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Lean Meets Theoretical Computer Science: Scalable Synthesis of Theorem Proving Challenges in Formal-Informal Pairs

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Abstract

Formal theorem proving (FTP) stands at the forefront of LLM reasoning, yet existing datasets are largely limited in scope due to their dependence on manual curation. We identify theoretical computer science (TCS) as a novel testbed with promising potential, as many TCS problems can be algorithmically modeled and automatically verified, thereby enabling scalable formalization with rigorous formal-informal alignment guarantees. We showcase this approach via two TCS problem modules: the Busy Beaver (BB) challenge and the Mixed BooleanArithmetic (MBA) challenge. We evaluate leading reasoning models and finetuned theorem provers on our dataset, where the best-performing DeepSeekProver-v2-671B attains only 57.5% on our BB challenge and no more than 12% on our MBA challenge. These results reveal substantial reasoning gaps beyond conventional static benchmarks. We call on the Lean community to further study the potential of TCS problems in the formal reasoning domain where our approach enables fully automated synthesis of arbitrarily many problems in their strictly aligned formal-informal pairs that are universally easy to verify yet systematically hard to prove.

1. Introduction

While Large Reasoning Models (LRMs) (Besta et al., 2025) are evolving at an unprecedented speed, this promising progress is increasingly shadowed by a critical asymmetry: the advancing momentum of frontier models is quickly outpacing our ability to accurately gauge the boundary of their reasoning capability, as evidenced by the rapid saturation of legacy benchmarks such as MATH (Hendrycks et al.,

2021) and GPQA (Rein et al., 2023).

Beyond conventional static benchmarks that evaluate on a final answer only, a natural next stage is to examine detailed machine proof to see if models are genuinely capable of making meaningful logical derivations. Formal Theorem Proving (FTP) (Chen et al., 2025) is emerging as a defining frontier for automating such proof validation by harnessing the power of interactive theorem provers such as Lean (de Moura & Ullrich, 2021) and Isabelle (Nipkow et al., 2002).

As a result, there's a critical need for large-scale, highquality datasets that bridge theorem proving problems between their formal-informal forms. Previous work such as MiniF2F (Zheng et al., 2022), ProofNet (Azerbayev et al., 2023), PutnamBench (Tsoukalas et al., 2024), and CombiBench (Liu et al., 2025) leveraged labor-intensive expert curation to formalize problems from math competitions and college courses, yet such public data sources may suffer from inter-annotator inconsistency and data contamination of the training corpora (Magar & Schwartz, 2022; Dong et al., 2024), where even slight data leakage can inflate model performance by up to 30% points (Dekoninck et al., 2024).

In light of these concerns, Theoretical Computer Science (TCS) emerges as a promising new testbed where many problems can be algorithmically modeled and verified, which enables scalable fully automated problem formalization using a modularized TCS problem such as the Halting Problem of Turing Machines. Furthermore, we can adjust the difficulty of synthesized problems by tuning complexity parameters such as the state count of a Turing Machine or the variable count in an algebraic expression. This parameterized setting also enables us to synthesize fresh problems from a infinitely vast problem space, which acts as a robust mitigation against data contamination. It's particularly worth noting that our synthesis does not rely on any LLMgenerated content in any steps, which would be unavoidably impacted by language model hallucination and potential regurgitation of training data.

In light of these concerns, our main contribution in this paper is threefold:

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$ \underbrace{ \begin{array}{ll} \mbox{Mixed Boolean-Arithmetic (MBA) Expression} \\ x_{+y=} \begin{cases} x \neg y - 1 & 2 \cdot \neg y - 11 \cdot \neg x + 9 \cdot \neg (x \lor y) \\ (x,y) + (x,y) \\ 2^*(x \lor y) - (x \circledcirc y) \\ 2^*(x \lor y) - (x \circledcirc y) \end{cases} & + 13 \cdot \neg (x \lor \neg y) + 2 \cdot (x \land y) \\ = 2 \cdot (x \lor y) \end{cases} $						<pre>theorem mba_chall (x y : BitVec 32) + 13#32 * ~~~(x by sorry</pre>	theorem mbs_challenge_3882c549 (x y: 18140c 32): 2432 *y - 11852 *x + 9832 *(x y) + 13822 *(x y) + 2832 * (x &&& y) = 2832 * (x y) := by sorry			/ let x, y be 32-bit bit-vectors. Prove the equivalence of the following two expressions: \$2\cdot \lnot y-11\cdot (lnot y-11\cdot \lnot x\lor y)^3\cdot \lnot (x\lor y)^3\cdot \lnot (x\lor y)^3\cdot (x\lor y)\$, \$2\cdot (x\lor y)\$, \$2\cdot (x\lor y)\$		
Problem Module	>	Parame	eter Instar	itiation		>	Formal Problem		>		Informal Description	
Susy-Beaver Machine (BB)												
HALT	State	Symbol	Next State	Nove	Write	def machine : Mach (000, _), [.zero	ine -> none			/ Prove the follow	ving Turing Machine with the trans	sition table halts.
	000	zero	HALT	-	-	(000, _), T.one	some ((881, by omega), (Turi > some ((888, by omega), (Turi	ing.Dir.right, Γ.one))		State Symbol Next S	State Move Write	
	000	one	001	left	one	(001, _), F.one (_+2, _), _ => b	> none v omega			898 zero HAL	T loft zoro	
200	001	zero	888	right	one		1 · · · · · · · · · · · · · · · · · · ·			-/ theorem machine_	halts : 3 n, (nth_cfg n).isNone :	= by sorry
HALT	001	one	HALT	-	-	sorry	its : 3 n, (nth_org n).iswone :	- by				

Figure 1. Complete Pipeline of our Synthesis Framework: We start with a problem module that can be instantiated by a rule-based system to generate theorem proving problem description in Lean code shown in the blue block and the same description in Markdown shown in the green blocks.

- We propose a contamination-resistant synthesis framework with adjustable difficulty that generates arbitrarily many theorem proving challenges in their rigorously aligned formal-informal pairs by leveraging TCS-inspired problem modules as shown in Figure 1.
- We evaluate a variety of frontier LRMs and LLM-based theorem provers. The best-performing DeepSeek-Prover-v2-671B attained best performance of 57.5% on our BB challenge and only 12% on our MBA challenge respectively, yet other theorem provers such as Kimina-Prover-Preview (Wang et al., 2025) and Goedel-Prover-SFT (Lin et al., 2025) struggle to resolve any of our synthesized problems, which may hint at how base model scaling could enhance capability of LLM-based theorem provers.
- We design a novel step-level task decomposition setting to gauge if models can effectively use a customized Out-Of-Distribution library of Lean lemma to resolve unseen problems, where best-performing model, OpenAI-o4-mini, showed 98.88% success rate. This reveals the critical bottleneck of the proof task lies in whole-proof level understanding and strategic planning as opposed to step-level problem-solving.

2. Related Work

Formal Theorem Proving (FTP). LLM has demonstrated promising potential in advancing the field of math-100 ematics (Polu & Sutskever, 2020) with the help of interactive theorem provers as endorsed by many world-leading mathematicians such as Peter Scholze (Scholze, 2022) and Terence Tao (Tao, 2025). By integrating FTP in various 104 contexts such as LLM-based Agents (Li et al., 2024a) and 105 Retrieval-Augmented Generation (RAG) (Zayyad & Adi, 106 2024), many downstream applications can be empowered such as code copilot (Murphy et al., 2024) and operations research (Yang et al., 2024). 109

Autoformalization. Autoformalization refers to the process of translating natural language into formal language, which is inherently challenging for human due to the complex syntax of FTP languages. While the synthetic data approach (Wu et al., 2021; Huang et al., 2024; Ying et al., 2024) attempted to leverage LLMs for this process (Li et al., 2024b; Wu et al., 2022; Lu et al., 2024), current progress is largely limited by expert annotation to proofread and correct LLM-generated formal contents, which is labor-intensive and exposed to inter-annotator inconsistencies. Therefore, we aim to automate the entire process of (in)formalization via a template-based approach to ensure rigorous alignment, rendering manual curation *an optional quality check* as opposed to *an expensive necessity*.

Benchmark Contamination. In light of rising concerns about whether our benchmarks reflect genuine reasoning capability of LLMs (Magar & Schwartz, 2022; Dong et al., 2024), various attempts were made to detect and mitigate data contamination (Dekoninck et al., 2024). For instance, LiveBench (White et al., 2024) aims to mitigate contamination by refreshing benchmark questions every 6 months, and MixEval (Ni et al., 2024) attempted to remove preference bias by adopting a mixture of benchmarks. Nevertheless, data contamination remains a persistent issue so long as the questions are sourced from the public Internet at large, including synthetic data reliant on LLM generation.

3. Methodology

3.1. The Busy Beaver (BB) Challenge

We showcase our approach based on the halting problem of the famous Busy Beaver Machine. Busy Beaver machines are simple yet powerful computation models as any Turingcomplete problems can be reduced to the Busy Beaver problem. Many research questions in modern mathematics, such as the Collatz Conjecture (Michel, 1993) and the famous
Goldbach Conjecture (Aaronson, 2020) have been proven
to be reducible to BB(6) and BB(27) respectively.

to be reducible to BB(6) and BB(27) respectively.

114 The Problem Module. A busy beaver machine is an N-115 state, 2-symbol Turing machine, where the Busy Beaver 116 function **BB**(N) (Harland, 2022) is defined as the maxi-117 mum number of steps an N-state halting machine can exe-118 cute before halt. In this challenge we instantiate with $N \leq 5$ 119 as BB(5) is currently the limit of frontier mathematics re-120 search (Aaronson, 2020), we note that this parameter N121 can be any natural number in principle. By setting this pa-122 rameter N we enable adjustable difficulty of synthesized 123 problems and the number of machines available grows expo-124 nentially with the N as detailed in Table 1, thereby ensuring 125 the infinite scalability of our synthesis. 126

n	Number of Machines
1	64
2	20,736
3	16,777,216
4	4,294,967,296

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Table 1. Number of Busy Beaver (BB) Machines for Increasing Values of N.

Challenge definition. We ask models to prove whether a given BB machine described by a state transition table halts or not.

141 Generate easy-to-verify ground-truth. In order to know 142 exactly whether a given Busy Beaver machine halts, we 143 execute the machine for BB(N) + 1 steps, where BB(N)144 is the Busy Beaver number for N-state machines, defined as 145 the maximum steps for any N-state Turing Machine to run 146 without halting, The numerical value of **BB**(N) ($N \le 5$) 147 are proven results in mathematics (Xu, 2024). BB Machines 148 that reaches halt state within BB(N) + 1 steps are halting, 149 otherwise non-halting by the definition of BB(N). 150

151 Synthesize hard-to-prove challenge. We instantiate a 152 Busy Beaver machine with a state transition table, which 153 is then used to generate both Lean and Markdown state-154 ments using an expert-defined template. This synthetic 155 framework ensures scalable generation of arbitrarily many 156 proof questions in rigorously aligned formal-informal pairs 157 as illustrated in Figure 1. Specifically, each BB machine 158 is uniquely defined by a State Transition Table containing 159 tuples in the form State \times Symbol \times State \times Move \times Symbol, 160 where State $\in \{0, 1, \dots, N - 1, \text{HALT}\}$, Symbol \in 161 {zero, one}, Move ∈ {left, right}, indicating a BB 162 machine at a certain state with head pointing to certain sym-163 bol needs to change to another state, write a symbol to the 164

original head position and move to left or right. To generate a N state BB machine, we randomly sample the remaining elements for all 2N transition tuples.

With the state transition table, we apply an expert-defined template to generate the proof challenge in Lean. The template contains all necessary definitions and two blanks to fill in for the machine definition and the halting/non-halting theorem, a sorry at the end indicates where models should fill in their proof. We also generate a Markdown description based on a rigorously aligned template as detailed in Appendix D. We provide a complete example of our BB Challenge with problem descriptions in both Lean-Markdown and model responses in Appendix C.

3.2. The Mixed Boolean-Arithmetic (MBA) Challenge

The Problem Module Mixed Boolean-Arithmetic (MBA) expressions combine arithmetic operators $(+, -, \times)$ with bitwise operations (\wedge (AND), \vee (OR), \oplus (XOR), \neg (NOT)) over integer variables, which form universal representations of polynomial functions over bitvectors (Reichenwallner & Meerwald-Stadler, 2022) used in cryptographic obfuscation (Liu et al., 2021).

MBA equations can be categorized into two types according to their construction:

Linear MBA equations. Equations of the form

$$\underbrace{\sum_{k} a_k \times e_k(x, y)}_{\text{Linear MBA expression A}} = \underbrace{\sum_{k} b_k \times e'_k(x, y)}_{\text{Linear MBA expression B}},$$

where each coefficient a_k , $b_k \in \{\pm 1, \pm 2, ..., \pm 11\}$. and each atomic boolean expression $e_k(x, y)$, $e'_k(x, y)$ have 16 options as below.

$$\left[\begin{array}{cccc} x & x \lor y & x \land y & x \oplus y \\ \neg x & x \lor \neg y & x \land \neg y & \neg (x \oplus y) \\ y & \neg (x \lor y) & x \land \neg x & \neg (x \land y) \\ \neg y & \neg (x \lor \neg y) & \neg (x \land \neg y) & \neg (x \land \neg x) \end{array} \right]$$

Nonlinear MBA equations. Equations in which each side may include products of MBA sub-expressions $(e_{k_1}(x, y) \times e_{k_2}(x, y))$ and arbitrarily nested bitwise operations, e.g. $10 \times \neg (1 \times (x \wedge y) \lor \neg ((-1) \times (x \lor \neg y)))).$

Dataset Generation In the first stage, we generate two-variable MBA equations following the MBA obfuscator protocol (Liu et al., 2021). Specifically, each equation is constructed by first generating a linear MBA expression that is identically zero, and then randomly moving a subset of terms to the right-hand side with their signs flipped. We then translate each equation into a Lean theorem paired with an informal Markdown description as illustrated in

Figure 1. Every variable and constant coefficient are declared as BitVec 32 so that all arithmetic and bitwise
operations are on 32-bit bitvectors modulo 2³². We ensure
infinite scalability by incrementing the number of variables
in the MBA expression, which guarantees a sufficiently large
problem space to mitigate contamination via combinatorial
explosion.

173 Challenge definition. We ask models to prove the equiva174 lence of two MBA expressions. Proofs must be constructed
175 step by step using lemmas for arithmetic, bitwise, and dis176 tributive identities to ensure genuine symbolic reasoning.
177 We explicitly discourage tactics such as bv_decide (which
178 invokes a SAT solver) and other automatic approaches.

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180 SAT solver. Lean provides a built-in tactic called 181 by_decide for automatically proving or disproving equalities 182 over fixed-width bitvectors (BitVec n). Internally, bv_decide 183 reduces the goal to a Boolean satisfiability problem (SAT) 184 by applying bit-blasting, a process that translates bitvec-185 tor operations into equivalent propositional logic formulas 186 over individual bits. The resulting Boolean formula is then 187 handed to an external SAT solver to check satisfiability. By 188 default, by_decide uses a 10-second timeout for the solver. 189

Generate easy-to-verify ground-truth. For any linear
 MBA equation

$$E_1(x,y) = E_2(x,y),$$

we normalize both sides into their *Weighted 2-DNF* (W2DNF):

W2DNF(E) =
$$\sum_{i,j\in\{0,1\}} c_{ij}(E) \left(\ell_i(x) \wedge \ell_j(y)\right),$$

where $\ell_0(z) = \neg z$, $\ell_1(z) = z$ and each $c_{ij}(E) \in \mathbb{Z}_{32}$ Thus the original equality $E_1 = E_2$ holds if and only if

$$c_{ij}(E1) = c_{ij}(E2)$$
 for all $i, j \in \{0, 1\}$.

Normalization steps are directly translated into a sequence of Lean tactics that Lean can verify as the ground-truth solution for the MBA challenge.

Customized lemma library. We curated a custom library containing all necessary lemmas to reduce any 2-variable linear MBA expression into weighted 2-DNF form without relying on any external theorem or lemma, which enabled us to automatically generate and verify all ground-truth proofs for our MBA challenge. The complete library is provided in Appendix F.

Step-level task decomposition. In order to test if models perform differently in handling step-level task comparing

to entire proof, we decompose each ground-truth proof into a sequence of step-level tasks. After each tactic is applied, Lean reports an unsolved goal. Whenever the left-hand side (LHS) or right-hand side (RHS) of the goal changes, we extract a step lemma according to the following rules:

- For LHS changes: The lemma's left-hand side matches the *previous* goal's LHS, and its right-hand side matches the *current* goal's LHS.
- For RHS changes: The lemma's left-hand side matches the *previous* goal's RHS, and its right-hand side matches the *current* goal's RHS.

For each problem, the final step (and *only* the final step) is always simp. All non-final tactics are exclusively one of three types: simp only, rw, or nth_rewrite, and crucially, each must use a lemma from our custom library. We provide a complete example of the step lemma challenge with model responses in Appendix C and results for this setting in 5.

4. Experimental

We report Pass@16 on various frontier models, which counts a case as successful if and only if at least one of the 16 attempts could pass Lean compiler verification, that is, no errors are reported and no 'sorry' is used in the proof.

While it's possible to set other n for Pass@n, we note that n = 16 is the common best practice for existing formal theorem proving benchmarks (Zheng et al., 2022; Tsoukalas et al., 2024; Liu et al., 2025), which strikes a balance of reasonable budget and non-deterministic inference. For unexpected failures such as Timeout, Out-Of-Memory and API error, we re-run each trial without counting the failed case into n = 16.

4.1. Evaluation Setup

Evaluated models. We evaluated both frontier generalpurpose reasoning models and LLM-based theorem provers. Dedicated formal theorem provers are fine-tuned using FTP data on base models such as DeepSeekMath (Shao et al., 2024). For general-purpose LRMs, we chose a mixture of advanced open-source and proprietary models: DeepSeek-R1-671B (DeepSeek-AI et al., 2025), QwQ-32B (Qwen, 2025), OpenAI-o3 and o4-mini (OpenAI, 2025), Both OpenAI models carry default settings of 200K context window, 100K max output tokens, and a knowledge cut-off date on June 1, 2024. For LLM-based theorem provers, we evaluated various frontier models including Goedel-Prover-SFT (Lin et al., 2025), Leanabelle-Prover (Zhang et al., 2025), Kimina-Prover-Preview-7B (Wang et al., 2025), DeepSeek-Prover-v2-7B, and DeepSeek-Prover-v2-671B (Ren et al., 2025).

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Model	BB(1)	BB(2)	BB(3)	BB(4)	Total
General LRMs					
DeepSeek-R1	21/50	12/50	10/50	12/50	55/200 (27.5%)
QwQ-32B-Preview	26/50	21/50	26/50	25/50	98/200 (49.0%)
OpenAI-o3	15/50	17/50	19/50	17/50	68/200 (34.0%)
OpenAI-04-mini	19/50	10/50	12/50	13/50	54/200 (27.0%)
Theorem Provers					
Goedel-Prover-SFT	0/50	0/50	0/50	0/50	0/200 (0.0%)
Leanabell-Prover-GD-RL	0/50	0/50	0/50	0/50	0/200 (0.0%)
Kimina-Prover-Preview-7B	0/50	0/50	0/50	0/50	0/200 (0.0%)
DeepSeek-Prover-v2-7B	9/50	9/50	10/50	10/50	38/200 (19.0%)
DeepSeek-Prover-v2-671B	34/50	30/50	26/50	25/50	115/200 (57.5%

Table 2. Pass@16 Results on BB Challenge, where each column represents an incremental setting for state count N as a complexity parameter.

Inference setting. For open-source models, we use greedy sampling to aid reproducibility, which is equivalent to fixing the sampling temperature to T = 0.0 as recommended by the model developers (DeepSeek-AI et al., 2025; Qwen, 2025) for math and coding tasks. Furthermore, We enable thinking mode for all models whenever possible and follow default settings on Reasoning Efforts, Context Length, Max Tokens, and System Prompts in model metadata.

We implemented our code under a Linux environment with Python 3.10. All open-source models are deployed using transformer library and PyTorch on a 4xGH200 server, with open-source models downloaded via huggingface-cli. The proprietary models are used directly via the OpenAI API. We prompted models to follow detailed instruction as in Appendix C.

After generation, model outputs are parsed to extract Lean proof, which is validated using a regular expression. The proof is then verified using Kimina-Lean-Server (Santos et al., 2025) built with Lean and Mathlib v4.19.0 via a RESTful API.

4.2. Results

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BB challenge. We report Pass@16 in Table 2 and analyze detailed failure modes in Section 4.4. Frontier LRMs
OpenAI-o3 and o4-mini have struggled to score past 35% on our BB challenge, marking a critical gap in formal reasoning capability despite rapid saturation on static benchmarks from public sources.

Among LLM-based theorem provers, best-performing DeepSeek-Prover-v2-671B (Ren et al., 2025) scored 57.5%, but we notice rapid performance degradation as models scale down to 7B, where advanced theorem provers such as Goedel-Prover-SFT (Lin et al., 2025), Leanabelle-ProverGD-RL (Zhang et al., 2025) and Kimina-Prover-Preview-7B (Wang et al., 2025) struggled to solve even 1 instance of our challenges.

Paradoxically, QwQ-32B (Qwen, 2025) attained best performance among general LRMs with only 32B parameters, which raises an intriguing question as to how scaling affects the performance of general reasoning models vs. dedicated theorem provers in a potentially different manner.

MBA challenge. We report Pass@16 in Table 5, revealing even more pronounced difficulties than BB challenge. Further, we decompose 10 randomly selected MBA challenge into 365 steps according to Section 3.2 and report step-level performance in Table 4.

Frontier LRMs including DeepSeek-R1 (DeepSeek-AI et al., 2025) and QwQ-32B (Qwen, 2025), struggled to solve any of our challenges, while OpenAI-o4-mini (OpenAI, 2025) solved only 6 problems.

Specialized theorem provers exhibited extreme stratification: DeepSeek-Prover-v2-671B (Ren et al., 2025) solved 12% of linear problems with lemmas, but failed all problems without lemmas and all non-linear problems. Smaller provers showed near-universal failure, with only Kimina-Prover-7B (Wang et al., 2025) solving a single instance. This demonstrates that even state-of-the-art formal systems struggle with fundamental algebraic reasoning when deprived of lemma support or faced with non-linear complexity.

4.3. Success Cases

We present a successful case of a proof of non-halting BB(4) machine and more cases in Appendix E. The model DeepSeekProver-v2-671B leveraged proof by induction and attempted to use various automated tactics, such as aesop

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Model	Linear w/ Lemma	Linear w/o Lemma	Non-Linear
Reasoning LLMs			
DeepSeek-R1	0/100	0/100	0/40
OpenAI-04-mini	2/100	4/100	0/40
QwQ-32B-Preview	0/100	0/100	0/40
Theorem Provers			
DeepSeek-Prover-v2-7B	0/100	0/100	0/40
Goedel-Prover	0/100	0/100	0/40
Kimina-Prover-7B	1/100	0/100	0/40
Leanabelle-Prover	0/100	0/100	0/40
DeepSeek-Prover-v2-671B	12/100	0/100	0/40

Table 3. Pass@16 Performance on MBA challenge. We evaluated all models using 2 parallel settings where models are tested with vs. without our customized lemma library as detailed in Section 3.2. This parallel setting aims to gauge their capability of in-context learning unseen lemma to tackle novel problems out of their training corpora.

Model	#Correct Steps
OpenAI-04-mini	352/356
DeepSeek-Prover-v2-671B	258/356

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Table 4. Step-level task performance on linear MBA where models are asked to choose an appropriate lemma from our customized lemma library for each step of the proof.

and omega, showing that a considerable manipulation of the automated tactic taxonomy.

```
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       DeepSeek-Prover-v2-671B:
       theorem machine_never_halts : ∀ n, (nth_cfg n).isSome
306
             \hookrightarrow := by
307
          intro n
308
         have h : ∀ n, (nth_cfg n).isSome := by
            intro n
309
            induction n with
             zero => simp [nth_cfg, init]
311
              succ n ih =>
              cases h1 : nth_cfg n with
312
              | none => simp all [nth cfg, step, machine, Cfg,
313
                    \hookrightarrowStmt, \Gamma, Fin.forall_fin_succ, Fin.
314
                    \hookrightarrow forall fin succ']
               | some cfg =>
315
                 \texttt{simp_all} [nth_cfg, step, machine, Cfg, Stmt, \Gamma,
316
                      \hookrightarrow Fin.forall_fin_succ, Fin.forall_fin_succ
                      \hookrightarrow'
                 <;>
318
                 (try cases cfg <;> simp_all [nth_cfg, step,
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                       \hookrightarrowmachine, Cfg, Stmt, \Gamma, Fin.
                      ↔ forall_fin_succ, Fin.forall_fin_succ'])
                 <;>
                 (try aesop)
                 <;>
                 (try omega)
                 <;>
324
                 (try aesop)
325
          exact h n
326
```

In this successful MBA case, the problem is simple enough that bv_decide is able to solve it within its default 10second timeout by leveraging a SAT solver.

```
o4-mini:

theorem mba_challenge_88282d89 (x y : BitVec 32) : 1#32

→ * --- (x &&& --- y) + 1#32 * --- (x ^^ y) - 3#32 *

→ (x ||| --- y) + 1#32 * --- (x ||| y) + 3#32 * (x

→ &&& --- (x ||| y) + 3#32 * (x &&& y) = 1#32 * --- (x |||

→ --- y) := by

bv_decide
```

This case is more complex such that bv_decide alone cannot solve. However, the combination of norm_num and bv_decide is sufficient to complete the proof. Notably, the sequence of have statements introducing previously proven lemmas is entirely unused, and the tactics following the first bv_decide are never executed, as the goal is already solved at that point. This suggests that the model remains heavily reliant on automated tactics and lacks a clear understanding of what these tactics actually do.

```
DeepSeek-Prover-v2-671B:
theorem mba_challenge_3165c251 (x y : BitVec 32) :
  -3#32 * (x | | | ~~~y) - 1#32 * x - 2#32 * y + 1#32 *
      \Rightarrow (x ||| y) + 2#32 * ~~~ (x ||| ~~~ y) + 2#32 *
                   ~y) + 6#32 * (x &&& y) = -2#32 * ~~~y
      ↔ (x & & & ^
       \hookrightarrow := by
 have h1 := bv32_not_xor_eq_or x y
  . . .
 have h_{21} := bv32\_sum\_all y x
 norm_num [Nat.add_assoc, Nat.add_comm, Nat.
       →add_left_comm, Nat.mul_assoc, Nat.mul_comm, Nat
       ↔.mul_left_comm] at *
  <;> simp_all (config := {decide := true})
  <;> bv decide
  <;> simp_all (config := {decide := true})
  <;> by decide
```

4.4. Failure Cases

Our experiments reveal several key failure modes of frontier models. These failure can be categorized into 4 major types with signature patterns as shown in Table 5. More cases in

330	Appendix E.	
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332	Error Message Type	%(#Errors)
333		
334	Irrelevant Hallucination	67.27% (122404)
335	Tactic Misuse	23.22% (42247)
336	Voluntary Give Up	4.88% (8871)
337	Type Mismatch	4.47% (8136)
338	Others	0.16% (300)

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Table 5. Summary of error type distribution for both BB and MBA Challenge.

343 Hallucination. Hallucination consistently appears within 344 7B theorem provers, where they often tried to use non-345 existent theorems or tactics. DeepSeek-Prover-v2-671B 346 has exhibited much stronger anti-hallucination capability 347 thanks to its large base model. 348

Here we show 2 cases where Goedel-Prover-SFT attempted 349 to prove by induction on a completely unrelated problem. 350 Similarly, Kimina-Prover-Preview tried to rename the given 351 theorem head nth_cfg to nth_configuration, which 352 led to an unsolved goal at the end of the proof. 353

```
354
         Goedel-Prover-SFT:
355
         theorem sequence_formula {a : \mathbb{N} \to \mathbb{N}} (h1 : a 1 = 1)
               (h_rec : \forall n : \mathbb{N}, n \geq 1 \rightarrow a (n + 1) = 2 * a n + 1)
356
                     \rightarrow
357
```

```
\forall n : \mathbb{N}, n \geq 1 \rightarrow a n = 2^n - 1 := by
```

359 Kimina-Prover-Preview:

```
360
      theorem machine_never_halts : ∀ n, (nth cfigurations n)
361
           ↔.isSome := by
        intro n
362
        induction n with
363
        zero =>
          simp [nth configurations]
364
        | succ n ih =>
365
          simp [nth configurations, ih]
          <;> aesop
367
```

368 For the MBA challenge, we show another failure case of 369 OpenAI-o4-mini where model hallucinates a non-existent 370 tactic bv_simp. 371

```
o4-mini:
theorem mba_challenge_14b066fa (x y : BitVec 32) :
                                                                                   \stackrel{\leftarrow}{\hookrightarrow} -1 \# 32 * - (x ^{-} (x ^{-} y) + 2 \# 32 * - x + 2 \# 32 * - (x ^{-} (x ^{-} y) + 2 \# 32 * (x ^{-} + 2 \# 32 * x + 3 \# 32 * (x ^{-} + 3 \# 
                                                                                      \begin{array}{c} \hookrightarrow & || | & \overbrace{\phantom{a}}^{r} y) & - 2 \# 32 \ \ast \ (x \ \land \land \land \ y) \ + \ 1 \# 32 \ \ast \ \overbrace{\phantom{a}}^{r} (x \ \&\&\& \\ \hookrightarrow \\ \frown x) \ - \ 5 \# 32 \ \ast \ y \ - \ 8 \# 32 \ \ast \ \overbrace{\phantom{a}}^{r} (x \ || \ y) \ - \ 2 \# 32 \ \ast \ (x \ || \ y) \ - \ 2 \# 32 \ \ast \ (x \ || \ y) \ - \ 2 \# 32 \ \ast \ (x \ || \ y) \ - \ 2 \# 32 \ \ast \ (x \ || \ y) \ - \ 2 \# 32 \ \ast \ (x \ || \ y) \ - \ 2 \# 32 \ \ast \ (x \ || \ y) \ - \ 2 \# 32 \ \ast \ (x \ || \ y) \ - \ 2 \# 32 \ \ast \ (x \ || \ y) \ - \ 2 \# 32 \ \ast \ (x \ || \ y) \ - \ 2 \# 32 \ \ast \ (x \ || \ y) \ - \ 2 \# 32 \ \ast \ (x \ || \ y) \ - \ 2 \# 32 \ \ast \ (x \ || \ y) \ - \ 2 \# 32 \ \ast \ (x \ || \ y) \ - \ 2 \# 32 \ \ast \ (x \ || \ y) \ - \ 2 \# 32 \ \ast \ (x \ || \ y) \ - \ 2 \# 32 \ \ast \ (x \ || \ y) \ - \ 2 \# 32 \ \ast \ (x \ || \ y) \ - \ 2 \# 32 \ \ast \ (x \ || \ y) \ - \ 2 \# 32 \ \ast \ (x \ || \ y) \ - \ 2 \# 32 \ \ast \ (x \ || \ y) \ - \ 2 \# 32 \ \ast \ (x \ || \ y) \ - \ 2 \# 32 \ \ast \ (x \ || \ y) \ - \ 2 \# 32 \ \ast \ (x \ || \ y) \ - \ 2 \# 32 \ \ast \ (x \ || \ y) \ - \ 2 \# 32 \ \ast \ (x \ || \ y) \ - \ 2 \# 32 \ \ast \ (x \ || \ y) \ (x \ || \
                                                                                     \Rightarrow x \&\&\& ~~y) + 3#32 * (x \&\&\& y) = -1#32 * ~~(x % % % % y)
                                                                                     ↔&&& ~~~y) := by
                                                                           bv_simp
                                                                           ring
```

Tactic misuse. Models showed a dangerous tendency to blindly apply automated proof tactics such as aesop (which automatically looks for search tactics recursively in a proof tree) without understanding the necessary conditions for aesop to be applicable, resulting in the failure of exhaustive search.

```
DeepSeek-Prover-v2-671B:
theorem machine_never_halts : ∀ n, (nth configurations
    ↔n).isSome := bv
  intro n
  . . .
    <;> aesop
```

In this MBA challenge example, this tendency is even more pronounced. The model gathers many lemmas into one simp_only call without checking their relevance and then blindly invokes ring. The proof is bloated with useless rewrites and heavy automation, yet still failsdemonstrating a failure to reason about lemma and tactic applicability.

```
o4-mini with lemmas:
theorem mba_challenge_080db093 (x y : BitVec 32) :
    -5#32 * ~~~y + 1#32 * ~~~ (x &&& ~~~x) + 4#32 * (x |||
                                 ↔x + 24#32 * ~~~ (x ||| y) + 22#32 * ~~~ (x |||
                                  ↔~~~y) + 13#32 * (x &&& ~~~y) + 6#32 * (x &&& y
                                  (\rightarrow) = -4#32 * ~~~ (x ^^ y) + 6#32 * (x ||| ~~~ y)
                                  \hookrightarrow := by
           simp only [bv32_and_not_self, bv32_not_and_self,

why the set of t
          simp only [bv32_x_distr, bv32_y_distr, ...] at *
          simp only [bv32_sum_all] at *
         ring
```

This sample illustrates a tactic misuse whereby_decide fails to solve the goal within the 10-second timeout. The failure highlights the limitations of relying solely on automated tactics for large or intricate goals.

```
o4-mini:
import Std.Tactic.BVDecide
/--
Let x,y be 32-bit bit-vectors. Prove the equivalence of
         \hookrightarrow the following two expressions: 7.x - 5.y - 2.(x\oplus
         \hookrightarrowy) - 6·¬(x \land ¬x) - 5·(x\lory) - 2·¬(x\landy) - (x\lor¬y) +
          \hookrightarrow 4 \cdot \neg y - 7 \cdot \neg (x \oplus y) + 13 \cdot \neg (x \vee y) + 21 \cdot \neg (x \vee \neg y) + 17 \cdot (x \wedge \neg y) 
         \hookrightarrowy) and -5 \cdot (x \land \neg y) + 1 \cdot \neg x
theorem mba_challenge_6f99807f (x y : BitVec 32) :
         \hookrightarrow ((7\#32 \ \star \ x) \ - \ (5\#32 \ \star \ y) \ - \ (2\#32 \ \star \ (x \ \widehat{} \ \widehat{} \ y)) \ -
         \hookrightarrow (6\#32 \ \star \ (\tilde{\ } \tilde{\ } (x \ \&\&\& \ (\tilde{\ } \tilde{\ } x)))) \ - \ (5\#32 \ \star \ (x \ \big| \ \big| \ y))
         ↔ - (2#32 * (~~~ (x &&& y))) - (1#32 * (x ||| (~
                                                                                                           ~у
         (\rightarrow))) + (4#32 * (~~~y)) - (7#32 * (~~~(x ~~y))) +
         \hookrightarrow (13\#32 \ \ast \ (\ \widetilde{\phantom{a}}\ \widetilde{\phantom{a}}\ (x \ | \ | \ y))) \ + \ (21\#32 \ \ast \ (\ \widetilde{\phantom{a}}\ \widetilde{\phantom{a}}\ (x \ | \ | \ |
         \hookrightarrow (\tilde{y}))) + (17#32 * (x \&\& y))) = ((-5#32) * (x \&\& w))) = ((-5#32) * (x \&\& w))) = ((-5#32) * (x \&\& w)))
         \hookrightarrow \&\&\& (\tilde{} (\tilde{} \tilde{} ))) + (1#32 * (\tilde{} \tilde{} \tilde{} x)) := by
   bv decide
```

Type mismatch. Type mismatch is a fundamental syntactic error arising from the type-dependent nature of Lean system, which directly reflects models' failure to understand and correctly apply respective Lean tactics in question. In this case, the 7B theorem-proving models failed to interpret and adapt to Leans inherent type rules, producing expressions whose inferred types did not match the expected ones. Fortunately, this type of error occurs rarely at 4.47% in the
big picture, which speaks to the promising progress that
frontier models have a considerably correct understanding
of the Lean tactic taxonomy.

```
389
389
390
Kimina-Prover-Preview:
theorem machine_never_halts : ∀ n, (nth_cfg n).isSome
391
392
intro n
induction n with
...
394
I succ n ih =>
395
simp [nth_cfg, step, machine]
exact ih
```

Voluntary give-up. In this case, the model voluntarily
chose to give up by leaving sorry under the proof goal
without even attempting to solve the problem with any tactics at all. This type of error makes up 4.88% of total errors,
which could be seen as a failure of instruction-following
often depicted by reasoning models comparing to generalpurpose LLMs.

5. Discussion

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The Automation Trap in Theorem Proving Our empirical analysis identifies a systematic overreliance on automated tactics as primary proof mechanisms across frontier models. Models predominantly deploy tactics such as aesop for recursive proof search and by_decide for SATbased solving as black-box oracles, demonstrating minimal comprehension of their formal operational boundaries. This dependency manifests in two critical failure modalities: (1) proofs that circumvent genuine deductive understanding when tactics succeed coincidentally, and (2) complete proof collapse when tactics fail without fallback mechanisms. Notably, models frequently generate elaborate lemma declarations while defaulting to brute-force tactic sequencinga pattern indicating a fundamental disconnect between syntactic manipulation and strategic reasoning that fundamentally undermines verification integrity.

The Reasoning Gap between Step-Level vs. Holistic Proof Task Our step-level task decomposition setting reveals a significant discrepancy between step-level performance and holistic proof synthesis with a simple overhead proof goal. Models demonstrate near-perfect capability in choosing unseen out-of-distribution lemma for atomic inference tasks yet exhibit catastrophic failure rates in composing these operations into complete proofs. This divergence indicates that the primary bottleneck resides not in local operations but in global proof planning and strategic integration. The persistent inability to reconcile stepwise correctness with end-to-end whole proof generation suggests reasoning capabilities of frontier models remain constrained in long contexts by insufficient strategic planning for orchestrating atomic transformations into coherent proof strategies when challenged with lengthy proofs containing multiple steps.

Contamination-Resistant Evaluation Framework Our methodology establishes a novel evaluation paradigm through the integration of Lean with Theoretical Computer Science. Our framework achieves infinite scalability via algorithmic problem generation from parameterized TCS modules, with granular difficulty modulation through computational parameters (e.g., Turing Machine state complexity, MBA expression depth). Automated verifiability provides ground-truth validation without human intervention, while dynamically generated problem spaces ensure intrinsic resistance to dataset contamination. By enabling rigorous formal-informal alignment absent expert curation, this TCS-inspired synthesis creates a sustainable evaluation ecosystem where benchmark freshness and complexity scales along with the progress of frontier theoretical computer science research.

6. Conclusion

We propose Theoretical Computer Science as a promising testbed for formal theorem proving, which by design is capable of utilizing modularized, fully automatic problem generation to systematically overcome contamination and scalability limitations in legacy benchmarks. Our TCSinspired modular synthesis paradigm enables the creation of infinitely scalable, formally rigorous problem spaces with adjustable complexity through computational parameters such as Turing Machine state configurations and MBA expression depth. Our experimental results demonstrate a profound reasoning gap: while models achieve near-perfect scores of 98.88% on atomic step-level tasks involving out-ofdistribution lemma selection, they collapse to a mere 12% success rate when synthesizing complete lengthy proofs. This drastic performance degradation highlights the devastating role of hallucination during long-context reasoning sequences, which may act as a roadblock for models to form any systematic strategies for tasks requiring lengthy whole proofs. We also reveal the dangerous tendency of frontier models' over-reliance on automated tactics like aesop and bv_decide without understanding their applicability with limitations. To tackle these challenges, we call on the Lean community to further explore the massive potential of theoretical computer science and its interplay with the realm of formal theorem proving, thereby leveraging the joint effort to advance both domains synergistically.

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• A. Limitations

While this work has been conducted according to best practices of previous work on formal theorem proving, there are several potential limitations:

⁴ Firstly, our evaluation for proprietary OpenAI models are conducted with their default configuration, combined with our
 ⁵ zero-temperature setting for open-sourced models to enhance reproducibility, all evaluated models may not have shared
 ⁶ completely identical settings due to the undisclosed parameter settings of proprietary models.

Meanwhile, in order to strike a balance between budgetary restraints and performance representativeness, we only selected best-performing models on mainstream formal theorem proving benchmarks such as PutnamBench (Tsoukalas et al., 2024) and miniF2F (Zheng et al., 2022) for evaluation. There may be merit in exploring how other frontier proprietary models such as Gemini-2.5 (Google DeepMind, 2025) and Claude-3.7-Sonnet (Anthropic, 2025) would perform on our dataset. Therefore, we plan to open-source our codebase and dataset to the community for researchers with ample resources to explore more models.

Lastly, while we leverage Lean compiler to automate proof validation, the proof is graded on a pass/fail basis as a whole. However, we note it's possible to implement a stepwise grading metric by dynamically masking each step in a whole proof and ask the model to fill in each step respectively, thereby gauging models' capability to implement key intermediate steps.

B. Automated Proof Validation

In our validation pipeline, we adopt the open-source Lean 4 server implementation from Kimina Lean Server (Santos et al., 2025). The Kimina Lean Server provides a Python interface allowing real-time feedback for generated proofs. With a Python function call verify, the server receives a list of Lean proofs and returns validation results for each proof. The server itself handles multiple requests efficiently by spreading verification across multiple Lean REPL processes.

C. Complete Example with Our Prompting Strategy

System Prompt We used default system prompts as in the evaluated models' metadata.

A complete BB example. Below we demonstrate a complete record of evaluation, including the problem statement in Lean 4 and Markdown, our evaluation prompt and the model response:

Lean Meets Theoretical Computer Science: Scalable Synthesis of Theorem Proving Challenges in Formal-Informal Pairs

```
def init (l : List \Gamma) : Cfg := ((0, by omega), Turing.Tape.mk<sub>1</sub> l)
def step (M : Machine) : Cfg \rightarrow Option Cfg :=
 fun (q, T)
                (M q T.head).map fun \langle q', a \rangle
                                                       (q', (T.write a.write).move a.move)
def machine : Machine
|\langle 000, \rangle, \Gamma.zero \Rightarrow \text{some } \langle \langle 000, \text{ by omega} \rangle, \langle \text{Turing.Dir.left}, \Gamma.zero \rangle \rangle
  \langle 000, \_ \rangle, \Gamma.one => none
|\langle 001, \_ \rangle, \Gamma.zero => none
|\langle 001, \_ \rangle, \Gamma.one => \text{ some } \langle \langle 000, \text{ by omega} \rangle, \langle \text{Turing.Dir.left, } \Gamma.one \rangle \rangle
| (_+2, _), _ => by omega
def nth_cfg : (n : Nat) -> Option Cfg
| 0 => init []
| Nat.succ n => match (nth_cfg n) with
                  | none => none
                  | some cfg => step machine cfg
/__
Prove the following Turing Machine with the transition table never halts.
| State | Symbol | Next State | Move | Write |
 -----|-----|-----|-----|
| 000 | zero | 000 | left | zero |
| 000 | one | HALT | - | - |
| 001 | zero | HALT | - | - |
| 001 | one | 000 | left | one |
theorem machine_never_halts : \forall n, (nth_cfg n).isSome := by
 sorry
• • •
You can make your own auxiliary corollaries and theorems to support the proof, instead of only completing the part
     ↔with the sorry. Please output the entire program and not just the last part. Please output only the program
     \hookrightarrow and add no other comment, such that your answer is a compilable lean code. Make sure to reason enough to make
     \hookrightarrow your code correct.
### Response:
```lean4
import Mathlib
import Aesop
set_option maxHeartbeats 0
open BigOperators Real Nat Topology Rat
/-- Given a sequence { a } with a_1 = 1 and a
 L_1 = 2a + 1,
 prove that a = 2^n - 1 for all n \ge 1 - /
theorem sequence_formula {a : \mathbb{N} \to \mathbb{N}} (h1 : a 1 = 1)
 (h_rec : \forall n : \mathbb{N}, n \geq 1 \rightarrow a (n + 1) = 2 * a n + 1) :
 \forall n : \mathbb{N}, n \geq 1 \rightarrow a n = 2^n - 1 := by
 /-
 We need to prove that for a sequence (\{a_n\}) defined by (a_1 = 1) and (a_{n+1} = 2a_n + 1), the
 \rightarrow general term \(a_n \) is given by \(a_n = 2^n - 1 \) for all \(n \geq 1 \).
 1. **Base Case**: For (n = 1), we have (a_1 = 1). This matches (2^1 - 1 = 1), so the base case holds.
 2. **Inductive Step**: Assume (a_n = 2^n - 1) holds for some (n \ge 1). We need to show it holds for (n \ge 1)
 \hookrightarrow + 1 \).
 - By the recurrence relation, \langle a_{n+1} \rangle = 2a_n + 1 \rangle.
 - Using the inductive hypothesis \ (a_n = 2^n - 1 \), we get:
 \ [
 a_{n+1} = 2(2^n - 1) + 1 = 2^{n+1} - 2 + 1 = 2^{n+1} - 1
 \backslash 1
 - Thus, \(a_{n+1} = 2^{n+1} - 1 \), completing the inductive step.
 By induction, (a_n = 2^n - 1) holds for all (n \ge 1).
 -/
 intro n hn
 induction' hn with n hn
 -- Base case: n = 1
 -- We know a 1 = 1, which matches 2^1 - 1 = 1
 simp all
 -- Inductive step: Assume a n = 2^n - 1, prove a (n + 1) = 2^n (n + 1) - 1
 cases n with
 zero =>
```

```
-- When n = 0, the induction hypothesis does not apply, so we directly use the initial condition
simp_all
succ n =>
-- For n = succ n, use the recurrence relation and the inductive hypothesis
simp_all [Nat.succ_eq_add_one, Nat.pow_succ, Nat.mul_succ]
-- Simplify the expression to match the form 2^(n + 1) - 1
ring
<;> omega
```

. . .

# **A complete step lemma challenge example.** Below we demonstrate a complete record of evaluation, including the problem statement in Lean 4 and Markdown, our evaluation prompt and the model response:

```
Theorem library:
```lean4
import Mathlib.Tactic.Lemma
import Mathlib.Tactic.NthRewrite
0[simp]
theorem bv32_and_not_self(x : BitVec 32) :
 x &&& ~~~x = 0 := by
 simp
0[simp]
theorem bv32_not_not(x : BitVec 32) :
   ~~~~x = x := by
  simp
@[simp]
theorem bv32_or_not_self(x : BitVec 32) :
 x ||| ~~~x = BitVec.allOnes 32 := by
 simp
0[simp]
theorem bv32_not_or_self(x : BitVec 32) :
   ``~ x ||| x = BitVec.allOnes 32 := by
  simp
0[simp]
theorem bv32_neg_mul (x y : BitVec 32) :
 -x * y = -(x * y) := by
  simp
theorem bv32_not_and (x y : BitVec 32) :
 ~~~ (x &&& y) = ~~~ x ||| ~~~ y := by
 rw [BitVec.not_and]
theorem bv32_not_or (x y : BitVec 32) :
  ~~~(x | | | y) = ~~~x &&& ~~~y := by
  rw [BitVec.not_or]
theorem bv32_not_xor_eq_or (x y : (BitVec 32)) :
  (x ^{(1)} y) = (x ^{(1)} x ^{(1)} x ^{(1)} x ^{(1)} y) = by
  ext i
  simp
  cases h_1 : x[i] <;> cases h_2 : y[i]
  simp
  simp
  simp
  simp
theorem bv32_xor_eq_or (x y : (BitVec 32)) :
 (x ^^^ y) = (~~~x &&& y) ||| (x && ~~y) := by
  ext i
  simp
  cases h_1 : x[i] <;> cases h_2 : y[i]
  simp
  simp
  simp
  simp
```

```
theorem bv32_x_distr (x y: BitVec 32) :
  x = (x &&& y) ||| (x &&& ~~~y) := by
  ext i
  simp
 simp [
          Bool.and or distrib left]
theorem bv32_y_distr (x y: BitVec 32) :
  y = (x \&\& y | | | ~~ x \&\& y) := by
  ext i
  simp
          Bool.and_or_distrib_right]
  simp [
theorem bv32_add_assoc (x y z : BitVec 32) :
 x + y + z = x + (y + z) := by
 rw [BitVec.add_assoc]
theorem bv32_add_comm(x y : BitVec 32) :
 x + y = y + x := by
 rw [BitVec.add_comm]
theorem bv32_add_neg_eq_sub {x y : BitVec 32} :
 x + -y = x - y := by
  rw [BitVec.add_neg_eq_sub]
theorem bv32_mul_comm (x y : BitVec 32) :
 x \star y = y \star x := by
 rw [BitVec.mul_comm]
theorem bv32_var_mul_comm (x y z: BitVec 32) :
  (x &&& y) * z = z * (x &&& y) := by
 rw [BitVec.mul_comm]
theorem bv32_mul_add (x y z : BitVec 32) :
 x * (y + z) = x * y + x * z := by
 rw [BitVec.mul_add]
theorem bv32_neg_eq_mul (x : BitVec 32) :
 -x = x * (BitVec.allOnes 32) := by
 rw [ BitVec.neg_one_eq_allOnes]
  rw [BitVec.mul_neg]
 rw [BitVec.mul_one]
theorem bv32_add_mul_one (x y : BitVec 32) :
 x + x + y = x + (1#32 + y) := by
 rw [BitVec.mul_add]
 rw [BitVec.mul_one]
/--
1: x &&& v
2: ~~~x &&& y
3: x &&& ~~~y
4: ~~~ x &&& ~~~y
theorem bv32_or_eq_add12 (x y : BitVec 32) :
 (x &&& y) ||| (~~~x &&& y) = (x &&& y) + (~~~x &&& y) := by
  apply Eq.symm
 apply BitVec.add_eq_or_of_and_eq_zero
 simp [
          BitVec.and_assoc]
  simp [BitVec.and_comm _ (~~~x)]
  simp [
          BitVec.and_assoc]
theorem bv32_or_eq_add13 (x y : BitVec 32) :
  (x \&\&\& y) ||| (x \&\&\& ~~~y) = (x \&\&\& y) + (x \&\&\& ~~~y) := by
  apply Eq.symm
  apply BitVec.add_eq_or_of_and_eq_zero
          BitVec.and_assoc]
  simp [
  simp [BitVec.and_comm _ x]
  simp [BitVec.and_assoc]
theorem bv32_or_eq_add14 (x y : BitVec 32) :
```

```
(x \&\&\& y) ||| (~~~x \&\&\& ~~~y) = (x \&\&\& y) + (~~~x \&\&\& ~~~y) := by
  apply Eq.symm
  apply BitVec.add_eq_or_of_and_eq_zero
  simp [ BitVec.and_assoc]
  simp [BitVec.and_comm _ (~~~x)]
  simp [ BitVec.and_assoc]
theorem bv32_or_eq_add21 (x y : BitVec 32) :
  (\tilde{\ }\tilde{\ }\tilde{\ }x \&\&\& \ y) ||| (x \&\&\& \ y) = (\tilde{\ }\tilde{\ }x \&\&\& \ y) + (x \&\&\& \ y) := by
  apply Eq.symm
  apply BitVec.add_eq_or_of_and_eq_zero
 simp [ BitVec.and_assoc]
 simp [BitVec.and_comm _ x]
  simp [ BitVec.and_assoc]
theorem bv32_or_eq_add23 (x y : BitVec 32) :
  (\tilde{\ }\tilde{\ }\tilde{\ }x \ \&\&\&\ y) \ |\ |\ | \ (x \ \&\&\&\ \tilde{\ }\tilde{\ }y) \ = \ (\tilde{\ }\tilde{\ }x \ \&\&\&\ y) \ + \ (x \ \&\&\&\ \tilde{\ }\tilde{\ }y) \ := \ by
  apply Eq.symm
  apply BitVec.add_eq_or_of_and_eq_zero
 simp [ BitVec.and_assoc]
  simp [BitVec.and_comm _ x]
  simp [
            BitVec.and_assoc]
theorem bv32_or_eq_add31 (x y : BitVec 32) :
  (x \&\&\& ~~~y) | | | (x \&\&\& y) = (x \&\&\& ~~~y) + (x \&\&\& y) := by
  apply Eq.symm
  apply BitVec.add_eq_or_of_and_eq_zero
  simp [
            BitVec.and_assoc]
  simp [BitVec.and_comm _ x]
           BitVec.and_assoc]
  simp [
  simp [BitVec.and assoc]
theorem bv32_or_eq_add32 (x y : BitVec 32) :
                                                 ····y) + (~~~x &&& y) := by
  (x &&& ~~~y) ||| (~~~x &&& y) = (x &&& ~~
  apply Eq.symm
 apply BitVec.add_eq_or_of_and_eq_zero
 simp [
            BitVec.and_assoc]
 simp [BitVec.and_comm _ (~~~x)]
  simp [ BitVec.and assoc]
theorem bv32_or_eq_add41 (x y : BitVec 32) :
  (\tilde{x} \times \tilde{x} \times \tilde{y}) = (\tilde{x} \times \tilde{x} \times \tilde{y}) + (\tilde{x} \times \tilde{x} \times \tilde{y}) = (\tilde{x} \times \tilde{x} \times \tilde{y}) + (\tilde{x} \times \tilde{x} \times \tilde{y}) = \mathbf{by}
  apply Eq.symm
  apply BitVec.add_eq_or_of_and_eq_zero
  simp [ BitVec.and_assoc]
  simp [BitVec.and_comm _ x]
  simp [
            BitVec.and assoc]
theorem bv32_or_eq_add_three (x y : BitVec 32) :
  (x | | | y) = (x \&\&\& ~~y) + (x \&\&\& y) + (~~x \&\&\& y) := by
  nth_rw 1 [bv32_y_distr x y]
  nth_rw 1 [bv32_x_distr x y]
 simp [ BitVec.or_assoc]
  simp [BitVec.or_comm _ (x &&& y)]
  simp [ BitVec.or_assoc]
  rw [BitVec.or_comm (x &&& y)]
  apply Eq.symm
  rw [BitVec.add_eq_or_of_and_eq_zero]
  rw [BitVec.add_eq_or_of_and_eq_zero]
  simp [ BitVec.and_assoc]
  simp [BitVec.and_comm _ x]
  simp [BitVec.and_assoc]
  rw [BitVec.add_comm]
  rw [ bv32_or_eq_add13]
  rw [
          bv32_x_distr x y]
  simp [ BitVec.and_assoc]
theorem bv32_sum_all (x y : BitVec 32) :
  (~~~x &&& ~~~y) + (~~~x &&& y) + (x &&& y) + (x &&& ~~~y) = BitVec.allOnes 32 := by
  simp [BitVec.add_comm _ (~~~x &&& y)]
  simp [BitVec.add_comm _ (x &&& _)]
  simp [ BitVec.add assoc]
```

```
rw [BitVec.add_eq_or_of_and_eq_zero]
        rw [ bv32_or_eq_add_three x y]
       nth_rw 1 [bv32_x_distr x y]
        simp [BitVec.or_comm _ y]
       nth_rw 1 [bv32_y_distr x y]
        simp [ BitVec.or assoc]
        simp [BitVec.or_comm _ (x &&& y)]
        simp [ BitVec.or_assoc]
        simp [BitVec.or_comm _ (~~~x &&& _)]
        simp [ BitVec.or_assoc]
        simp [BitVec.or_comm _ (~~~x &&& y)]
        rw [ bv32_x_distr (~~~x) y]
       rw [BitVec.or_assoc]
       rw [ bv32_x_distr x y]
       simp
                                    by32 or eg add three x vl
       rw [
       simp [ BitVec.not_or]
theorem bv32_self_eq_neq_mul (x: BitVec 32):
      x = -x * (BitVec.allOnes 32) := by
       rw [BitVec.neg mul]
       rw [BitVec.mul_comm]
     rw [ BitVec.neg_mul]
       simp [ BitVec.neg_one_eq_allOnes]
theorem bv32_not_self_and_not (x y : BitVec 32) :
                 (x \&\&\& ~~x) = (~~x \&\&\& ~~y) + (~~x \&\&\& y) + (x \&\&\& y) + (x \&\&\& ~~y) := by
       rw [bv32_not_and]
     rw [BitVec.not not]
  rw [bv32_not_or_self]
   rw [bv32_sum_all]
Let x, y be 32-bit bit-vectors. Prove the equivalence of the following two expressions: $2\cdot \lnot (x\land \lnot y
                   ↔)-1\cdot (x\lor \lnot y)-7\cdot \lnot (x\oplus y)+11\cdot \lnot (x\land y)-5\cdot \lnot (x\lor y)-13\cdot \
                   \hookrightarrow lnot (x\lor \lnot y)+6\cdot (x\land y)$, $10\cdot (x\land \lnot y)$
_ /
theorem mba_challenge_02a2f35e (x y : BitVec 32) : 2#32 * ~~~ (x &&& ~~~y) - 1#32 * (x ||| ~~~y) - 7#32 * ~~~ (x ^^^
                                                                                      ~~ (x &&& y) - 5#32 * ~~~ (x ||| y) - 13#32 * ~~~ (x ||| ~~~ y) + 6#32 * (x && y) = 10#32 * (x && 
                 ⇔y) + 11#32 *
                 \hookrightarrow \tilde{} 
       simp only [ bv32_add_neg_eq_sub] /- step 1 -/
simp only [ bv32_neg_mul] /- step 2 -/
       simp only [bv32_not_and] /- step 3 -/
       simp only [bv32_not_or] /- step 4 -/
        sorry
lemma mba_challenge_02a2f35e_lhs_step_1 (x y : BitVec 32) : 2#32 * <sup>---</sup>(x &&& <sup>---</sup>y) - 1#32 * (x ||| <sup>---</sup>y) - 7#32 * 
→<sup>---</sup>(x ^^ y) + 11#32 * <sup>---</sup>(x &&& y) - 5#32 * <sup>---</sup>(x ||| y) - 13#32 * <sup>---</sup>(x ||| <sup>---</sup>y) + 6#32 * (x &&& y) = 2#32
                                   \rightarrow
                   (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 
       simp only [ bv32_add_neg_eq_sub]
lemma mba_challenge_02a2f35e_lhs_step_2 (x y : BitVec 32) : 2#32 * ~~~ (x &&& ~~~ y) + -(1#32 * (x ||| ~~~ y)) + -(7#32
                  \begin{array}{c} \longrightarrow \\ & & & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & & & \\ & & & & & \\ & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & & \\ & & & 
       simp only [
                                                                bv32_neg_mul]
lemma mba_challenge_02a2f35e_lhs_step_3 (x y : BitVec 32) : 2#32 * <sup>---</sup>(x &&& <sup>---</sup>y) + -1#32 * (x ||| <sup>---</sup>y) + -7#32 *
                  →2#32 * (~~
                 \leftrightarrow (x ||| y) + -13#32 * (x ||| ~~ y) + 6#32 * (x &&& y) := by
       simp only [bv32_not_and]
lemma mba_challenge_02a2f35e_lhs_step_4 (x y : BitVec 32) : 2#32 * (~~x ||| ~~~y) + -1#32 * (x ||| ~~y) + -7#32
                  \begin{array}{c} \leftrightarrow \ast & (1 - 1) + 1 + 32 \ast (1 - 1) + 1 + 32 \ast
       simp only [bv32 not or]
lemma mba_challenge_02a2f35e_lhs_step_5 (x y : BitVec 32) : 2#32 * (~~x ||| ~~~y) + -1#32 * (x ||| ~~y) + -7#32
                                            (x ^^^ y) + 11#32 * (~~~x ||| ~~~y) + -5#32 * (~~~x &&& ~~y) + -13#32 * (~~~x &&& ~~
                 \hookrightarrow *
                                                                                                                                                                                                                                                                                                                                                                                                                                ~v) + 6#32 * (x
```

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```
↔ &&& y) = 2#32 * (~~x ||| ~~~y) + -1#32 * (x ||| ~~y) + -7#32 * (~~x &&& ~~y ||| x &&& y) + 11#32 *
                           \hookrightarrow (\bar{\ } x | | | \bar{\ } x | | | = 1 
                        simp only [<Theorem here>]
              ...
              You are proving a single step of theorem 'mba_challenge_02a2f35e'. Based on the previous steps, select exactly one
                          ↔ appropriate theorem from the Theorem library above and insert it in place of <Theorem here> to complete the
                          ⇔proof of lemma 'mba_challenge_02a2f35e_lhs_step_5'. Do not modify any code from previous theorems or lemmas.
                          \hookrightarrow {\tt You} are also not allowed to add any other tactics to the proof body.
              ### Response:
              You need the lemma that rewrites \overline{(x \wedge y)} into (\overline{x \& \& \cdots y}) ||| (x & & y). That is
             bv32_not_xor_eq_or
              So your step 5 becomes:
1000 lemma mba_challenge_02a2f35e_lhs_step_5 (x y : BitVec 32) :
                   \begin{array}{c} (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (-7) + (
                simp only [bv32_not_xor_eq_or]
              This completes the requested rewrite.
```

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D. Template-Based Formal-Informal Translation

²⁰⁹ We use the following Python program to produce problem descriptions in rigorously aligned Lean-Markdown pair.

```
import srsly
from tqdm import tqdm
output_dir = "busy_beaver/prompts_to_run"
tables = list(srsly.read_jsonl("busy_beaver/bb_with_table.jsonl"))
template = """Complete the following Lean 4 code:
```lean4
{lean_code}
• • •
You can make your own auxiliary corollaries and theorems to support the proof, instead of only completing the part
 -with the sorry. Please output the entire program and not just the last part. Please output only the program
 ↔ and add no other comment, such that your answer is a compilable lean code. Make sure to reason enough to make
 ↔ your code correct.
....
informal_tmplate = """
/--
{informal}
-/
....
for problem in tables:
 lean_path = problem["file_name"]
 file_name = lean_path.split("/")[-1]
 out_path = f"{output_dir}/{file_name.removesuffix('.lean')}.txt"
 is_halting = True
 if "nonhalting" in file_name:
 is_halting = False
 informal_head = "Prove the following Turing Machine with the transition table " + (
 "halts." if is_halting else "never halts."
)
 # print(out_path)
 lean_code = None
 with open(lean_path, "r") as f:
 lean_code = f.read().removeprefix("\n")
 assert lean_code != None
 informal = "/-- \n" + informal_head + "\n" + problem["table"] + "-/\n"
 with open(out_path, "w") as f:
 f.write(
 template.format(
 lean_code=lean_code.replace(
```

```
 045
 "theorem machine_", informal + "theorem machine_"

 046
).replace("\n\ndef nth_cfg", "\ndef nth_cfg")

 047
 .replace("\n\n/--", "\n/--")

 048
)

 049
)

 050
 pass
```

# **E. More Success and Failure Cases**

<sup>4</sup> We demonstrate additional full record of evaluation, including problem statements in their Lean-Markdown pair and model responses for both successful and failed evaluation cases. The comprehensive record of model responses for cases can be found in the results folder of our dataset.

### E.1. Success Case

#### <sup>0</sup> E.1.1. DEEPSEEK-PROVER-V2-671B/BB-4STATE-CASE107-NONHALTING

This is a trivial non-halting case, meaning there is no "HALT" entry in the transition table. It can therefore be resolved via a single structural induction. Although the proof completes, warning messages appear, such as "aesop: failed to prove the goal after exhaustive search", "(try aesop) tactic does nothing", and "this tactic is never executed". These suggest the model does not fully reason about the proof and instead relies on automated tactics, hoping some may resolve the goal.

```
import Mathlib.Computability.TuringMachine
inductive \Gamma
 zero
 one
 deriving DecidableEq
instance : Inhabited \Gamma := \langle \Gamma. zero \rangle
structure Stmt where
 move : Turing.Dir
 write : \Gamma
def Machine := Fin 4 \rightarrow \Gamma \rightarrow Option (Fin 4
 Stmt)
structure Cfg where
 q: Fin 4
 Tape : Turing.Tape \Gamma
def init (1 : List \Gamma) : Cfg := ((0, by omega), Turing.Tape.mk₁ 1)
def step (M : Machine) : Cfg \rightarrow Option Cfg :=
 fun (q, T)
 (M q T.head).map fun \langle q', a \rangle
 (q', (T.write a.write).move a.move)
def machine : Machine
 | (000, _), Γ.zero => some ((001, by omega), (Turing.Dir.left, Γ.one))
 (000, _), \Gamma.one => some ((001, by omega), (Turing.Dir.right, <math>\Gamma.one))
 \langle 001, _ \rangle, \Gamma.zero => some \langle \langle 000, by omega \rangle, \langle Turing.Dir.right, \Gamma.one \rangle \rangle
 (001, _), \Gamma.one => some ((003, by omega), (Turing.Dir.left, <math>\Gamma.one))
 (002, _), \Gamma.zero => some ((001, by omega), (Turing.Dir.right, <math>\Gamma.zero))
 (002, _), \Gamma.one => some ((000, by omega), (Turing.Dir.right, \Gamma.zero))
 (003, _), \Gamma.zero => some ((000, by omega), (Turing.Dir.left, <math>\Gamma.zero))
 (003, _), \Gamma.one => some ((001, by omega), (Turing.Dir.left, <math>\Gamma.zero))
| \langle _+4, _ \rangle, _ => by omega
def nth_cfg : (n : Nat) -> Option Cfg
| 0 => init []
| Nat.succ n => match (nth_cfg n) with
 none => none
 | some cfg => step machine cfg
/--
Prove the following Turing Machine with the transition table never halts.
| State | Symbol | Next State | Move | Write |
```

```
|-----|-----|-----|
| 000 | zero | 001 | left | one
 000 | one | 001 | right | one |
 001 | zero | 000 | right | one |
 001 | one | 003 | left | one |
| 002 | zero | 001 | right | zero
 002 | one | 000 | right | zero
 003 | zero | 000 | left | zero |
| 003 | one | 001 | left | zero |
theorem machine_never_halts : \forall n, (nth_cfg n).isSome := by
 intro n
 have h : ∀ n, (nth_cfg n).isSome := by
 intro n
 induction n with
 | zero => simp [nth_cfg, init]
 | succ n ih =>
 cases h1 : nth_cfg n with
 | \text{ none } => \textbf{simp_all} \text{ [nth_cfg, step, machine, Cfg, Stmt, } \Gamma, \text{ Fin.forall_fin_succ, Fin.forall_fin_succ']}
 | some cfg =>
 simp_all [nth_cfg, step, machine, Cfg, Stmt, \Gamma, Fin.forall_fin_succ, Fin.forall_fin_succ']
 (try cases cfg <;> simp_all [nth_cfg, step, machine, Cfg, Stmt, Γ, Fin.forall_fin_succ, Fin.forall_fin_succ
 \hookrightarrow' 1)
 <;>
 (try aesop)
 <;>
 (try omega)
 <;>
 (try aesop)
 exact h n
```

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### E.2. Failure Case

E.2.1. DEEPSEEK-PROVER-V2-671B/BB-2STATE-CASE102-NONHALTING

This is a case where the Turing machines state remains fixed at 000. A correct proof requires showing that the machine consistently executes the first rule of the transition table. The model attempts a single structural induction; however, in the inductive case *succ* n *ih*, it leaves two unsolved goals *False*. These cannot be resolved via the induction hypothesis, suggesting that the model fails to generalize inductive reasoning in this setting.

```
import Mathlib.Computability.TuringMachine
 inductive \Gamma
 zero
 one
 deriving DecidableEg
 instance : Inhabited \Gamma := \langle \Gamma. zero \rangle
 structure Stmt where
 move : Turing.Dir
 write : \Gamma
 def Machine := Fin 2 \rightarrow \Gamma \rightarrow \text{Option} (Fin 2 Stmt)
 structure Cfg where
 q : Fin 2
 Tape : Turing.Tape \Gamma
 def init (1 : List \Gamma) : Cfg := ((0, by omega), Turing.Tape.mk₁ 1)
 def step (M : Machine) : Cfg \rightarrow Option Cfg :=
 fun (q, T)
 (M q T.head).map fun (q', a)
 (q', (T.write a.write).move a.move)
 def machine : Machine
1152 | \langle 000, _ \rangle, \Gamma.zero => some \langle \langle 000, \text{ by omega} \rangle, \langle Turing.Dir.left, \Gamma.zero \rangle \rangle
 | (000, _), \Gamma.one => none
 |\langle 001, \rangle, \Gamma.zero \Rightarrow none
```

```
|\langle 001, _ \rangle, \Gamma.one => some \langle \langle 000, \text{ by omega} \rangle, \langle Turing.Dir.left, \Gamma.one \rangle \rangle
 |\langle +2, -\rangle, - \rangle by omega
 def nth_cfg : (n : Nat) -> Option Cfg
 | 0 => init []
 | Nat.succ n => match (nth cfg n) with
 none => none
 | some cfg => step machine cfg
1162 /--
 Prove the following Turing Machine with the transition table never halts.
 | State | Symbol | Next State | Move | Write |
 |-----|-----|-----|
 | 000 | zero | 000 | left | zero |
 | 000 | one | HALT | - | - |
 | 001 | zero | HALT | - | - |
 | 001 | one | 000 | left | one |
 -/
 theorem machine_never_halts : \forall n, (nth_cfg n).isSome := by
 intro n
 have h : ∀ n, (nth_cfg n).isSome := by
 intro n
 induction n with
 zero =>
 simp [nth cfg, init]
 succ n ih =>
 simp_all [nth_cfg, step, machine, Cfg.q, Cfg.Tape, Turing.Tape.move, Option.isSome]
 <;> aesop
 exact h n
```

#### E.2.2. GOEDEL-PROVER/BB-2STATE-CASE102-NONHALTING

<sup>80</sup> The model produced proof of a completely unrelated theorem about sequences. This seems to be a hallucination, where <sup>81</sup> the model matched a common pattern like *theorem...by sorry* and filled in a generic proof without understanding the <sup>82</sup> actual task. This shows a key limitation of small provers: Without symbolic grounding or verification, they can only match <sup>83</sup> surface-level patterns rather than truly reasoning.

```
import Mathlib
import Aesop
set_option maxHeartbeats 0
open BigOperators Real Nat Topology Rat
/-- Given a sequence { a } with a_1 = 1 and a
 L_1 = 2a + 1,
 prove that a = 2^n - 1 for all n > 1 - /
theorem sequence_formula {a : \mathbb{N} \to \mathbb{N}} (h1 : a 1 = 1)
 (h_rec : \forall n : \mathbb{N}, n \geq 1 \rightarrow a (n + 1) = 2 * a n + 1) :
 \forall n : \mathbb{N}, n \geq 1 \rightarrow a n = 2^n - 1 := by
 /-
 We need to prove that for a sequence (\{a_n\}) defined by (a_1 = 1) and (a_{n+1} = 2a_n + 1), the
 \hookrightarrowgeneral term \(a_n \) is given by \(a_n = 2^n - 1 \) for all \(n \geq 1 \).
 1. **Base Case**: For (n = 1), we have (a_1 = 1). This matches (2^1 - 1 = 1), so the base case holds.
 2. **Inductive Step**: Assume (a_n = 2^n - 1) holds for some (n \ge 1). We need to show it holds for (n \ge 1)
 \hookrightarrow + 1 \).
 - By the recurrence relation, \ (a_{n+1} = 2a_n + 1 \).
 - Using the inductive hypothesis (a_n = 2^n - 1), we get:
 1 /
 a_{n+1} = 2(2^n - 1) + 1 = 2^{n+1} - 2 + 1 = 2^{n+1} - 1
 \backslash]
 - Thus, (a_{n+1} = 2^{n+1} - 1), completing the inductive step.
 By induction, (a_n = 2^n - 1) holds for all (n \ge 1).
 intro n hn
 induction' hn with n hn
 -- Base case: n = 1
 -- We know a 1 = 1, which matches 2^1 - 1 = 1
 simp all
 -- Inductive step: Assume a n = 2^n - 1, prove a (n + 1) = 2^n (n + 1) - 1
 cases n with
```

```
110 | zero =>
111 -- When n = 0, the induction hypothesis does not apply, so we directly use the initial condition
112 simp_all
113 -- For n = succ n, use the recurrence relation and the inductive hypothesis
114 simp_all [Nat.succ_eq_add_one, Nat.pow_succ, Nat.mul_succ]
115 -- Simplify the expression to match the form 2^(n + 1) - 1
116 ring
116 <;> omega
```

# E.2.3. KIMINI-PROVER-7B/BB-4STATE-CASE122-NONHALTING

The model just outputs *sorry*, which means it didnt complete the proof. This might be because it couldnt figure out how to reason about the problem, or because it has seen *sorry* used as a placeholder in Lean and assumed that was enough to count as a valid answer.

```
import Mathlib.Computability.TuringMachine
 inductive \Gamma
 zero
 one
 deriving DecidableEq
 instance : Inhabited \Gamma := \langle \Gamma. zero \rangle
 structure Statement where
 move : Turing Dir
 write : \Gamma
 def Machine := Fin 4 \rightarrow \Gamma \rightarrow Option (Fin 4 Statement)
 structure Cfg where
 q : Fin 4
 Tape : Turing Tape \Gamma
 def init (l : List \Gamma) : Cfg := ((0, by omega), (Turing Dir.right, \Gamma.zero))
 def step (M : Machine) : Cfg \rightarrow Option Cfg :=
 fun (q, T)
 (M q T.head).map fun \langleq^{\prime}, a
angle
 \langle q', (T.map a).move a \rangle
 def machine : Machine
 |\langle 000, \rangle, \Gamma.zero => \text{ some } \langle \langle 001, by omega \rangle, \langle Turing Dir.right, \Gamma.zero \rangle \rangle
 \langle 000, _ \rangle, \Gamma.one => some \langle \langle 003, \text{ by omega} \rangle, \langle \text{Turing Dir.left, } \Gamma.\text{zero} \rangle \rangle
 \langle 001, _ \rangle, \Gamma.zero => some \langle \langle 003, \text{ by omega} \rangle, \langle \text{Turing Dir.left, } \Gamma.one \rangle \rangle
 \langle 001, _ \rangle, \Gamma.one => some \langle \langle 002, \text{ by omega} \rangle, \langle \text{Turing Dir.right}, \Gamma.zero \rangle \rangle
 \langle 002, _ \rangle, \Gamma.zero => some \langle \langle 003, by omega \rangle, \langle Turing Dir.left, \Gamma.zero \rangle \rangle
 (002, _), \Gamma.one => some ((001, by omega), (Turing Dir.left, <math>\Gamma.one))
 |\langle 003, _ \rangle, \Gamma.zero => some \langle \langle 001, \text{ by omega} \rangle, \langle \text{Turing Dir.left, } \Gamma.one \rangle \rangle
 | (003, _), Γ.one => some ((000, by omega), (Turing Dir.right, Γ.zero))
 | \langle_+4\,, _\rangle\,, _ => by omega
 def nth configurations (n : Nat) : Option Cfg :=
 0 => init []
 Nat.succ n => match (nth configurations n) with
 | none => none
 | some cfg => step machine cfg
 /--
 Prove the following Turing Machine with the transition table never halts.
 | State | Symbol | Next State | Move | Write |
 -----|-----|------|-----|
 | 000 | zero | 001 | right | zero |
 | 000 | one | 003 | left | zero |
 | 001 | zero | 003 | left | one
 | 001 | one | 002 | right | zero
 | 002 | zero | 003 | left | zero |
 002
 | one | 001 | left | one |
1262 | 003 | zero | 001 | left | one |
1263 | 003 | one | 000 | right | zero |
```

```
1265 theorem machine_never_halts : ∀ n, (nth configurations n).isSome := by
1266 sorry
```

```
1269 F. Customized Lemma Library.
```

```
import Mathlib.Tactic.NthRewrite
1272 @[simp]
1273 theorem bv32_and_not_self(x : BitVec 32) :
 x &&& ~~~x = 0 := by
 simp
 0[simp]
 theorem bv32_not_not(x : BitVec 32) :
        ~~~~~x = x := by
      simp
     0 [simp]
1280 theorem bv32_or_not_self(x : BitVec 32) :
      x ||| ~~~x = BitVec.allOnes 32 := by
       simp
     0[simp]
     theorem bv32_not_or_self(x : BitVec 32) :
       ~~~x ||| x = BitVec.allOnes 32 := by
 simp
1287 @[simp]
1288 theorem bv32_neg_mul (x y : BitVec 32) :
 -x * y = -(x * y) := by
 simp
 theorem bv32_not_and (x y : BitVec 32) :
 ···· (x &&& y) = ···· x ||| ···· y := by
 rw [BitVec.not_and]
1294 theorem bv32_not_or (x y : BitVec 32) :
       ~~~ (x | | | y) = ~~~ x &&  ~~~ y := by
       rw [BitVec.not_or]
     theorem bv32_not_xor_eq_or (x y : (BitVec 32)) :
        ~~~(x ^^^ y) = (~~~x &&& ~~y) ||| (x && y) := by
 ext i
 simp
 cases h_1 : x[i] <;> cases h_2 : y[i]
 simp
 simp
 simp
 simp
 theorem bv32_xor_eq_or (x y : (BitVec 32)) :
 (x \land \land \gamma) = (\land \land \land \land \varphi) = (\land \land \land \land \land \varphi) = (x \land \land \land \land \varphi) = by
 ext i
 simp
 cases h_1 : x[i] <;> cases h_2 : y[i]
 simp
 simp
 simp
 simp
 theorem bv32_x_distr (x y: BitVec 32) :
 x = (x \&\&\& y) || | (x \&\&\& ~~~y) := by
 ext i
 simp
 Bool.and_or_distrib_left]
 simp [
 theorem bv32_y_distr (x y: BitVec 32) :
 y = (x & & & y | | | ~~~x & & & y) := by
 ext i
 simp
```

```
simp [Bool.and_or_distrib_right]
 theorem bv32_add_assoc (x y z : BitVec 32) :
 x + y + z = x + (y + z) := by
 rw [BitVec.add_assoc]
 theorem bv32_add_comm(x y : BitVec 32) :
 x + y = y + x := by
 rw [BitVec.add_comm]
 theorem bv32_add_neg_eq_sub {x y : BitVec 32} :
 x + -y = x - y := by
 rw [BitVec.add_neg_eq_sub]
 theorem by32 mul comm (x v : BitVec 32) :
 x * y = y * x := by
 rw [BitVec.mul_comm]
 theorem bv32_var_mul_comm (x y z: BitVec 32) :
 (x \& \& & y) * z = z * (x \& \& & y) := by
 rw [BitVec.mul_comm]
 theorem <code>bv32_mul_add</code> (x y z : BitVec 32) :
 x * (y + z) = x * y + x * z := by
 rw [BitVec.mul_add]
 theorem bv32_neg_eq_mul (x : BitVec 32) :
 -x = x * (BitVec.allOnes 32) := by
 rw [BitVec.neg_one_eq_allOnes]
 rw [BitVec.mul_neg]
 rw [BitVec.mul_one]
1345 theorem bv32_add_mul_one (x y : BitVec 32) :
 x + x * y = x * (1#32 + y) := by
 rw [BitVec.mul_add]
 rw [BitVec.mul_one]
 /--
 1: x &&& y
 2: ~~~x &&& y
 3: x &&& ~~~y
 4: ~~~x &&& ~~~y
 -/
1353 theorem bv32_or_eq_add12 (x y : BitVec 32) :
 (x & & & y) | | | (~~~x & & & y) = (x & & & y) + (~~~x & & & y) := by
 apply Eq.symm
 apply BitVec.add_eq_or_of_and_eq_zero
 simp [BitVec.and assoc]
 simp [BitVec.and_comm _ (~~~x)]
 simp [BitVec.and_assoc]
1359 theorem bv32_or_eq_add13 (x y : BitVec 32) :
 apply Eq.symm
 apply BitVec.add_eq_or_of_and_eq_zero
 simp [BitVec.and_assoc]
 simp [BitVec.and_comm _ x]
 simp [BitVec.and_assoc]
1365 theorem bv32_or_eq_add14 (x y : BitVec 32) :
 apply Eq.symm
 apply BitVec.add_eq_or_of_and_eq_zero
 simp [BitVec.and_assoc]
 simp [BitVec.and_comm _ (~~~x)]
 simp [BitVec.and_assoc]
1371 theorem bv32_or_eq_add21 (x y : BitVec 32) :
 (\tilde{\ }\tilde{\ }\tilde{\ }x &&& \tilde{\ }y) | | (x &&& \tilde{\ }y) = (\tilde{\ }\tilde{\ }x &&& \tilde{\ }y) + (x && \tilde{\ }x && \tilde{\ }y) := by
 apply Eq.symm
 apply BitVec.add_eq_or_of_and_eq_zero
```

```
simp [
 BitVec.and assocl
 simp [BitVec.and_comm _ x]
 simp [BitVec.and_assoc]
1378 theorem bv32_or_eq_add23 (x y : BitVec 32) :
 (~)
 apply Eq.symm
 apply BitVec.add_eq_or_of_and_eq_zero
 simp [BitVec.and_assoc]
 simp [BitVec.and_comm _ x]
 simp [BitVec.and_assoc]
1384 theorem bv32_or_eq_add31 (x y : BitVec 32) :
 (x \&\&\& ~~~ y) | | | (x \&\&\& y) = (x \&\&\& ~~ y) + (x \&\&\& y) := by
 apply Eq.symm
 apply BitVec.add_eq_or_of_and_eq_zero
 simp [
 BitVec.and_assoc]
 simp [BitVec.and_comm _ x]
 simp [BitVec.and_assoc]
 simp [BitVec.and_assoc]
1391 theorem bv32_or_eq_add32 (x y : BitVec 32) :
 (x \&\&\& ~~y) = (x \&\&\& ~~y) + (~~x \&\&\& y) := by
 apply Eq.symm
 apply BitVec.add_eq_or_of_and_eq_zero
 simp [BitVec.and assoc]
 simp [BitVec.and_comm _ (~~~x)]
 simp [
 BitVec.and_assoc]
1397 theorem bv32_or_eq_add41 (x y : BitVec 32) :
 apply Eq.symm
 apply BitVec.add_eq_or_of_and_eq_zero
 BitVec.and_assoc]
 simp [
 simp [BitVec.and_comm _ x]
 simp [
 BitVec.and_assoc]
1403 theorem bv32_or_eq_add_three (x y : BitVec 32) :
 (x | | | y) = (x \&\&\& ~~y) + (x \&\&\& y) + (~~x \&\&\& y) := by
 nth_rw 1 [bv32_y_distr x y]
 nth_rw 1 [bv32_x_distr x y]
 simp [
 BitVec.or_assoc]
 simp [BitVec.or_comm _ (x &&& y)]
 simp [BitVec.or_assoc]
 rw [BitVec.or_comm (x &&& y)]
 apply Eq.symm
 rw [BitVec.add_eq_or_of_and_eq_zero]
 rw [BitVec.add_eq_or_of_and_eq_zero]
 simp [BitVec.and assoc]
 simp [BitVec.and_comm _ x]
 simp [BitVec.and_assoc]
 rw [BitVec.add_comm]
 rw [bv32_or_eq_add13]
 rw [bv32_x_distr x y]
 simp [
 BitVec.and_assoc]
1417 theorem bv32_sum_all (x y : BitVec 32) :
 (~~~x &&& ~~~y) + (~~~x &&& y) + (x &&& y) + (x &&& ~~~y) = BitVec.allOnes 32 := by
 simp [BitVec.add_comm _ (~~~x &&& y)]
 simp [BitVec.add_comm _ (x &&& _)]
 simp [BitVec.add_assoc]
 rw [BitVec.add_eq_or_of_and_eq_zero]
 rw [bv32_or_eq_add_three x y]
 nth_rw 1 [bv32_x_distr x y]
 simp [BitVec.or_comm _ y]
 nth_rw 1 [bv32_y_distr x y]
 BitVec.or_assoc]
 simp [
 simp [BitVec.or_comm _ (x &&& y)]
 simp [BitVec.or assoc]
 simp [BitVec.or_comm _ (~~~x &&& _)]
 simp [BitVec.or_assoc]
 simp [BitVec.or_comm _ (~~~x &&& y)]
```

1430	rw [ bv32_x_distr (~~~x) y]
1431	rw [ <b>BitVec.</b> or_assoc]
1432	rw [ bv32_x_distr x y]
1433	rw [ bv32 or eq add three x v]
1434	<pre>simp [ BitVec.not_or]</pre>
1435	
1436	<pre>theorem bv32_self_eq_neg_mul (x: BitVec 32):     x = -x * (BitVec allOnes 32) := bv</pre>
1437	rw [ <b>BitVec.</b> neg_mul]
1438	rw [ <b>BitVec.</b> mul_comm]
1/130	rw [ BitVec.neg_mul]
1440	simp [ bitvec.neg_one_eq_arrones]
1441	<pre>theorem bv32_not_self_and_not (x y : BitVec 32) :</pre>
1///2	$\sum_{x \in X} (x \& \& \& x = x) = (\sum_{x \in X} \& \& \& x = y) + (\sum_{x \in X} \& \& \& y) + (x \& \& \& y) + (x \& \& \& x = y) = by$
1///3	rw [bv32_not_and] rw [ <b>BitVec</b> .not not]
1443	rw [bv32_not_or_self]
1444	rw [bv32_sum_all]
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