IMPROVER: AGENT-BASED AUTOMATED PROOF OPTIMIZATION

Anonymous authorsPaper under double-blind review

ABSTRACT

Large language models (LLMs) have been used to generate formal proofs of mathematical theorems in proofs assistants such as Lean. However, we often want to optimize a formal proof with respect to various criteria, depending on its downstream use. For example, we may want a proof to adhere to a certain style, or to be declaratively structured, concise, or contain minimal dependencies. Having suitably optimized proofs is also important for learning tasks, especially since human-written proofs may not optimal for that purpose. To this end, we study a new problem of automated proof optimization: rewriting a proof so that it is correct and optimizes for an arbitrary criterion, such as length or declarativity. As a first method for automated proof optimization, we present ImProver, a large-languagemodel agent that rewrites proofs to optimize arbitrary user-defined metrics in Lean. We find that naively applying LLMs to proof optimization falls short, and we incorporate various improvements into ImProver, such as the use of symbolic Lean context in a novel Chain-of-States technique, as well as error-correction and retrieval. We test ImProver on rewriting real-world undergraduate, competition, and research-level mathematics theorems, finding that ImProver is capable of rewriting proofs so that they are substantially shorter and more declarative in structure.

1 Introduction

The fundamental virtue of a mathematical proof is that it provides certainty: a deductive argument shows that the assumptions of a mathematical statement logically guarantee the conclusion. In practice, however, informal, natural-language proofs are prone to imprecision, ambiguity, and error. Using a formal language such as Lean (Moura & Ullrich, 2021) removes such ambiguity and imprecision and enables a proof assistant to verify correctness down to the primitives of a formal axiomatic system.

Although any two correct formal proofs of a statement equally establish the validity of their conclusion, there are various criteria on which one of them may be preferred over another. When an expert formalizer finishes a proof, they always go back and revise it, aiming, for example, to improve readability and robustness. Instructors show their students how to shorten their proofs and structure them better, and the maintainers of Lean's Mathlib (mathlib Community, 2020) demand revisions to submissions to improve their robustness and adhere to style guidelines.

To this end, we study a new problem of *automated proof optimization*: rewriting a proof so that it is correct and optimizes a user-specified criterion such as length or readability. To mathematicians and formalizers, the ability to improve proofs automatically is invaluable to the maintenance and development of libraries for research and pedagogy alike. For example, the development of Mathlib as an evolving corpus maintained by hundreds of human formalizers requires strict guidelines to ensure efficient and generalized theorems - a task that proof optimizers can excel at automating, in order to generate proofs that rely on existing lemmas with concision and generalizability.

Moreover, automated proof optimization is not only useful in its own right, but also for the purposes of improving AI that can find proof on its own. At the very least, it provides a form of data augmentation: the limited amount of formal training data is currently a bottleneck for machine learning, and our methods provide ways of generating additional data automatically. More interestingly, our methods also provide a means of optimizing training data. For example, other work (Jiang et al., 2023)

suggests that a promising means for generating formal proofs is to have an LLM sketch a high-level outline of a proof that can be filled in by symbolic automated reasoning methods. For that purpose, it is useful to have a corpus of proofs that are written in such a structured form. Our methods provide means of generating such proofs from less structured ones.

Our work shows that naively applying LLMs to proof optimization falls short, often resulting in incorrect or poorly optimized proofs. We develop various improvements that can be applied on top of a black-box language model, including Chain-of-States prompting – an analogy to chain-of-thought prompting (Wei et al., 2022) that shows intermediate proof states, contextual information, error-correction, and retrieval. We incorporate these into ImProver: a large language model agent that rewrites proofs to optimize arbitrary user-defined metrics in Lean. We test ImProver on rewriting real-world undergraduate theorems, competition problems, and research-level mathematics, finding that ImProver is capable of rewriting proofs so that they are substantially shorter and more declarative in style.¹

Original (human-written)

054

055

056

057

058

060

061

062

063

064

065

066 067

068 069

070

071

073

074

075

076

077

079

081

082

083

084

085

087

088

089 090 091

092 093

094

095

096

097

098

100

101

102

103

104

105

106

107

ImProver (length-optimized)

```
lemma lemma0 {\alpha : Type} {p : \alpha \rightarrow \alpha \rightarrow \text{Prop}}
                                                           lemma lemma0 {\alpha : Type} {p : \alpha \rightarrow \alpha \rightarrow Prop}
    (h1 : \forall x, \exists! y, p x y)
                                                                 (h1 : \forall x, \exists! y, p x y)
     (h2 : \forall x y, p x y \leftrightarrow p y x) :
                                                                 (h2 : \forall x y, p x y \leftrightarrow p y x) :
    ∀ x, Classical.choose
                                                                ∀ x, Classical.choose
         (h1 (Classical.choose (h1
                                                                      (h1 (Classical.choose (h1
     x).exists)).exists=x := by
                                                                 x).exists)).exists=x := by
  -- PROOF START
                                                              -- PROOF START
  intro x
                                                              intro x
  obtain \langle y, h1e, h1u \rangle := h1 x
                                                              obtain \langle y, hle, hlu \rangle := hl x
             : Classical.choose (h1 x).exists =
                                                             rw [hlu _ (Classical.choose_spec _)]
     v :=
                                                              obtain (w, hle', hlu') := hl y
    hlu _ (Classical.choose_spec (h1
                                                              rw [hlu' _ ((h2 _ _).mpr hle)]
exact hlu' _ (Classical.choose_spec _)
                                                             rw [hlu'
    x).exists)
  rw [h2']
  obtain (w, hle', hlu') := hl y
  have h4 := Classical.choose_spec (h1
    v).exists
  have hxw : x = w := by
    apply hlu'
    rw [h2]
    exact hle
  rw [hxw]
  exact hlu' _ h4
```

Figure 1: ImProver automatically rewrites formal proofs to optimize a criterion such as length or readability while remaining correct. In this example, ImProver optimizes a human-written lemma from the 2022 International Math Olympiad (Question 2, solution from Compfiles (David Renshaw, 2024)) for length. ImProver's optimized proof is correct and more concise.

2 RELATED WORK

Recently there has been wide interest in automating theorem proving in interactive proof assistants; see (Lu et al., 2023; Li et al., 2024) for surveys. Indeed, at a high level, proof assistants constitute a sound verifier in a prover-verifier game (Anil et al., 2021), suggesting that a machine-learning based prover that interfaces with such a verifier is a natural next step for formal reasoning systems.

A typical approach to developing machine learning provers (Polu & Sutskever, 2020) is to train on a large corpus of mathematical proofs such as Lean's Mathlib (mathlib Community, 2020; Han et al., 2022; Polu et al., 2022; Lample et al., 2022; Yang et al., 2023; Hu et al., 2024). A model learns from the distribution of proofs in the corpus, such as Mathlib-style proofs. Recently, the AlphaProof (AlphaProof & Teams, 2024) system was shown to produce proofs with an arcane, non-human structure and syntax. We consider the new problem of rewriting a proof to optimize a metric, such as rewriting a proof into a more declarative or more concise one. Proof optimization is more general than theorem proving, since we can also rewrite an empty proof to optimize correctness. Finally, there is a rich literature on the varied styles of (human) formal proofs (e.g., (Autexier & Dietrich, 2010; Wiedijk, 2004)). Our model, ImProver, builds on neural theorem proving techniques

¹Code is available at [link removed for anonymity]

including full proof generation (Jiang et al., 2023; First et al., 2023), conditioning on example proofs (Jiang et al., 2023), retrieval (Yang et al., 2023; Thakur et al., 2024), and preceding file context (First et al., 2023; Hu et al., 2024), as well as error correction (Madaan et al., 2023; Chen et al., 2023) and documentation retrieval (Zhou et al., 2023) from code generation. ImProver brings these code generation techniques, along with new Chain-of-States prompting and meta-programmed contextual information, into a unified proof optimization agent.

3 AUTOMATED PROOF OPTIMIZATION WITH ImProver

Given a theorem statement x, additional context c, and an initial proof y_0 , proof optimization consists of generating a new proof y that is correct and minimizes (or maximizes) a metric $\mu(x, c, y_0, y) \to \mathbb{R}$.

3.1 METRICS

By varying the metric, we can perform tasks such as shortening proofs, making them more declarative

in structure, or even automated proving. We consider 3 metrics:

Length Metric: The length metric measures the number of tactic invocations in the tactic proof, aiming to reduce the proof's length while ensuring its correctness. Note that shorter proofs often represent more efficient proofs.

Declarative Metric: We aim to rewrite proofs to be written in a declarative style (Autexier & Dietrich, 2010; Wiedijk, 2004), which is related to the number of independent subproofs in a proof. Intuitively, this corresponds with a sense of structure for the proof, and can be interpreted as being more readable, explicit, or modular in style. Concretely, we evaluate declarativity using the ratio of number of explicitly typed have tactics to total number of tactic invocations.

Completion Metric: The completion of a proof simply describes its correctness. This is a trivial metric which measures the number of errors present. The completion metric is used for concretely viewing proof optimization as a generalization of neural theorem proving.

Our goal here has been to provide a flexible means to optimize proofs with respect to any metric that might prove useful. The particular metrics we use here are intentionally simplistic, in that they are used only to test and evaluate the method. The task of designing metrics that correspond more accurately to human criteria or are optimal for various training tasks is left to later work as what defines a good metric are dependent on the use case.

 Additionally, we note the possibility of degenerate solutions, as in, generations of proofs that score highly on a certain metric, while not corresponding to the intuitive sense of that metric. For example, overuse of have statements can greatly increase the declarativity of the proof, despite not being used in the proof's deductive process whatsoever. It is undesirable for a model to generate such degenerate solutions, and to account for this, we guide the model with many human-written examples of each metric in question, rather than requiring it to solely maximize a reward function. For more complex, user-defined metrics, the possibilities for degenerate solutions only increases, and as such, guiding models using concrete examples as well as using reward models rather than reward functions to score metrics may mitigate the risks of such degenerate solutions.

3.2 Improver

We develop several improvements that can be applied to a black-box LLM generator $y_{out} \sim G(\cdot|x_{in})$, such as GPT-4 (OpenAI et al., 2024), and specify ImProver with respect to these parameters. The explicit prompts and templates that are sent to the LLM can be found in (§A).

3.2.1 Chain-of-States Prompting

Typical formal proofs are a sequence of tactics (akin to steps) and *states* that show the hypotheses and goals at each step. The intermediate states often contain valuable information (e.g., an expression after it has been simplified) that is not present in the tactics. To allow the model to reason about these intermediate goals and hypotheses, we use tools from Lean metaprogramming to automatically annotate each proof state as a comment prior to each tactic. We refer to this method as *Chain-of-*

Without Chain-of-States

162

163

164

165

166

167

168

169

170

171

172

173

174

175

176

177178

179

180 181

182 183

185

187

188

189

190

191

192

193

194

195 196

197

199

200

201

202

203

204

205

206207

208209

210

211

212

213

214

215

With Chain-of-States

```
rintro x ((xs, xt) | (xs, xu))

use xs; left; exact xt
                                                            rintro x (\langle xs, xt \rangle \mid \langle xs, xu \rangle)
  . use xs; right; exact xu
                                                            case inl.intro
                                                            \alpha : Type u_1
                                                            s t u : Set \alpha
                                                            x : \alpha
                                                            \mathsf{xs}\;:\;\mathsf{x}\;\in\;\mathsf{s}
                                                            xt : x \in t
                                                            \vdash x \in s \cap (t \cup u)
                                                            case inr.intro
                                                            \alpha : Type u_1
                                                            stu: Set \alpha
                                                             x : \alpha
                                                            \mathsf{xs}\; :\; \mathsf{x}\; \in\; \mathsf{s}
                                                            \vdash x \in s \cap (t \cup u)
                                                            · use xs; left; exact xt
                                                            Goals Solved!
                                                             . use xs; right; exact xu
                                                             Goals Solved!
```

Figure 2: A Lean proof (left) with Chain-of-States prompting annotations (right).

States (CoS) prompting since it makes intermediate states explicit, akin to how chain-of-thought prompting (Wei et al., 2022) makes intermediate steps of a solution explicit.

These states are extracted directly and symbolically from the underlying Lean compilation steps using Lean's rich metaprogramming suite. The implementation of this extraction system is modeled from the work (Kim Morrison, 2024). Specifically, in the compiler's elaboration and evaluation stages – where the parsed theorem code is first converted into concrete syntax trees (in practice, Syntax objects) and abstract syntax trees (Expr objects) – we convert the CST and AST output objects into the relevant proof data and proof states in the form of proof trees (Lean.Elab.InfoTree). These proof trees contain detailed context and information on a tactic-by-tactic level relating to the modification of the proof state, metavariable context, and proof correctness.

After state extraction is completed and cached for efficient future access, we annotate the proof text itself to contain the intermediate states in the form as comments. Figure 2 shows an example.

This explicit reasoning aims to help the generator model construct more optimized proofs via additional symbolic data.

3.2.2 Output formatting.

LLM outputs often contain ancillary and syntactically invalid content, especially before and after the actual proof. Additionally, by applying additional structure to the LLM outputs, we may hope to generate more structured proofs. To analyze this hypothesis, we introduce two additional output formats in addition to the standard string output: string list and string tree. The former enforces the model output of a proof to be a tactic sequence represented as a list of strings, and the latter enforces proofs to be written as proof trees, represented as a tree of strings.

3.2.3 Sampling Method

We also introduce different methods of sampling between many (sequential or parallel) LLM inference calls, involving best-of-n and iterative refinement implementations, as well as combinations thereof.

Best-of-n. The best-of-n technique generates multiple (n) calls to the language model and selects the "best" via a simple selection policy that first prioritizes output correctness, and secondly prioritizes the evaluated metric delta score.

Using a temperature value of 1, we ensure that our n calls to the model are diverse, as the temperature hyperparameter (ranging between 0 and 2) controls the randomness of the outputs. The default

value of 1 ensures that outputs are sufficiently random without sacrificing accuracy and generating unpredictable behavior. Moreover, this allows for sufficient variance that the best-of-n scoring function has many distinct inputs to choose from.

More specifically, our scoring function is given by the 2-ary comparison function S, whose arguments are output objects y, y'.

$$S(y,y') = \begin{cases} \max(y,y', \text{key: } x \mapsto \mu(x)), & E(y) = E(y') = 0 \\ y, & E(y) = 0, E(y') > 0 \\ y', & E(y) > 0, E(y') = 0 \\ \min(y,y', \text{key: } x \mapsto E(x)), & E(y) = E(y') > 0 \end{cases}$$

Where $\mu(x)$ is the metric score of x, and E(x) is the number of errors in x. This comparison function can be extended to evaluate the best output of any finite n via induction.

Error correction and Refinement. Inspired by self-debugging techniques in code generation (Madaan et al., 2023; Chen et al., 2023), ImProver identifies and corrects errors in the generated proofs by iteratively refining its outputs. The refinement process relies on user-defined parameters n and prev_num to specify the number of iterations and the number of previous iterations' data to forward, respectively. Each iteration carries information on the last prev_num iterations, including input, output, metric score, correctness, and error messages.

Combination Sampling and Compound Prompt Functions. Compound prompt functions utilize the curried nature of the back-end implementations of best-of-n and refinement to nest these techniques within one another. For example:

 $best_of_n$ ((refinement, m), n) is a compound sampling method that run a best-of-n, where each call is a m-step refinement.

refinement ((best_of_n, m), n) is a compound sampling method that runs a n-step refinement, where each call is a best-of-m call to the LLM.

Note that with each of these compound prompt functions, there are always a total of mn iterations.

3.2.4 RETRIEVAL

ImProver uses MMR (Maximum Marginal Relevance)-based (Carbonell & Goldstein, 1998) retrievalaugmented generation to select relevant examples and documents. More specifically, for a userspecified k, example retrieval selects the k most relevant examples of proof optimization on a specific metric. additionally, document retrieval extracts information using MMR from a pair of fixed (vector) databases for the specified metric. The databases store syntactically chunked data from the Theorem Proving in Lean (TPiL) handbook – containing syntax guides and tactic explanations – and the Mathlib mathematics libary – containing thousands of theorems and lemmas.

The Mathlib retriever finds the top k documents that score the highest MMR score against the current theorem, the TPiL retriever finds the top k documents that score the highest MMR score against the current theorem in context and all current error messages. This retrieval process helps in generating more contextually accurate prompts that allow the language model to better correct its own errors as well as find useful lemmas to reference.

4 EXPERIMENTS

We test ImProver on rewriting real-world undergraduate theorems, competition problems, and research-level mathematics and compare its results to those of the base GPT-40 and GPT-40-mini models. We examine the optimization capabilities of ImProver for the length and declarative metrics - studying the effectiveness in maintaining the correctness of the tactic proof while making it more concise as well as making it more declarative in style and structure.

4.1 SETUP

Our experimentation is split into three distinct stages. We first perform ablation testing on the ImProver model parameters (§3.2) to ensure that ImProver's parameter specification is the optimal one with respect to correctness and metric optimization score. We then evaluate this optimal parameter combination on datasets of varying complexity and analyze the performance and results thereof. Lastly, we note the performance of ImProver in NTP applications in comparison to the base GPT-40 and GPT-40-mini models.

Datasets. We evaluate ImProver on subsets of the Mathematics in Lean (MIL) (leanprover-community, 2024), Compfiles (David Renshaw, 2024), and Mathlib (mathlib Community, 2020) datasets. Details of the datasets used in each experiment is included in appendix B.1.

Models. Our base generator uses GPT-4o (OpenAI et al., 2024) (gpt-4o-2024-08-06). Since no prior methods currently exist for automated proof optimization, we consider a prompted GPT-4o without the improvements described in (§3.2) as our baseline. Additionally, the baseline and ImProver both receive a prompt containing instructions to optimize for the given metric, with the theorem statement, context, and initial proof. ImProver augments this prompt with the data from the improvements described in §3.2. Additional input information is detailed in appendix A.

Performance metrics. Since proof optimization is a new task, we define four performance metrics for measuring aspects of correctness and improvement.

First, we define *improvement* for length as percentage change in length, $\frac{\mu_{\rm len}(y_0) - \mu_{\rm len}(y)}{\mu_{\rm len}(y_0)} \times 100$. For readability, we use the difference, $\mu_{\rm read}(y) - \mu_{\rm read}(y_o)$. If no correct output is generated by the model for a specific theorem, improvement is defined to be zero. We define *nonempty improvement* as the improvement restricted to theorems for which some output has nonzero improvement. Intuitively, improvement is the expected improvement in metric score from the input to output, accounting for errors in the generation. The nonempty improvement score is the expected improvement in metric score, given that there are no errors in the generation.

Additionally, the *accuracy* is the percentage of theorems in the dataset which the model was able to generate a correct output for. The *improved accuracy* is the percentage of theorems in the dataset which the model was able to generate a correct output for, as well as improve the metric to be nonzero.

4.1.1 ABLATIONS

When performing our ablation studies, we used a fixed dataset (MIL; see appendix B.1) and metric (length) and varied the parameters of all the features to find the optimal combination. However, as there are over 8640 possible combinations, rather than test all combinations, we evaluate using a factorial testing method.

Testing Groups.

We define the following testing groups with the specified parameter combinations:

GPT-4o-mini/GPT-4o: This varies the GPT-4o model, outputting a string with no other features.

Output and CoS: We evaluate the effects of different output formatting styles (string, string list, string tree) and CoS (True, False), with the model fixed as GPT-40, with no other features enabled.

Example Retrieval: We evaluate the effects of increasing the number of examples provided (multishot prompting) in the range of 0, 3, 5, 7, and 10, with the model fixed as GPT-40, CoS and output formatting fixed as the best combination from the previous test, and no other features enabled.

Sampling Method: Here, we evaluate the effects of best-of-n and refinement for a fixed n=5. Additionally we test on the refinement cases if forwarding the most recent iteration result, or all previous iteration results is the best, and if we should keep the best out of the iterations, or the most recent. The model is fixed as GPT-40, CoS, output formatting, and examples are fixed as the best combination from the previous test, and no other features enabled.

n and Model: Here, we evaluate the effects of larger n values and different models. We test n=3,5,7,10,15 on GPT-40 and GPT-40-mini, as well as n=20 for GPT-40-mini (as it is of a

Table 1: Average Proof optimization results.

Metric	Model	Improvement	Nonempty Improvement	Accuracy	Improved Acc.
Length	GPT-40	3.7	15.15	26.36%	8.31%
	ImProver	20.96	55.29	100.0 %	35.44 %
Readability	GPT-40	2.21	8.02	18.75%	6.13 %
	ImProver	9.34	30.53	100.0 %	24.56 %

Table 2: MIL Proof optimization results.

Metric	Model	Improvement	Nonempty Improvement	Accuracy	Improved Acc.
Length	GPT-40	6.25	18.58	37.5%	14.42%
	ImProver	30.54	56.56	100.0%	50.0%
Declarativity	GPT-40	4.18	14.48	28.85%	11.54%
	ImProver	13.45	30.97	100.0%	34.21 %

far lower token cost). CoS, output formatting, examples, and sampling method are fixed as the best combination from the previous test, and no other features enabled.

Combos and RAG: We evaluate combination methods refinement (best_of_m',m) and best_of_m' (refinement (m)), for $m \neq m'$ with mm' equal to the optimal value m from the previous test. We also test the effect of enabling document retrieval. Model, CoS, output formatting, examples, n, and sampling method are fixed as the best combination from the previous test.

Selection. For each testing group, we select the best parameter combination - which is then held as constant for the testing of all future testing groups - based on the combination that has the maximal improvement score. This improvement score represents the expected improvement in metric score, accounting for possible errors in the generation; selecting the parameter combination with the highest such score allows for rewarding both generation accuracy and large improvements in the metric score.

Comparing this with the other three performance metrics, accuracy is not prefered as a selection heuristic, as by simply returning the initial input, we can get 100% accuracy. Improved accuracy accounts for this by only counting theorems that has some positive improvement in metric score in the calculation, but this does not reward larger improvements to metric score any differently than smaller ones. Conversely, nonempty improvement ignores incorrect generations, so it is also not preferable for selection. The improvement score accounts for all this, rewarding correct generations and discouraging incorrect ones, and placing a higher weight to larger improvements in metric score.

Ablation datasets. We evaluate our ablations on a subset of MIL as detailed in appendix B.1.

4.2 RESULTS

ImProver is capable of optimizing proofs in all settings. From Table 2, Table 3, and Table 4, we can see that ImProver is capable of optimizing proofs on all datasets for both the length and declarative metrics. Furthermore, Table 1 shows that across all metrics, ImProver significantly outperforms GPT-40 on proof optimization tasks on every experimental measure – aggregated from all datasets. Additionally, from Table 2, Table 3, and Table 4, we can see that ImProver outperforms GPT-40 on each dataset as well. We proceed to analyze this data and its implications.

Length optimization. First focusing on the length metric, we see that ImProver outperforms GPT-40 with respect to the improvement score by 566% (aggregated over all datasets). Additionally, we are guaranteed that ImProver produces a correct output, although that output may just be the same as the input. However, 35.44% of the time, it generates a correct output that is not the same length as the input, and in that case, we expect an average of a 55.29% reduction in length. Comparing this with GPT-40, we conclude that not only can ImProver optimize at a higher level on arbitrary theorems, but its ability to generate nontrivial correct outputs is far greater in comparison to GPT-40.

Declarativity optimization. Declarativity optimization is similar, with ImProver outperforming GPT-40 by 423%. Moreover, the accuracy, improved accuracy, and nonempty improvement disparities for declarativity parallel those of the length tests. However, it should be noted that for both GPT-40

378 379

380 381 382 384 385

386 387 388

389 390 391 392

400

401

402 403 404 405 406 407

408 409 410 411 412 413

416 417 418 419

414

415

421 422 423

424

425

426

427

428

429

430

431

420

Table 3: Compfiles Proof optimization results.

Metric	Model	Improvement	Nonempty Improvement	Accuracy	Improved Acc.
Length	GPT-40	2.75	30.7	11.54%	5.13%
	ImProver	18.86	54.48	100.0%	34.62 %
Declarativity	GPT-40	0.39	3.38	14.1%	1.28%
	ImProver	5.74	24.89	100.0%	19.23 %

Table 4: Mathlib Proof optimization results.

Metric	Model	Improvement	Nonempty Improvement	Accuracy	Improved Acc.
Length	GPT-40	0.0	0.0	16.67%	0.0%
	ImProver	6.19	53.65	100.0%	11.54%
Declarativity	GPT-40	0.0	0.0	4.65%	0.0%
	ImProver	4.63	33.19	100.0%	11.63%

and ImProver, the accuracy and improved accuracy scores were markedly smaller for declarativity than length optimization. This suggests that for both models, it was generally more "difficult" to generate a correct output, and moreover, generate a correct output with a better metric score than the input, for declarativity optimization than length optimization. In other words, optimizing for declarativity is more difficult for the underlying generator than optimizing for length. However, we speculate with higher-quality prompts and metrics, this disparity can be minimized. Regardless, we note that different metrics can be less likely to be correctly optimized, and that model performance is correlated with the metric it seeks to optimize – both for GPT-40 and ImProver.

Optimization varies based on dataset difficulty. Additionally noting Table 2, Table 3, and Table 4, we observe that the improvement score for both metrics for both GPT-40 and ImProver is highest for the MIL dataset, lower for Compfiles, and the lowest on the Mathlib theorems. This suggests that the expected improvement in metric score decreases with higher difficultly – with undergraduate-level theorems having a significantly higher expected improvement than research-level theorems. However, it should be noted that for both metrics, the nonempty improvement of ImProver stayed consistent, whereas for GPT-40, it followed the aforementioned trend of decreasing with difficulty, Similarly, the accuracy and improved accuracy scores for both metrics and models decreased with higher difficulty datasets (disregarding ImProver's accuracy scores, as they are ensured to be 100%). This suggests that although the base GPT-40 generator is less likely to generate a correct output for higher difficulty datasets, the improvements that ImProver makes to the base generator allows it to maintain its improvement in the metric score whenever a correct output is generated. As such, we can speculate that the bottleneck in the improvement score is not the model's ability to optimize the proof for a metric, but rather its ability to generate a new correct proof at all. As such, we conjecture that with more capable generator models, the accuracy – and thus, the improvement score – in optimization tasks will continue to increase, until the improvement scores match the nonempty improvement.

Overall, we conclude that although the performance of both ImProver and GPT-40 decreases on length and declarativity optimization on more difficult datasets, ImProver significantly outperforms GPT-40 on all datasets for length and declarativity optimization.

4.2.1 ABLATION TESTING

We perform ablation studies using a subset of the MIL dataset as discussed in §4.1.1. The results of this factorial study are aggregated in Table 5. We measure the baseline results from the GPT-40 and GPT-40-mini models, noting that GPT-40 is the better-scoring model (with respect to the improvement score). Thus, fixing this model, we vary the output formatting type and if CoS is enabled, and determine that outputting string list with CoS enabled maximizes the improvement score. Fixing these parameters, we now vary the number of examples retrieved, noting that prompting with 10 examples maximizes the improvement score. Fixing this parameter, we vary the sampling methods (excluding compound methods and fixing n=5) and observe that best-of-n is the best parameter combination. Now, as GPT-4o-mini is significantly less computationally expensive than its GPT-40 counterpart, we test both models with the sample method fixed to best-of-n, and vary n=1,3,5,7,10,15, and for GPT-40-mini, also n=20. We conclude that GPT-40 with n=15 is

432 433 434

436 437

438

439

440

441

Table 5: Ablation results. Each cell in the ablation tests shows best / worst, which are the best and worst parameter combinations in the test group.

	Improvement	Nonempty Improve.	Accuracy	Improved Acc.				
GPT-4o-mini	0	0	3.62%	0%				
GPT-40	7.03	19.67	35.77%	15.33%				
+ Output and CoS	8.04 / 6.31	12.38 / 14.17	64.96% / 44.53%	21.17% / 16.06%				
+ Example Retrieval	9.34 / 5.67	14.7 / 8.44	63.5% / 67.15%	21.9% / 16.79%				
+ Sampling Method	15.35 / 9.34	18.44 / 14.7	83.21% / 63.5%	36.5% / 21.9%				
+ n and Model	23.51 / 3.65	26.28 / 4.63	89.47% / 78.95%	45.61% / 8.77%				
+ Combos and RAG	34.88 / 28.25	57.56 / 33.48	60.61% / 84.38%	54.55% / 53.12%				
ImProver	34.88	57.56	100%	54.55%				

442 443 444 445

446

448 449

Table 6: CoS Declarativity Ablation results.

	Improvement	Nonempty Improve.	Accuracy	Improved Acc.
GPT-40	4.97	15.89	37.5%	12.5%
ImProver, CoS Disabled	9.23	24.61	100.0%	28.12%
ImProver	16.69	31.42	100.0%	46.88%

450 451 452

453

454

455

456

457

458

459

460

461

462

463

464

465

466

467

468

469 470

471

472

473

474

475

476

the most effective. Fixing these parameters, we consider all mixed compound sampling methods with and without document retrieval enabled, concluding that a 5-step refinement with best-of-3 on each iteration, with RAG enabled, is the optimal combination.

Thus, as we can see from Table 5, the optimal parameter combination comes from gpt-4o outputting as a string list with CoS, RAG, 10 examples, 5-step refinement with each iteration being a best-of-3 evaluation. Changing any one of these parameters them leads to a reduction in performance. Additional ablation data can be found at (§B.2).

Declarativity and Chain-of-States (CoS) Ablation. We additionally examine the effects of disabling CoS on declarativity optimization tasks, as we speculate that CoS has a high impact on the performance of declarativity optimization tasks, as the proof states that are embedded due to CoS seem to be a critical aspect to generating the explicit declarations that the declarative metric measures.

We confirm this result by considering Table 6 and observe that enabling CoS nearly doubles the improvement score, and significantly improves the nonempty improvement score, suggesting that CoS has a large impact on optimizing for the declarative metric, as conjectured. However, we also note a significant increase in improved accuracy, which suggests that embedding the chain of states also improves the ability of the model to generate nontrivial correct outputs, implying that the symbolic information contained in the states are critical to effectively making a proof more declarative.

Syntax Guidance Ablation. We examine the effects of syntax guidance on ImProver's performance. To test this, we consider a subset of MIL (B.1), and optimize for length with and without error message forwarding. Considering the results of this ablation in Table 7, we observe that without syntax guidance and error forwarding, the ability of the model to improve the metric score is approximately unchanged, but there is a significant 13% spike in improved accuracy. This signifies that the syntax guidance improves the model's ability to generate correct results – as is expected – but does not improve the model's ability to optimize proofs assuming correct generations. This ensures that the large improvement in performance compared to GPT-40 is not solely due to simple syntax guidance, but moreso caused by improvements like CoS, example retrieval, retrieval, etc.

477 478 479

4.2.2 NEURAL THEOREM PROVING EVALUATION

480 481 482

483

484

485

We evaluate ImProver's neural theorem proving (NTP) performance using the completion metric on a subset from MIL with empty input proofs (B.1). Table 8 shows the accuracy on the dataset split by topic for both ImProver and GPT-4o. ImProver substantially outperforms GPT-4o across all topics, with an 80% increase in accuracy compared to the base model, showing that proof optimization systems do indeed generalize NTP systems.

Table 7: Syntax Guidance Ablation results.

	Improvement	Nonempty Improve.	Accuracy	Improved Acc.
GPT-40	11.00	25.94	42.42%	21.21%
ImProver, No Syntax Guidance	23.42	49.97	100.0%	46.88%
ImProver	28.94	48.74	100.0%	59.38%

Table 8: Proof generation results. Each cell shows percent accuracy.

MIL	Set Theory	Group Theory	Overall
GPT-40	18.18%	25%	21.73%
ImProver	45.45 %	33.33 %	39.13 %

4.3 QUALITATIVE RESULTS

Next, we discuss qualitative examples showing the improvements from ImProver in proof optimization. Additional examples can be found in §B.3.

Compfiles Length Optimization. Consider Figure 1, a lemma from the 2022 IMO Question 2 (Compfiles) that we optimize for length. ImProver halves thr proof from 12 tactics to 6. Here, ImProver makes multiple nontrivial optimizations, such as eliminating the h2' and h4 and hxw hypotheses, as well as fully generating proof terms for specific rewrites and other tactics.

MIL Declarativity Optimization. Consider Figure 3, a result from MIL that we optimize for the declarative metric. This original proof carried a score of 0, as it has no have statements. In comparison, after applying ImProver, the model explicitly defines hypotheses for use in the latter half of the proof; these hypotheses can easily be converted into standalone lemmas for reuse.

Original (human-written)

```
def iso1 [Fintype G] (h : Disjoint H K) (h' :
        card G = card H * card K)
: K \( \simes \) G / H := by
    apply MulEquiv.ofBijective
        ((QuotientGroup.mk' H).restrict K)
    rw [bijective_iff_injective_and_card]
    constructor
    rw [\( \simes \) ker_eq_bot_iff, (QuotientGroup.mk'
        H).ker_restrict K]
    simp [h]
    symm
    exact aux_card_eq h'
```

ImProver (declarativity-optimized)

```
def iso1 [Fintype G] (h : Disjoint H K) (h' :
     card G = card H * card K)
: K ≃* G / H := by
 have injectivity : Function.Injective
     ((QuotientGroup.mk' H).restrict K) := by
    rw [\leftarrow ker_eq_bot_iff, (QuotientGroup.mk'
    H).ker restrict K]
    simp [h]
 have card_eq : card (G / H) = card K := by
   exact aux_card_eq h'
  apply MulEquiv.ofBijective
    ((QuotientGroup.mk' H).restrict K)
  rw [bijective_iff_injective_and_card]
  constructor
 exact injectivity
  symm
 exact card eq
```

Figure 3: Optimizing a group-theoretic result from MIL Chapter 8 Section 1 for declarativity.

5 CONCLUSION

In this paper, we introduced ImProver, a novel agent-based tool for automated proof optimization in Lean. By incorporating CoS, RAG, and other features, ImProver significantly outperforms base language models in proof optimization over undergraduate, competition, and research-level problems.

However, ImProver is limited by its high cost and slow runtime, which is exacerbated by its reliance on black-box LLM's. We intend to address this inefficiency in future work by applying fine-tuning and RL on a smaller model to match performance at a lower cost.

ImProver demonstrates its ability to generate substantially shorter and more declarative proofs while maintaining correctness. As such, we believe that ImProver sets the stage for further work on proof optimization to advance the study and use of AI in mathematics.

562

563 564

565

566

567 568

569

570 571

572

573

574 575

576

577 578

579

580

581

582 583

584

585 586

588 589

590

592

540 REFERENCES 541 542 AlphaProof and AlphaGeometry Teams. Al achieves silver-medal standard solving international mathematical olympiad problems. https://deepmind.google/discover/blog/ 543 ai-solves-imo-problems-at-silver-medal-level/, 2024. 544 Cem Anil, Guodong Zhang, Yuhuai Wu, and Roger Grosse. Learning to give checkable answers with 546 prover-verifier games, 2021. URL https://arxiv.org/abs/2108.12099. 547 548 Serge Autexier and Dominik Dietrich. A tactic language for declarative proofs. In Matt Kaufmann 549 and Lawrence C. Paulson (eds.), *Interactive Theorem Proving*, pp. 99–114, Berlin, Heidelberg, 550 2010. Springer Berlin Heidelberg. 551 Jaime Carbonell and Jade Goldstein. The use of mmr, diversity-based reranking for reordering 552 documents and producing summaries. In Proceedings of the 21st Annual International ACM SIGIR 553 Conference on Research and Development in Information Retrieval, SIGIR '98, pp. 335–336, 554 New York, NY, USA, 1998. Association for Computing Machinery. ISBN 1581130155. doi: 555 10.1145/290941.291025. URL https://doi.org/10.1145/290941.291025. 556 Xinyun Chen, Maxwell Lin, Nathanael Schärli, and Denny Zhou. Teaching large language models to 558 self-debug, 2023. URL https://arxiv.org/abs/2304.05128. 559 560

- David Renshaw. compfiles. https://github.com/dwrensha/compfiles, 2024.
 - Emily First, Markus N. Rabe, Talia Ringer, and Yuriy Brun. Baldur: Whole-proof generation and repair with large language models, 2023.
 - Jesse Michael Han, Jason Rute, Yuhuai Wu, Edward Ayers, and Stanislas Polu. Proof artifact cotraining for theorem proving with language models. In International Conference on Learning Representations, 2022. URL https://openreview.net/forum?id=rpxJc9j04U.
 - Jiewen Hu, Thomas Zhu, and Sean Welleck. minictx: Neural theorem proving with (long-)contexts, 2024. URL https://arxiv.org/abs/2408.03350.
 - Albert Qiaochu Jiang, Sean Welleck, Jin Peng Zhou, Timothee Lacroix, Jiacheng Liu, Wenda Li, Mateja Jamnik, Guillaume Lample, and Yuhuai Wu. Draft, sketch, and prove: Guiding formal theorem provers with informal proofs. In The Eleventh International Conference on Learning Representations, 2023. URL https://openreview.net/forum?id=SMa9EAovKMC.
 - Kim Morrison. lean-training-data. https://github.com/kim-em/ lean-training-data, 2024.
 - 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. In Alice H. Oh, Alekh Agarwal, Danielle Belgrave, and Kyunghyun Cho (eds.), Advances in Neural Information Processing Systems, 2022. URL https://openreview.net/forum? id=J4pX8Q8cxHH.
 - mathematics in lean. leanprover-community. https://github.com/ leanprover-community/mathematics_in_lean, 2024.
 - Zhaoyu Li, Jialiang Sun, Logan Murphy, Qidong Su, Zenan Li, Xian Zhang, Kaiyu Yang, and Xujie Si. A survey on deep learning for theorem proving, 2024.
 - Pan Lu, Liang Qiu, Wenhao Yu, Sean Welleck, and Kai-Wei Chang. A survey of deep learning for mathematical reasoning. In Anna Rogers, Jordan Boyd-Graber, and Naoaki Okazaki (eds.), Proceedings of the 61st Annual Meeting of the Association for Computational Linguistics (Volume 1: Long Papers), pp. 14605–14631, Toronto, Canada, July 2023. Association for Computational Linguistics. doi: 10.18653/v1/2023.acl-long.817. URL https://aclanthology.org/ 2023.acl-long.817.

595

596

597

600

601

602 603

604

605

608

609

610

611

612

613

614

615

616

617

618

619

620

621

622

623

625

626

627

630

631

632

633

634

635

636

637

638

640

641

642

645

646

647

Aman Madaan, Niket Tandon, Prakhar Gupta, Skyler Hallinan, Luyu Gao, Sarah Wiegreffe, Uri Alon, Nouha Dziri, Shrimai Prabhumoye, Yiming Yang, Shashank Gupta, Bodhisattwa Prasad Majumder, Katherine Hermann, Sean Welleck, Amir Yazdanbakhsh, and Peter Clark. Self-refine: Iterative refinement with self-feedback. In *Thirty-seventh Conference on Neural Information Processing Systems*, 2023. URL https://openreview.net/forum?id=S37hOerQLB.

The mathlib Community. The lean mathematical library. In *Proceedings of the 9th ACM SIGPLAN International Conference on Certified Programs and Proofs*, POPL '20. ACM, January 2020. doi: 10.1145/3372885.3373824. URL http://dx.doi.org/10.1145/3372885.3373824.

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*, pp. 625–635, Berlin, Heidelberg, 2021. Springer-Verlag. ISBN 978-3-030-79875-8. doi: 10.1007/978-3-030-79876-5_37. URL https://doi.org/10.1007/978-3-030-79876-5_37.

OpenAI, Josh Achiam, Steven Adler, Sandhini Agarwal, Lama Ahmad, Ilge Akkaya, Florencia Leoni Aleman, Diogo Almeida, Janko Altenschmidt, Sam Altman, Shyamal Anadkat, Red Avila, Igor Babuschkin, Suchir Balaji, Valerie Balcom, Paul Baltescu, Haiming Bao, Mohammad Bavarian, Jeff Belgum, Irwan Bello, Jake Berdine, Gabriel Bernadett-Shapiro, Christopher Berner, Lenny Bogdonoff, Oleg Boiko, Madelaine Boyd, Anna-Luisa Brakman, Greg Brockman, Tim Brooks, Miles Brundage, Kevin Button, Trevor Cai, Rosie Campbell, Andrew Cann, Brittany Carey, Chelsea Carlson, Rory Carmichael, Brooke Chan, Che Chang, Fotis Chantzis, Derek Chen, Sully Chen, Ruby Chen, Jason Chen, Mark Chen, Ben Chess, Chester Cho, Casey Chu, Hyung Won Chung, Dave Cummings, Jeremiah Currier, Yunxing Dai, Cory Decareaux, Thomas Degry, Noah Deutsch, Damien Deville, Arka Dhar, David Dohan, Steve Dowling, Sheila Dunning, Adrien Ecoffet, Atty Eleti, Tyna Eloundou, David Farhi, Liam Fedus, Niko Felix, Simón Posada Fishman, Juston Forte, Isabella Fulford, Leo Gao, Elie Georges, Christian Gibson, Vik Goel, Tarun Gogineni, Gabriel Goh, Rapha Gontijo-Lopes, Jonathan Gordon, Morgan Grafstein, Scott Gray, Ryan Greene, Joshua Gross, Shixiang Shane Gu, Yufei Guo, Chris Hallacy, Jesse Han, Jeff Harris, Yuchen He, Mike Heaton, Johannes Heidecke, Chris Hesse, Alan Hickey, Wade Hickey, Peter Hoeschele, Brandon Houghton, Kenny Hsu, Shengli Hu, Xin Hu, Joost Huizinga, Shantanu Jain, Shawn Jain, Joanne Jang, Angela Jiang, Roger Jiang, Haozhun Jin, Denny Jin, Shino Jomoto, Billie Jonn, Heewoo Jun, Tomer Kaftan, Łukasz Kaiser, Ali Kamali, Ingmar Kanitscheider, Nitish Shirish Keskar, Tabarak Khan, Logan Kilpatrick, Jong Wook Kim, Christina Kim, Yongjik Kim, Jan Hendrik Kirchner, Jamie Kiros, Matt Knight, Daniel Kokotajlo, Łukasz Kondraciuk, Andrew Kondrich, Aris Konstantinidis, Kyle Kosic, Gretchen Krueger, Vishal Kuo, Michael Lampe, Ikai Lan, Teddy Lee, Jan Leike, Jade Leung, Daniel Levy, Chak Ming Li, Rachel Lim, Molly Lin, Stephanie Lin, Mateusz Litwin, Theresa Lopez, Ryan Lowe, Patricia Lue, Anna Makanju, Kim Malfacini, Sam Manning, Todor Markov, Yaniv Markovski, Bianca Martin, Katie Mayer, Andrew Mayne, Bob McGrew, Scott Mayer McKinney, Christine McLeavey, Paul McMillan, Jake McNeil, David Medina, Aalok Mehta, Jacob Menick, Luke Metz, Andrey Mishchenko, Pamela Mishkin, Vinnie Monaco, Evan Morikawa, Daniel Mossing, Tong Mu, Mira Murati, Oleg Murk, David Mély, Ashvin Nair, Reiichiro Nakano, Rajeev Nayak, Arvind Neelakantan, Richard Ngo, Hyeonwoo Noh, Long Ouyang, Cullen O'Keefe, Jakub Pachocki, Alex Paino, Joe Palermo, Ashley Pantuliano, Giambattista Parascandolo, Joel Parish, Emy Parparita, Alex Passos, Mikhail Pavlov, Andrew Peng, Adam Perelman, Filipe de Avila Belbute Peres, Michael Petrov, Henrique Ponde de Oliveira Pinto, Michael, Pokorny, Michelle Pokrass, Vitchyr H. Pong, Tolly Powell, Alethea Power, Boris Power, Elizabeth Proehl, Raul Puri, Alec Radford, Jack Rae, Aditya Ramesh, Cameron Raymond, Francis Real, Kendra Rimbach, Carl Ross, Bob Rotsted, Henri Roussez, Nick Ryder, Mario Saltarelli, Ted Sanders, Shibani Santurkar, Girish Sastry, Heather Schmidt, David Schnurr, John Schulman, Daniel Selsam, Kyla Sheppard, Toki Sherbakov, Jessica Shieh, Sarah Shoker, Pranav Shyam, Szymon Sidor, Eric Sigler, Maddie Simens, Jordan Sitkin, Katarina Slama, Ian Sohl, Benjamin Sokolowsky, Yang Song, Natalie Staudacher, Felipe Petroski Such, Natalie Summers, Ilya Sutskever, Jie Tang, Nikolas Tezak, Madeleine B. Thompson, Phil Tillet, Amin Tootoonchian, Elizabeth Tseng, Preston Tuggle, Nick Turley, Jerry Tworek, Juan Felipe Cerón Uribe, Andrea Vallone, Arun Vijayvergiya, Chelsea Voss, Carroll Wainwright, Justin Jay Wang, Alvin Wang, Ben Wang, Jonathan Ward, Jason Wei, CJ Weinmann, Akila Welihinda, Peter Welinder, Jiayi Weng, Lilian Weng, Matt Wiethoff, Dave Willner, Clemens Winter, Samuel Wolrich, Hannah Wong, Lauren Workman, Sherwin Wu, Jeff Wu, Michael Wu, Kai Xiao, Tao Xu, Sarah Yoo, Kevin Yu, Qiming

- Yuan, Wojciech Zaremba, Rowan Zellers, Chong Zhang, Marvin Zhang, Shengjia Zhao, Tianhao Zheng, Juntang Zhuang, William Zhuk, and Barret Zoph. Gpt-4 technical report, 2024. URL https://arxiv.org/abs/2303.08774.
- Stanislas Polu and Ilya Sutskever. Generative language modeling for automated theorem proving, 2020.
- Stanislas Polu, Jesse Michael Han, Kunhao Zheng, Mantas Baksys, Igor Babuschkin, and Ilya Sutskever. Formal mathematics statement curriculum learning, 2022.
- Amitayush Thakur, George Tsoukalas, Yeming Wen, Jimmy Xin, and Swarat Chaudhuri. An in-context learning agent for formal theorem-proving, 2024.
- Jason Wei, Xuezhi Wang, Dale Schuurmans, Maarten Bosma, brian ichter, Fei Xia, Ed H. Chi, Quoc V Le, and Denny Zhou. Chain of thought prompting elicits reasoning in large language models. In Alice H. Oh, Alekh Agarwal, Danielle Belgrave, and Kyunghyun Cho (eds.), *Advances in Neural Information Processing Systems*, 2022. URL https://openreview.net/forum?id=_VjQlMeSB_J.
- Freek Wiedijk. Formal proof sketches. In Stefano Berardi, Mario Coppo, and Ferruccio Damiani (eds.), *Types for Proofs and Programs*, pp. 378–393, Berlin, Heidelberg, 2004. Springer Berlin Heidelberg. ISBN 978-3-540-24849-1.
- Kaiyu Yang, Aidan Swope, Alex Gu, Rahul Chalamala, Peiyang Song, Shixing Yu, Saad Godil, Ryan Prenger, and Anima Anandkumar. LeanDojo: Theorem proving with retrieval-augmented language models. In *Neural Information Processing Systems (NeurIPS)*, 2023.
- Shuyan Zhou, Uri Alon, Frank F. Xu, Zhengbao Jiang, and Graham Neubig. Docprompting: Generating code by retrieving the docs. In *The Eleventh International Conference on Learning Representations*, 2023. URL https://openreview.net/forum?id=ZTCxT2t2Ru.

A PROMPTS

In this appendix, we note the prompts used by ImProver both for general LLM prompting, as well as the metric-specific prompts.

A.1 TEMPLATE

For the main prompt sent to the LLM on each sample, we build a prompt string using a chat prompt template that is then invoked at runtime to fill in the variables.

Namely, these variables include the set of metric prompts, previous results, input theorem, context, a syntax documents, Mathlib documents, and examples.

The prompt template is a conversation of the format:

Placeholder: All metric prompts with a 'System' role

System: You will be given the proof context (i.e. the lean file contents/imports leading up to the theorem declaration) wrapped by <CONTEXT>...</CONTEXT>.

You will be given the previous *num_prev* input/output pairs as well as their metric (metric.name) score and correctness score, as well as any error messages, for your reference to improve upon. Each of these previous results will be wrapped with <PREV I=0></PREV I=0>,...,<PREV I=num_prev-1></PREV I=num_prev-1>, with I=num_prev-1 being the most recent result.

Remember to use lean 4 syntax, which has significant changes from the lean 3 syntax. To assist with the syntax relating to the current theorem and current error messages, you will be given *num_syntax_docs* documents to refer to for fixing these syntax issues. Each of these documents will be wrapped with <SYNTAX_DOC>...</SYNTAX_DOC>.

You will also receive *num_mathlib_docs* documents relevant to the current theorem to help with formulating your modified proof. Each of these will be wrapped with <CONTENT_DOC>...</CONTENT_DOC>

You will also receive *num_examples* examples of input-output pairs of proofs that were optimized for the *metric* metric. Each of these will be wrapped with <EXAM-PLE>...</EXAMPLE>

You will be given the tactic states as comments for reference. The current theorem will be wrapped in <CURRENT>...</CURRENT>

System: Output format instructions

Placeholder: All retrieved syntax documentation
Placeholder: All retrieved mathlib documentation

Placeholder: All retrieved examples

User: <CONTEXT> context </CONTEXT>
Placeholder: Previous results and inputs/outputs
Placeholder: All metric prompts with a 'User' role

User: <CURRENT> theorem </CURRENT>

This prompt is then invoked and sent to the language model by filling in all the variables and placeholders. Notably, when we invoke the chain given by chain |llm|parser, we throttle the invocation with a randomized exponential rate limit throttling to account for API rate limits, especially in highly-parallelized requests like when benchmarking over a large number of theorems.

A.2 METRIC PROMPTS

Length Metric

System: You are an AI assistant who shortens Lean 4 proofs while ensuring their correctness. You will aim to reduce the number of lines of the tactic proof while ensuring that it properly compiles in Lean 4.

User: Shorten the current theorem (wrapped in <CURRENT>...</CURRENT>) to be as short in length—measured in the number of lines of the proof—as possible, while also ensuring that the output is still syntactically correct."

Declarativity Metric

System: You are an AI assistant who rewrites Lean 4 proofs to be more readable while ensuring their correctness. We measure readablity by considering the ratio of the number of explicitly typed have tactics against the total number of tactics in the proof, as this is proportional to whether a proof is declarative in style, and thus, readable.

User: Rewrite the current theorem (wrapped in <CURRENT>...</CURRENT>) so it is more readable and declarative and modular.

Completion Metric

System: You are an AI assistant who automatically solves Lean 4 proofs (as in, generates the tactic proof) and ensures its correctness. You will receive a Lean 4 proof you must modify to eliminate any errors so that it compiles correctly and eliminate any "sorry"s with full proofs.

User: Rewrite the current theorem (wrapped in <CURRENT>...</CURRENT>) so it is a formal, complete, and correct Lean 4 proof by filling in its tactic proof.

A.3 METRIC EXAMPLES

In this section, we illustrate side-by-side examples of metric optimization. These examples are part of a larger set of examples provided to the model as described in $\S A.1$.

Length Metric As shown in Figure 4, we provide the model an example of using more advanced tactics like rintro and inlining apply statements to shorten the proof from 5 tactics to 2.

Suboptimal

Length Optimized

```
example : (P \rightarrow Q) \land (Q \rightarrow R) \rightarrow P \rightarrow R := by intro h p reases h with \langle a,b \rangle apply b apply a exact p
```

Figure 4: A human-written example of length optimization.

Declarative Metric

As shown in Figure 5, we provide the model an example of adding an intermediate result hp_nq with an explicitly written type of P → ¬Q. Additionally, we show the model an example of simplifying tactics and external lemmas and dependencies to solve the problem in a more direct, declarative, and readable manner.

Suboptimal

Declarativity Optimized

```
example (h : \neg (P \land Q)) : \neg P \lor \neg Q := by push_neg at h exact not_or_of_imp h exact (P \land Q) : \neg P \lor \neg Q := by intro p q exact (P \land Q) : \neg P \lor \neg Q := by intro p q exact h (P, Q) by_cases hp:P . right exact hp_nq hp . left exact hp
```

Figure 5: A human-written example of declarativity optimization.

Completion Metric

As shown in Figure 6, we provide the model an example of showing a property about Set's, an externally defined datastructure, using simple tactics and forward reasoning, without external lemmas.

Suboptimal

Completion Optimized

```
example \{\alpha: \text{Type*}\}\ (s: \text{Set }\alpha): s\cap s=s

:= by
sorry

example \{\alpha: \text{Type*}\}\ (s: \text{Set }\alpha): s\cap s=s
:= by
ext x

constructor
. intro h
reases h with \langle \text{hs,} \_ \rangle
exact hs
. intro h
constructor
. exact h
exact h
```

Figure 6: A human-written example of proof completion.

B ADDITIONAL EXPERIMENTAL RESULTS

In this section, we provide more detailed information on the experimental setup and results used to evaluate ImProver.

B.1 Dataset Details

Main Datasets We evaluate our experiments on subsets of the following datasets:

Mathematics in Lean (MIL) (leanprover-community, 2024): this dataset contains pedagogical solutions of common undergraduate-level exercises, and as such contains many declarative, yet verbose and inefficient proofs. We use exercise solutions from set theory, elementary number theory, group theory, topology, differential calculus, and integration & measure theory. This dataset contains theorems at an undergraduate-level of complexity. For our main results, we evaluated on 72 theorems from exercise solutions from MIL chapters 4, 5, 8, 9, and 10.

Compfiles (David Renshaw, 2024): Solutions of International Mathematics Olympiad (IMO) and American Mathematics Olympiad (USAMO) competition problems from 2016 to 2024. This is a dataset of internationally-renowned competitive math problems, many of which are readable and declarative, yet quite verbose. This dataset contains theorems of a competitive format, and although they contain concepts only at a high-school level, the logical complexity of internationally-renowned competition results is far above that. For our main results, we used all 26 theorems and lemmas from the Compfiles database of complete solutions to the International Mathematics Olympiad (IMO) and the American Mathematics Olympiad (USAMO) from 2016-2024.

Mathlib (mathlib Community, 2020): Mathlib contains many advanced results at the forefront of mathematics, and has been at the center of research-level formalizations. These proofs are concise and generalized - which often comes at the cost of readability, declarativity, and understandability. These results and theorems often are at the cutting edge of research and a highest level of complexity compared the the other two datasets.

For our main results, we evaluated our methods on 43 advanced research-level proofs from Mathlib/AlgebraicTopology/FundamentalGroupoid. This is the most difficult dataset.

Ablation Datasets

We evaluate our ablations on a subset of MIL. Additional details on this subset is included in appendix B.1. However, due to the increase in model calls for larger n values, we switch a representative sample of this subset for some test groups. Namely,

GPT-4o-mini, GPT-4o, Output and Cos, Example Retrieval, and Sampling Method are tested on the 133 theorems in the solutions of C03_Logic, C04_Sets_and_Functions, and C05_Elementary_Number_Theory.

n and Model are tested on 55 theorems from a representative sample of the aforementioned, and Combos and RAG are tested on a representative sample of 32 theorems from the aforementioned.

Additionally, we note that both the Declarativity/CoS ablation and the Syntax Guidance ablation are performed on the same 32 theorems sample as mentioned above.

Completion Datasets

We evaluate our completion/NTP dataset on 23 exercises from Mathematics in Lean. Namely, we consider a representative sample of 12 exercises in group theory (Chapter 8), 11 exercises in set theory (Chapter 4). Moreover, we ensure that all these theorems have an empty proof.

This experiment is intended to be an initial evaluation to show that automated proof optimization systems can generalize neural theorem proving, however, future work will explore the ability of ImProver to perform neural theorem proving on more real-world datasets and compete against specialized NTP models.

B.2 ABLATION DETAILS

We now proceed to show detailed results from our ablation testing.

Table 9: Output and Chain-of-States Ablations

Output Format	CoS	Improvement	Nonempty Improve.	Accuracy	Improved Acc.
string	True	7.53	16.12	46.72%	16.79%
string	False	7.03	19.67	35.77%	15.33%
string list	True	8.04	12.38	64.96%	21.17%
string list	False	7.04	13.58	51.82%	18.98%
string tree	True	7.62	15.34	49.64%	18.25%
string tree	False	6.31	14.17	44.53%	16.06%

By Table 9, we see that the optimal combination in this testing group is a string list output format with CoS enabled. Fix these values for all future tests.

Table 10: Example Retrieval Ablations

Examples	Improvement	Nonempty Improve.	Accuracy	Improved Acc.
0	5.67	8.44	67.15%	16.79%
3	8.49	13.68	62.04%	19.71%
5	8.38	12.9	64.96%	21.17%
7	7.56	12.04	62.77%	19.71%
10	9.34	14.7	63.5%	21.9%

With the previous optimal parameters fixed, run the ablation on the number of examples. By Table 10, we see that the optimal combination in this testing group is 10 examples. Fix this value for all future tests.

Table 11: Sampling Method Ablations

Method	Forward	Keep Best	Improvement	Nonempty Improve.	Accuracy	Improved Acc.
None	N/A	N/A	9.34	14.7	63.5%	21.9%
refinement	1	False	14.76	30.63	48.18%	30.66%
refinement	5	False	12.5	20.88	59.85%	30.66%
refinement	1	True	14.95	14.95	100.0%	30.66%
refinement	5	True	13.15	13.15	100.0%	29.93%
best-of-n	N/A	N/A	15.35	18.44	83.21%	36.5%

Note that forward and keep-best values are parameters for refinement of how many previous iterations to forward, and whether to keep the most recent or the best iteration in subsequent refinement steps.

Now, with the previous optimal parameters fixed, run the ablation on the sample method. By Table 11, we see that the optimal combination in this testing group is best-of-n. Fix this value for all future tests.

Table 12: Model and *n* Ablations

Model	n	Improvement	Nonempty Improve.	Accuracy	Improved Acc.
gpt-4o	3	19.66	24.36	80.7%	38.6%
gpt-4o	5	20.12	24.97	80.56%	36.11%
gpt-4o	7	22.44	27.21	82.46%	42.11%
gpt-4o	10	21.73	25.28	85.96%	40.35%
gpt-4o	15	23.51	26.28	89.47%	45.61%
gpt-4o-mini	3	3.65	4.63	78.95%	8.77%
gpt-4o-mini	5	5.12	6.21	82.46%	10.53%
gpt-4o-mini	7	3.65	4.34	84.21%	8.77%
gpt-4o-mini	10	4.99	5.69	87.72%	12.28%
gpt-4o-mini	15	4.35	5.06	85.96%	12.28%
gpt-4o-mini	20	4.87	5.56	87.72%	14.04%

With the previous optimal parameters fixed, run the ablation on the value of n and model. By Table 12, we see that the optimal combination in this testing group is GPT-40 with n=15. Fix this value for all future tests.

Table 13: RAG and Combination Sampling Method Ablations

Combination	m	m'	RAG	Improvement	Nonempty Improve.	Accuracy	Improved Acc.
best-of-n(refinement)	3	5	True	33.78	33.78	100.0%	50.0%
best-of-n(refinement)	3	5	False	31.23	31.23	100.0%	46.88%
best-of-n(refinement)	5	3	True	31.85	31.85	100.0%	50.0%
best-of-n(refinement)	5	3	False	31.35	31.35	100.0%	50.0%
refinement(best-of-n)	3	5	True	32.66	51.32	63.64%	48.48%
refinement(best-of-n)	3	5	False	32.88	50.1	65.62%	53.12%
refinement(best-of-n)	5	3	True	34.88	57.56	60.61%	54.55%
refinement(best-of-n)	5	3	False	29.54	49.75	59.38%	43.75%
best-of-n	N/A	15	True	29.64	32.71	90.62%	56.25%
best-of-n	N/A	15	False	28.25	33.48	84.38%	53.12%

With the previous optimal parameters fixed, run the ablation on the combination methods and if RAG is enabled. By Table 13, we see that the optimal combination in this testing group is a 5-step refinement with each iteration being a best-of-3 call, with RAG enabled.

B.3 ADDITIONAL QUALITATIVE EXAMPLES

In this section, we provide additional qualitative examples demonstrating the improvements ImProver achieves in proof optimization.

Compfiles: Length Optimization See (§4.3)

Compfiles: Declarativity Optimization Consider Figure 7, in which a lemma from the 2019 IMO problem 1 (from the Compfiles dataset) is optimized for declarativity. This introduces multiple new hypotheses, which generalize a linear_property of the functions, and then reuses and instantiates that (and others, too) hypothesis throughout the proof, creating a significantly more declarative proof.

MIL: Length Optimization Consider Figure 8, which optimizes an exercise solution from MIL Chapter 8, Section 1 (Group theory) for length, eliminating simp calls and introducing proof terms into the structure of the proof to shorten it from 9 tactic invocations to 7.

Original (human-written)

972

973

974

975

976

977

978

979

980

981

982

983

984

985 986

987 988

989

990

991

992

993

994

995

996 997

998 999

1000

1001

1002

1003

1004 1005

1007

1008

1009

1010

1011

1012

1013

1014

1015

1016

1017

1018

1019

1020

1021

1022 1023

1024 1025

ImProver (declarativity-optimized)

```
lemma additive_to_int_linear (f : \mathbb{Z} \to \mathbb{Z}) (h:
                                                            lemma additive_to_int_linear (f : \mathbb{Z} \,\to\, \mathbb{Z}) (h:
                                                               \forall (x y : \mathbb{Z}), f (x + y) = f x + f y):
\exists c, \forall a, f a = c * a := by
   \forall (x y : \mathbb{Z}), f (x + y) = f x + f y):
\exists c, \forall a, f a = c * a := by
  let g := AddMonoidHom.toIntLinearMap 
                                                              let g := AddMonoidHom.toIntLinearMap 
    AddMonoidHom.mk' f h
                                                                 AddMonoidHom.mk' f h
                                                              have linear_property : \forall a, f a = g a := by
  refine \langle f 1, fun a => ?_{}\rangle
  change \dot{g} a = g 1 * a
                                                                intro a
  rw [mul_comm, ← smul_eq_mul, ←
                                                                rf1
     LinearMap.map_smul, smul_eq_mul, mul_one]
                                                              have g_smul : \forall a, ga = g1 * a := by
                                                                 intro a
                                                                 rw [mul_comm, ← smul_eq_mul, ←
                                                                  LinearMap.map_smul, smul_eq_mul, mul_one]
                                                               refine \langle f 1, fun a => ?_{\rangle}
                                                              have f_eq_g : f a = g a := linear_property a
                                                              have g_a = q : g = g : 1 * a := g_smul a
                                                              rw [f_eq_g, linear_property 1, g_a_eq]
```

Figure 7: Optimizing a lemma from IMO 2019 P1 for declarativity

Original (human-written)

ImProver (length-optimized)

```
example (\varphi: \mathsf{G} \to \star \mathsf{H}) (\psi: \mathsf{H} \to \star \mathsf{K}) (S:
        Subgroup G) :
                                                                                                   example (\varphi: \mathsf{G} \to \star \mathsf{H}) (\psi: \mathsf{H} \to \star \mathsf{K}) (S:
       \operatorname{map}\ (\psi.\operatorname{comp}\ \varphi)\ \operatorname{S}\ =\ \operatorname{map}\ \psi\ (\operatorname{S}.\operatorname{map}\ \varphi)\quad :=\ \operatorname{by}
                                                                                                            Subgroup G) :
                                                                                                           \operatorname{map}\ (\psi.\operatorname{comp}\ \varphi)\ \mathsf{S}\ =\ \operatorname{map}\ \psi\ (\mathsf{S}.\operatorname{map}\ \varphi) \qquad :=
   ext x
   simp only [mem_map]
   constructor
   \cdot rintro \langle y, y_in, hy\rangle
                                                                                                       simp only [mem_map]
   exact \langle \varphi y, \langle y, y_in, rfl\rangle, hy\rangle rintro \langle y, \langle z, z_in, hz\rangle, hy\rangle
                                                                                                       constructor
                                                                                                     rintro \langle y, y_in, hy \rangle; exact \langle \varphi y, \langle y, y_in, \rangle
       use z, z_in
                                                                                                            rfl\rangle, hy\rangle
       calc \psi.comp \varphi z = \psi (\varphi z) := rfl
                                                                                                      rintro (y, (z, z_in, hz), hy); exact (z,
                                        = \psi y := by congr
                                                                                                           z_in, (congr_arg \psi hz).trans hy\rangle
```

Figure 8: Optimizing a lemma from the solutions of MIL CH08 S01 for length

MIL: Length Optimization 2 Consider Figure 8, which optimizes an exercise solution from MIL Chapter 8, Section 1 (Group theory) for length, converting a full tactic proof into a single proof term to shorten it from 28 tactic invocations to 1. Note that the model does not have access to the Lean commands that symbolically generate proof terms, and therefore generates and estimates the proof term entirely by itself.

Original (human-written)

ImProver (length-optimized)

```
example : s \setminus t \cup t \setminus s = (s \cup t) \setminus (s \cap t)
                                                                   example : s \setminus t \cup t \setminus s = (s \cup t) \setminus (s \cap t)
      := by
  ext x: constructor
                                                                     exact Set.ext fun x => \langle fun h => h.elim \rangle
  · rintro (\langle xs, xnt \rangle \mid \langle xt, xns \rangle)
                                                                         (fun (xs, xnt) \Rightarrow (Or.inl xs, fun (_, xt) =
     · constructor
                                                                          > xnt xt) (fun \langle xt, xns \rangle => \langle Or.inr xt,
        left
                                                                         fun \langle xs, _{\rangle} => xns xs \rangle),
        exact xs
                                                                      fun \langle h, nxst \rangle => h.elim (fun xs => Or.inl \langle
        rintro (_, xt)
                                                                         xs, fun xt => nxst \langle xs, xt \rangle \rangle) (fun xt =>
       contradiction
                                                                         Or.inr \langle xt, fun xs \Rightarrow nxst \langle xs, xt \rangle \rangle \rangle
     . constructor
       right
        exact xt.
       rintro (xs, _)
        contradiction
  rintro (xs | xt, nxst)
  · left
     use xs
     intro xt
     apply nxst
     constructor <;> assumption
   . right; use xt; intro xs
     apply nxst
     constructor <;> assumption
```

Figure 9: Optimizing a lemma from MIL CH04 S01 solution for length

MIL: Declarativity Optimization See (§4.3)

Mathlib: Length Optimization Consider Figure 10, which optimizes a theorem in algebraic topology from mathlib for length, eliminating simp calls and combining tactics to shorten it from 3 tactic invocations to 1.

Original (human-written)

1026

1027

1028

1029 1030

1031

1032

1033

1034

1035

1036

1037

1038 1039

1040

1041 1042

1043

1044

1045

1046 1047

1048

1049

1050

1051 1052

1053

1054

1055

1056

1057

1059

1061

1062

1063

1064

1065

1066

1067 1068

1069

1070

1071 1072

1074

1075

1076

1077

1078

1079

ImProver (length-optimized)

```
/-- If `f(p(t) = q(q(t))` for two paths `p`
     and 'q', then the induced path homotopy
                                                    /-- If f(p(t) = g(q(t)) for two paths p
     classes
                                                        and 'q', then the induced path homotopy
`f(p)` and `q(p)` are the same as well,
                                                         classes
    despite having a priori different types
                                                    f(p) and g(p) are the same as well,
                                                        despite having a priori different types
theorem heq_path_of_eq_image : HEq ((\pi_m
     f).map [p]) ((\pi_m g).map [q]) := by
                                                    theorem heq_path_of_eq_image : HEq ((\pi_m
  simp only [map_eq, \leftarrow
                                                       f).map \llbracket p \rrbracket) ((\pi_m \ g).map \llbracket q \rrbracket)
     Path.Homotopic.map_lift]; apply
                                                      exact Path.Homotopic.hpath_hext hfg
     Path.Homotopic.hpath_hext; exact hfg
```

Figure 10: Optimizing a theorem from Mathlib/FundamentalGroupoid/InducedMaps for length

Mathlib: Declarativity Optimization Consider Figure 11, a theorem from Mathlib that we optimize for declarativity.

This original proof carried a score of 0, as it does not contain any declarative statements. It is concise and efficient, however, it is difficult to understand and read.

After optimizing for declarativity, we see that the model did not change the structure of the proof. Rather, it added an intermediate declaration so that users can better understand the state after the convert. This intermediate tactic greatly helps in the understandability and clarity of the proof.

Original (human-written)

ImProver (declarativity-optimized)

```
/-- Another version of
                                                         /-- Another version of
     `simply_connected_iff_paths_homotopic` -/
                                                               `simply_connected_iff_paths_homotopic` -/
theorem simply_connected_iff_paths_homotopic'
                                                         theorem simply_connected_iff_paths_homotopic'
     {Y : Type*} [TopologicalSpace Y] :
                                                               {Y : Type*} [TopologicalSpace Y] :
    \texttt{SimplyConnectedSpace Y} \; \leftrightarrow \;
                                                              \texttt{SimplyConnectedSpace} \ \texttt{Y} \ \longleftrightarrow \\
      PathConnectedSpace Y ∧ ∀ {x y : Y} (p<sub>1</sub>
                                                               PathConnectedSpace Y \land \forall \{x \ y : Y\} (p<sub>1</sub>
     p_2 : Path x y), Path.Homotopic p_1 p_2 :=
                                                               p2 : Path x y), Path. Homotopic p1 p2
                                                           convert
  convert
     simply_connected_iff_paths_homotopic (Y
                                                               simply_connected_iff_paths_homotopic (Y
     := Y)
                                                               := Y)
  simp [Path.Homotopic.Quotient,
                                                           have h1 : \forall x y : Y, Subsingleton
     Setoid.eq_top_iff]; rfl
                                                              (Path.Homotopic.Quotient x y) \leftrightarrow \forall {p<sub>1</sub> p<sub>2</sub>
                                                               : Path x y}, Path.Homotopic p_1 p_2 := by
                                                              intro x v
                                                              simp [Path.Homotopic.Quotient,
                                                               Setoid.eq_top_iff]
                                                              rfl
                                                            simp only [h1]
```

 $Figure \ 11: Optimizing \ a \ theorem \ from \ \texttt{Mathlib/FundamentalGroupoid/SimplyConnected} \ for \ declarativity$

Full Proof Generation. We analyze the application of ImProver to neural theorem proving in the MIL example from Figure 12. This theorem relating to group theory originally has no proof, however, ImProver generates one from scratch. This generated proof is verified to be correct by Lean, utilizing all the included hypotheses as well as a retrieved mathlib theorem.

Original (human-written)

ImProver (completeness-optimized)

```
example (\varphi: G \to * H) (S T : Subgroup H) (hST : S \leq T) : comap \varphi S \leq comap \varphi T := by sorry := by intro g simp only [mem_comap] intro hS exact hST hS
```

Figure 12: Solving a group theorem exercise from MIL Chapter 8 Section 1 for declarativity.