Automated Deduction—CADE 28: 28th International Conference on Automated Deduction, Virtual Event, July 12–15, 2021, Proceedings 28*, pages 625–635. Springer, 2021.
- Lawrence C Paulson. *Isabelle: A generic theorem prover*. Springer, 1994.
- Bruno Barras, Samuel Boutin, Cristina Cornes, Judicaël Courant, Jean-Christophe Filliatre, Eduardo Gimenez, Hugo Herbelin, Gerard Huet, Cesar Munoz, Chetan Murthy, et al. *The Coq proof assistant reference manual: Version 6.1*. PhD thesis, Inria, 1997.
- Z. Z. Ren, Zhihong Shao, Junxiao Song, Huajian Xin, Haocheng Wang, Wanbiao Zhao, Liyue Zhang, Zhe Fu, Qihao Zhu, Dejian Yang, Z. F. Wu, Zhibin Gou, Shirong Ma, Hongxuan Tang, Yuxuan Liu, Wenjun Gao, Daya Guo, and Chong Ruan. Deepseek-prover-v2: Advancing formal mathematical reasoning via reinforcement learning for subgoal decomposition, 2025. URL <https://arxiv.org/abs/2504.21801>.
- Yong Lin, Shange Tang, Bohan Lyu, Jiayun Wu, Hongzhou Lin, Kaiyu Yang, Jia Li, Mengzhou Xia, Danqi Chen, Sanjeev Arora, et al. Goedel-prover: A frontier model for open-source automated theorem proving. *arXiv preprint arXiv:2502.07640*, 2025.
- Huajian Xin, ZZ Ren, Junxiao Song, Zhihong Shao, Wanbiao Zhao, Haocheng Wang, Bo Liu, Liyue Zhang, Xuan Lu, Qiushi Du, et al. Deepseek-prover-v1.5: Harnessing proof assistant feedback for reinforcement learning and monte-carlo tree search. *arXiv preprint arXiv:2408.08152*, 2024a.
- Haiming Wang, Huajian Xin, Zhengying Liu, Wenda Li, Yinya Huang, Jianqiao Lu, Zhicheng Yang, Jing Tang, Jian Yin, Zhenguo Li, et al. Proving theorems recursively. *arXiv preprint arXiv:2405.14414*, 2024.
- Chenyang An, Zhibo Chen, Qihao Ye, Emily First, Letian Peng, Jiayun Zhang, Zihan Wang, Sorin Lerner, and Jingbo Shang. Learn from failure: Fine-tuning llms with trial-and-error data for intuitionistic propositional logic proving. *arXiv preprint arXiv:2404.07382*, 2024.
- Huajian Xin, Daya Guo, Zhihong Shao, Zhizhou Ren, Qihao Zhu, Bo Liu, Chong Ruan, Wenda Li, and Xiaodan Liang. Deepseek-prover: Advancing theorem proving in llms through large-scale synthetic data. *arXiv preprint arXiv:2405.14333*, 2024b.

- Kaiyu Yang, Gabriel Poesia, Jingxuan He, Wenda Li, Kristin Lauter, Swarat Chaudhuri, and Dawn Song. Formal mathematical reasoning: A new frontier in ai. *arXiv preprint arXiv:2412.16075*, 2024a.
- The mathlib Community. The Lean mathematical library. In *Proceedings of the 9th ACM SIGPLAN International Conference on Certified Programs and Proofs*, CPP 2020, pages 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>.
- 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.
- Huaiyuan Ying, Zijian Wu, Yihan Geng, Jiayu Wang, Dahua Lin, and Kai Chen. Lean workbook: A large-scale lean problem set formalized from natural language math problems. *arXiv preprint arXiv:2406.03847*, 2024.
- Logan Murphy, Kaiyu Yang, Jialiang Sun, Zhaoyu Li, Anima Anandkumar, and Xujie Si. Autoformalizing euclidean geometry. *arXiv preprint arXiv:2405.17216*, 2024.
- Kefan Dong and Tengyu Ma. Stp: Self-play llm theorem provers with iterative conjecturing and proving. *arXiv e-prints*, pages arXiv–2502, 2025.
- Gabriel Poesia, David Broman, Nick Haber, and Noah Goodman. Learning formal mathematics from intrinsic motivation. *Advances in Neural Information Processing Systems*, 37:43032–43057, 2024.
- 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.
- Zijian Wu, Suozhi Huang, Zhejian Zhou, Huaiyuan Ying, Jiayu Wang, Dahua Lin, and Kai Chen. Internlm2. 5-stepprover: Advancing automated theorem proving via expert iteration on large-scale lean problems. *arXiv preprint arXiv:2410.15700*, 2024.
- Ran Xin, Chenguang Xi, Jie Yang, Feng Chen, Hang Wu, Xia Xiao, Yifan Sun, Shen Zheng, and Kai Shen. Bfs-prover: Scalable best-first tree search for llm-based automatic theorem proving. *arXiv preprint arXiv:2502.03438*, 2025.
- Chris Hokamp and Qun Liu. Lexically constrained decoding for sequence generation using grid beam search. *arXiv preprint arXiv:1704.07138*, 2017.
- An Yang, Beichen Zhang, Binyuan Hui, Bofei Gao, Bowen Yu, Chengpeng Li, Dayiheng Liu, Jianhong Tu, Jingren Zhou, Junyang Lin, Keming Lu, Mingfeng Xue, Runji Lin, Tianyu Liu, Xingzhang Ren, and Zhenru Zhang. Qwen2.5-math technical report: Toward mathematical expert model via self-improvement. *arXiv preprint arXiv:2409.12122*, 2024b.
- Kunhao Zheng, Jesse Michael Han, and Stanislas Polu. Minif2f: a cross-system benchmark for formal olympiad-level mathematics. *arXiv preprint arXiv:2109.00110*, 2021.
- 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.
- Kaiyu Yang, Aidan Swope, Alex Gu, Rahul Chalamala, Peiyang Song, Shixing Yu, Saad Godil, Ryan J Prenger, and Animashree Anandkumar. Leandojo: Theorem proving with retrieval-augmented language models. *Advances in Neural Information Processing Systems*, 36:21573–21612, 2023.

- Haohan Lin, Zhiqing Sun, Sean Welleck, and Yiming Yang. Lean-star: Learning to interleave thinking and proving. *arXiv preprint arXiv:2407.10040*, 2024.
- Dominique Pastre. Automated theorem proving in mathematics. *Annals of Mathematics and Artificial Intelligence*, 8:425–447, 1993.
- Carsten Schürmann and Frank Pfenning. Automated theorem proving in a simple meta-logic for If. In *International Conference on Automated Deduction*, pages 286–300. Springer, 1998.
- K Rustan M Leino. Automating theorem proving with smt. In *International Conference on Interactive Theorem Proving*, pages 2–16. Springer, 2013.
- 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.
- Jingyuan Zhang, Qi Wang, Xingguang Ji, Yahui Liu, Yang Yue, Fuzheng Zhang, Di Zhang, Guorui Zhou, and Kun Gai. Leanabell-prover: Posttraining scaling in formal reasoning. *arXiv preprint arXiv:2504.06122*, 2025.
- Haiming Wang, Mert Unsal, Xiaohan Lin, Mantas Baksys, Junqi Liu, Marco Dos Santos, Flood Sung, Marina Vinyes, Zhenzhe Ying, Zekai Zhu, et al. Kimina-prover preview: Towards large formal reasoning models with reinforcement learning. *arXiv preprint arXiv:2504.11354*, 2025a.
- Ruida Wang, Rui Pan, Yuxin Li, Jipeng Zhang, Yizhen Jia, Shizhe Diao, Renjie Pi, Junjie Hu, and Tong Zhang. Ma-lot: Multi-agent lean-based long chain-of-thought reasoning enhances formal theorem proving. *arXiv preprint arXiv:2503.03205*, 2025b.
- Jianqiao Lu, Yingjia Wan, Zhengying Liu, Yinya Huang, Jing Xiong, Chengwu Liu, Jianhao Shen, Hui Jin, Jipeng Zhang, Haiming Wang, et al. Process-driven autoformalization in lean 4. *arXiv preprint arXiv:2406.01940*, 2024.
- Woosuk Kwon, Zhuohan Li, Siyuan Zhuang, Ying Sheng, Lianmin Zheng, Cody Hao Yu, Joseph E. Gonzalez, Hao Zhang, and Ion Stoica. Efficient memory management for large language model serving with pagedattention. In *Proceedings of the ACM SIGOPS 29th Symposium on Operating Systems Principles*, 2023.
- Haiming Wang, Huajian Xin, 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.
- Zhihong Shao, Peiyi Wang, Qihao Zhu, Runxin Xu, Junxiao Song, Xiao Bi, Haowei Zhang, Mingchuan Zhang, YK Li, Y Wu, et al. Deepseekmath: Pushing the limits of mathematical reasoning in open language models. *arXiv preprint arXiv:2402.03300*, 2024.

## A Appendix

### A.1 Prompts used for policy model

For the policy model, we use the similar prompt template as in GPT-f [Polu and Sutskever, 2020], where the prompt only describes the current proof state without introducing any additional information. The template and an example are shown below:

*Template:*

```
[GOAL]
<state>
[PROOFSTEP]
```

*Example:* (aime\_1983\_p1 in MiniF2F)

```
[GOAL]
x y z w :  $\mathbb{N}$ 
ht :  $1 < x \wedge 1 < y \wedge 1 < z$ 
hw :  $0 \leq w$ 
h0 :  $\text{Real.log } \uparrow w / \text{Real.log } \uparrow x = 24$ 
h1 :  $\text{Real.log } \uparrow w / \text{Real.log } \uparrow y = 40$ 
h2 :  $\text{Real.log } \uparrow w / \text{Real.log } (\uparrow x * \uparrow y * \uparrow z) = 12$ 
 $\vdash \text{Real.log } \uparrow w / \text{Real.log } \uparrow z = 60$ 
[PROOFSTEP]
```

### A.2 Case study

Below we present two example proofs generated by our model on MiniF2F and ProofNet, respectively.

Example: amc12a\_2009\_p6 in MiniF2F

```
theorem amc12a_2009_p6
  (m n p q :  $\mathbb{R}$ )  $\mathbb{R}$ 
  (h0 :  $p = 2 \wedge m$ )
  (h1 :  $q = 3 \wedge n$ ) :
   $p^{(2 * n)} * (q^m) = 12^{(m * n)}$  := by
  subst_vars
  simp [mul_comm, Real.rpow_mul]
  have h0 :  $(0 : \mathbb{R}) < 2$  := by norm_num
  have h1 :  $(0 : \mathbb{R}) < 3$  := by norm_num
  field_simp [Real.rpow_def_of_pos, h0, h1]
  rw [← Real.exp_add]
  rw [mul_comm]
  rw [
    show  $(n * 2 * (\text{Real.log } 2 * m) + \text{Real.log } 3 * n * m) = (\text{Real.log } 12 * m * n)$  by
    have h3 :  $\text{Real.log } 12 = \text{Real.log } (2 \wedge 2 * 3)$  := by norm_num
    rw [h3]
    field_simp [Real.log_mul, Real.log_rpow, mul_assoc]
    ring_nf
  ]
```

Example: Rudin\_exercise\_4\_11a in ProofNet

```

theorem exercise_4_11a
{X : Type*} [MetricSpace X]
{Y : Type*} [MetricSpace Y]
(f : X → Y) (hf : UniformContinuous f)
(x : ℕ → X) (hx : CauchySeq x) :
CauchySeq (λ n => f (x n)) :=
  rw [Metric.cauchySeq_iff] at hx ⊢,
  intro ε hε,
  obtain ⟨δ, hδ, hδ'⟩ := Metric.uniformContinuous_iff.mp hf ε hε,
  obtain ⟨N, hN⟩ := hx δ hδ,
  exact ⟨N, fun m hm n hn => hδ' <| hN _ hm _ hn⟩

```

### A.3 Our DoBeVi REPL

To enable better interaction with Lean 4 prover and visualization of the search process, we develop Dojo-BeamSearch-Visualization (DoBeVi) REPL, a tool built upon a simplified and customized version of LeanDojo [Yang et al., 2023]. The tool consists of two main components: *interactive theorem proving environment* and *visualization module*.

#### A.3.1 Interactive theorem proving environment

In the component of interactive theorem proving environment, we present a streamlined adaptation of the LeanDojo framework, establishing a lightweight but robust foundation for distributed interactive theorem proving. Our implementation retains two core functionalities from LeanDojo:

- AST extraction and semantic analysis of target Lean files with precise theorem declaration identification.
- Core interactive logic execution via the `lean_dojo_repl` custom tactic.

In our DoBeVi REPL refines the architecture by removing three categories of non-essential components from LeanDojo:

- Partial initialization workflows.
- Premise and dependency tracking modules.
- Secondary data processing components.

Then we add the following new useful features for better interaction with the prover:

- Proof state tracking using globally unique identifiers (excluding `ProofFinish` nodes).
- Decoupled session management architecture enabling parallel theorem processing.
- Resilient recovery mechanisms for:
  - Tactic execution timeouts.
  - Lean process failures.

After that, the DoBeVi provides an optimized architecture that reduces runtime overhead while maintaining stable interfaces for integrating model-based theorem proving components.

#### A.3.2 Visualization of the search tree

The visualization module serves to clearly illustrate the entire proof search process by graphically representing the evolving search tree structure. In this module, each proof state encountered during the search is abstracted as a node in a graph, and each proof step applied to transition between states is represented as a directed edge. To better reflect the semantics of the search process, nodes are categorized into three types:

- **Prooffinished node:** Indicates that the proof has been successfully completed at this node.

- Error node: Represents a failed search node due to errors such as Lean syntax errors, timeouts, or unexpected crashes of the Lean process.
- Open node: Denotes an intermediate state that can still be expanded during the search.

Similarly, edges are divided into two categories:

- Tree edge: Connects to a previously unseen state, resulting in the creation of a new node. Tree edges are essential for expanding the search space and discovering new proof paths.
- Back edge: Leads to a state that has already been visited earlier in the search process. Back edges help identify convergence and redundancy in the search, enabling cycle detection and pruning.

Although the structure is referred to as a "search tree", it is, strictly speaking, a directed acyclic graph (DAG). This distinction stems from two key characteristics:

- Non-tree structure: Different but semantically similar proof steps may both lead from the same current state to the same next state, resulting in multiple paths converging to a single node. The property that there are no loops inside the tree is violated.
- Acyclic design: Cycles in the search path (e.g.,  $s_1 \rightarrow s_2 \rightarrow \dots \rightarrow s_1$ ) are explicitly detected and pruned in advance, as we consider such loops to be semantically meaningless and computationally redundant.

This visualization module is part of the DoBeVi system, which is organized in a modular fashion. The system consists of the following four components:

- Search tree module: Defines the core data structures, including Node, Edge, and the overall Tree layout.
- Tactic generation module: Interfaces with LLMs. Given the current state as input, it returns a set of candidate proof steps along with their associated scores. This module is extensible and allows users to integrate custom models as needed.
- Search strategy module: Specifies the logic for node expansion. We provide several default strategies such as Best-First Search, which always expands the node with the highest current score that has not yet been explored. Users are free to implement additional strategies tailored to their tasks.
- Visualization module: Responsible for rendering the entire search tree graphically, enabling an intuitive understanding of the search process and state transitions.

Figure 3 presents the visualization result of applying the Best-First Search strategy to the problem `amc12_2000_p6` from the MiniF2F dataset. Node IDs increment from 0, indicating the order in which nodes were expanded during the search. In this example, the search sequentially expanded nodes with IDs 0, 3, 11, 14, 16, 19, and 21, ultimately completing the proof successfully after the seventh expansion.

In summary, this module visualizes the search tree to record the entire search process, making it easier to review after execution and to inspire the design of better search and pruning strategies.

#### A.4 Detailed experimental settings

In our experiments, similar to most tree search methods, we separate the tree search and model generation components to improve overall evaluation efficiency. We refer to the implementation in ReProver [Yang et al., 2023] and use Python’s Ray <sup>5</sup> and vLLM [Kwon et al., 2023] libraries to implement the system. We launch multiple processes for tree search, where each process pulls unprocessed theorems from a queue and uses LeanDojo as the interaction tool between Python and the Lean 4 prover. When fetching proof steps, multiple tree search workers share several asynchronous LLM engines launched by vLLM, with one LLM instance deployed per GPU. In practice, we use dozens of tree search processes to maximize GPU utilization. For each search, we set a global timeout of 1,800 seconds; if the search time exceeds this value, the search process is forcibly terminated.

<sup>5</sup><https://github.com/ray-project/ray>





For each proof step, we impose a timeout of 20 seconds. While there are occasional cases - such as when using `aesop` - where longer execution times may be required, we consider any proof step exceeding this threshold as a timeout. This constraint is intended to prevent individual proof steps from disproportionately consuming the overall time budget.

During tree search, we use the REPL functionality provided by DoBeVi (Appendix A.3). When executing proof steps, errors can broadly be categorized into two types: (1) syntax errors or similar issues that directly cause the Lean 4 prover to return an error, which are usually caught quickly with an error message; and (2) timeout errors. To prevent infinite loops caused by certain tactics, we set a timeout for tactic execution. If such a timeout occurs, the Lean 4 prover becomes unable to execute new proof steps, forcing the entire proof process to stop. To handle this, we save the proof context before executing each tactic; if a timeout occurs, we restart the Lean REPL environment and restore the context. This avoids cases where a proof that should have succeeded with tree search ultimately fails just because a faulty tactic caused the Lean 4 prover to hang.

In addition, based on observations of certain failure cases during tree search, we identified an important phenomenon: erroneous proof steps tend to appear in batches. Specifically, when performing beam search from an proof state, if several consecutive proof steps are incorrect, it is highly likely that the remaining proof steps in the beam will also be incorrect. This pattern may stem from the fact that the current proof state represents an out-of-distribution input for the policy model, making it difficult for the model to generate valid Lean 4 code. Under such circumstances, these erroneous proof steps can substantially consume the global timeout allocated for the tree search, leading to inefficient exploration. To mitigate this issue, we adopt an early termination strategy: during expansion at a given state, if the number of incorrect child nodes exceeds a predefined threshold (usually  $0.5 \times$  beam size), we immediately discard the current node from further search. We found that this pruning technique did not degrade overall proving performance while significantly reducing computational time.

Regarding the choice of hyperparameters in the adaptive beam size strategy, we set  $B_{\max} = 16$ ,  $B_{\min} = 4$ , and  $\lambda = 15$  for MiniF2F, and  $B_{\max} = 48$ ,  $B_{\min} = 24$ , and  $\lambda = 2$  for ProofNet.

## A.5 Unsuccessful attempts and discussions

**Separating tactics and premises.** In our early experiments, we explored a more straightforward separation of tactics and premises. Specifically, we adopted a two-model design: one model directly outputs a valid tactic to serve as the starting token of the code, while a second model, analogous to the policy model, completes the required premises. However, this approach yielded unsatisfactory results. We frequently observed that the second model either failed to generate complete premises or produced outputs that violated the Lean 4 grammar. A key challenge lies in the highly imbalanced data distribution for a model that generates only tactics without premises. To quantify this imbalance, we analyzed the STP dataset and computed the tactic usage statistics, presented in Appendix A.6. For example, tactics like `rw` and `have` appear in nearly every proof context, leading the model to overwhelmingly favor these high-frequency tactics. In contrast, the policy model must guide the proof state toward completion, which does not always align with simply selecting the most common tactics. This mismatch introduces conflicting objectives that ultimately degrade performance. Therefore, we conclude that forcibly separating the generation of tactics and premises is infeasible. Instead, it may be more effective to adopt external augmentation strategies, such as the retrieval-augmented generation (RAG) method in Yang et al. [2023] or the lemma library construction approach in Wang et al. [2023].

**An ineffective scoring function.** One major drawback of tree search methods compared to whole-proof methods lies in the complexity of the neural-symbolic system: it involves many interacting components, making it difficult to diagnose failure modes when performance is suboptimal. In some cases, the coupling between components may even be inherently unavoidable. As discussed in the main text, we identify several key factors in tree search methods that have a non-negligible impact on performance:

- **Policy model.** As the actor in the system, the policy model is clearly the most critical determinant of overall performance.

- **Scoring function (sometimes value network).** The scoring function determines the order in which nodes are expanded within the tree structure. In some cases, a value network may be used for scoring instead of a rule-based method.
- **Beam size.** The beam size represents a special type of budget. As discussed in Section 4.3, increasing the beam size does not necessarily lead to better results. On the contrary, for certain settings, a small beam size (such as 4) can sometimes unlock greater potential from the policy model. Moreover, the empirically optimal beam size varies across benchmarks and is not a fixed value.
- **Other budget-related factors.** These include parameters like  $K$ ,  $E$ , and the timeout threshold. Compared to the previous factors, these are relatively straightforward: given fixed settings for other components, larger budgets generally increase the likelihood of achieving better results.

In our early experiments, we hypothesized that the problem setting resembled reinforcement learning, and thus sought inspiration from algorithms such as GRPO Shao et al. [2024]. We aimed to avoid introducing a separate value network, instead using the average performance of a set of actions generated by the actor as a scoring criterion. Concretely, for any intermediate proof state  $s$ , we computed the following score:

$$\text{score}(s) = \frac{1}{B} \sum_{i=1}^B \log P_{\theta}(t_i | s) \quad (3)$$

Here,  $\theta$  denotes the policy model’s parameters, and  $P_{\theta}(t_i | s)$  represents the joint probability of the  $i$ -th beam. The intuition behind this scoring function is that, on an average sense, higher beam probabilities suggest that the policy model is more likely to have encountered similar examples during training. Therefore, the current proof state  $s$  is more likely to lie on a path leading to proof completion.

However, subsequent experiments indicate that the evaluation results obtained using this scoring function are nearly indistinguishable from those derived using Equation 1, suggesting that this approach may not be particularly effective within the context of tree search methods.

**Dynamic beam size via *top\_p* strategy.** Another adaptive beam search strategy we explored is inspired by the *top\_p* (nucleus sampling) strategy commonly used in decoding. Specifically, after normalizing the joint probabilities of each beam, we sort the beams by their joint probabilities and then filter out beams with lower probabilities according to the *top\_p* threshold.

Considering all of the strategies we experimented with, we conclude that the scoring function (Equation 1) used in current tree search methods still suffers from significant shortcomings. As a result, the experimental outcomes of these various approaches showed little impact on performance.

## A.6 Tactic usage statistics on the STP dataset

We performed a comprehensive scan of all tactics used across the entire STP dataset, identifying a total of 173 unique tactics. By applying a threshold of  $\mathcal{P} = 0.999$  under the *top\_p* strategy to exclude infrequently used tactics, we obtained a final set of 60 common tactics. The frequency distribution of these tactics is shown in Figure 4.

## A.7 Search depth statistics on the MiniF2F benchmark

We conducted experiments using our policy model on the MiniF2F benchmark with varying beam sizes during search. The results, shown in Figure 5, indicate that under a fixed maximum number of expansions, smaller beam sizes tend to produce proving paths with greater search depth.

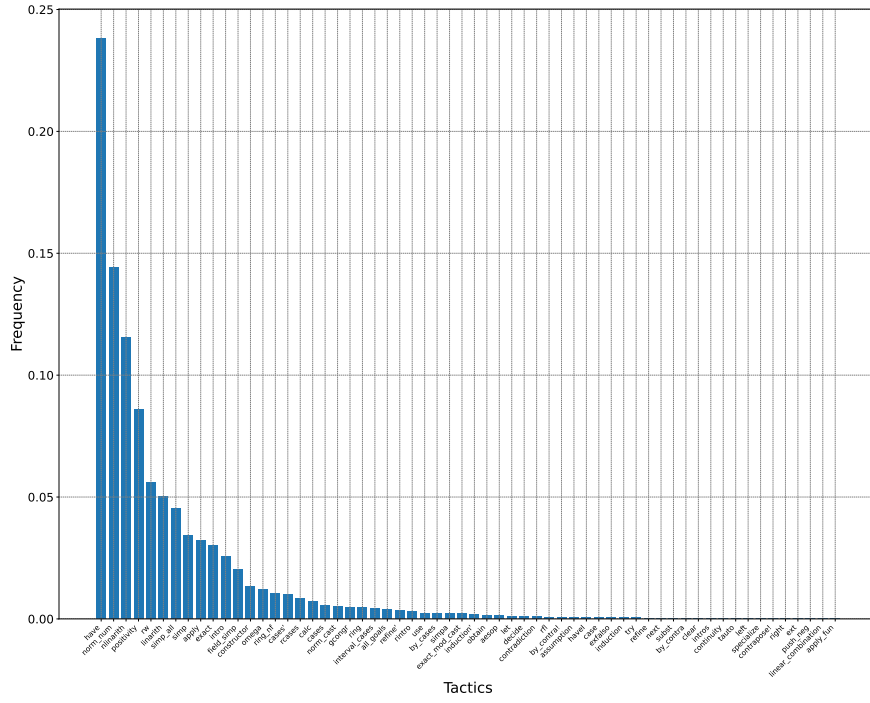


Figure 4: Distribution of the top 60 most frequent tactics in the STP dataset.

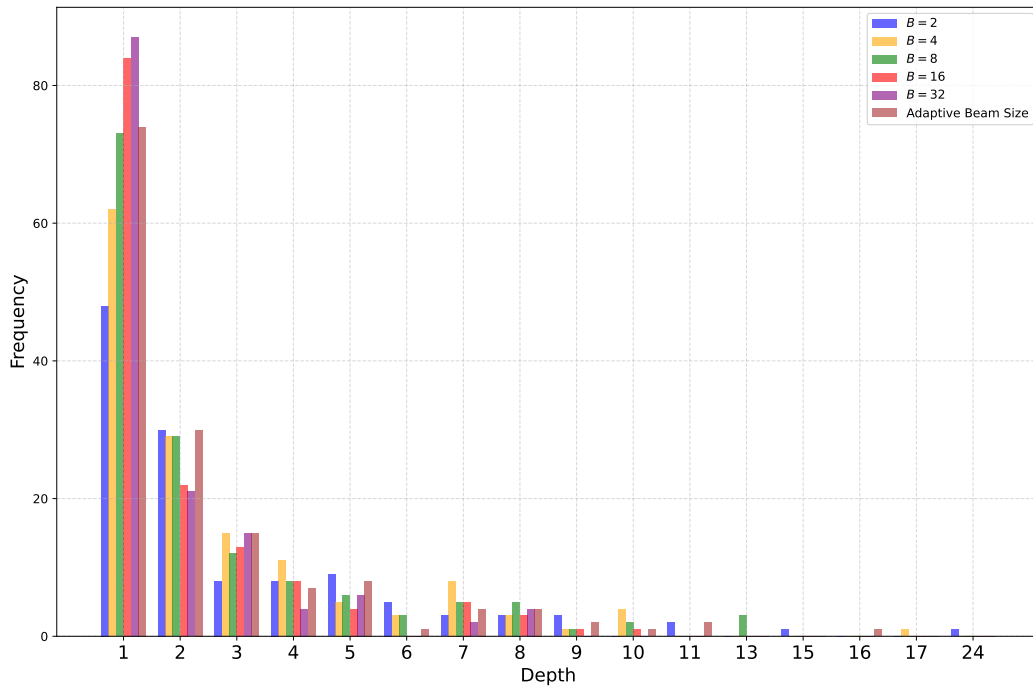


Figure 5: Frequency distribution of search depths of proving paths generated by our policy model on the MiniF2F benchmark, with the maximum number of expansions fixed at 600 ( $E = 600$ ).