# Towards Automated Functional Equation Proving: A Benchmark Dataset and A Domain-Specific In-Context Agent

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Abstract. Automated Theorem Proving (ATP) faces significant challenges due to the vast action space and the computational demands of proof generation. Recent advances have utilized Large Language Models (LLMs) for action selection in ATP, but these methods often require substantial computational resources. This study introduces the Functional Equation Automated Solver (FEAS), an agent that builds on the CO-PRA in-context learning framework within the Lean environment. FEAS innovates by refining prompt generation and response parsing mechanisms, integrating domain-specific heuristics for functional equations, and introducing the FunEq dataset—a rigorously curated collection of functional equation problems categorized into three difficulty levels. The agent's performance is evaluated against established baselines using this dataset, demonstrating improvements in theorem proving accuracy, particularly with the integration of functional equation-specific heuristics. Our results highlight the effectiveness of FEAS in generating and formalizing high-level proof strategies into Lean proofs, emphasizing the potential of tailored approaches in domain-specific ATP challenges.

#### 1 Introduction

Automated theorem proving (ATP) has long been a challenging endeavor in computer science [6]. Formalizing mathematics for efficient machine processing presents a significant hurdle, further complicated by the inherent infinite nature of the action space for proof construction. Interactive theorem provers (ITPs) like Lean [13], Coq [7], Isabelle [22], and HOL4 [18] offer a solution by facilitating formal proofs through user-guided application of tactics until the desired goals are achieved.

Recent efforts have explored the use of Large Language Models (LLMs) as action selectors to address the vast action space in ATP [17] [5]. These approaches involve training LLMs from scratch [11] or fine-tuning pre-trained models [1] to generate plausible actions within the context of formal proofs. However, such methods often incur significant computational costs.

In-context learning, exemplified by the COPRA agent [19], presents a promising avenue to overcome the computational bottleneck. This approach has demonstrated success in other domains like machine translation and code generation [14].

Evaluating the capabilities of these algorithms may relies on challenging problems encountered in high school math Olympiads. The International Mathematical Olympiad (IMO) [8] represents the pinnacle of difficulty in this domain. Notably, AlphaGeometry [20] recently achieved progress in automated theorem proving for geometric problems using LLMs with a competitive performance comparing to IMO participant. However, the field of functional equations, another core topic within IMO's algebraic domain involving finding all unknown functions satisfying specific conditions, remains largely unexplored in the realm of automated theorem proving.

In this project, we build upon the foundation of the COPRA in-context learning agent [19], working specifically within the Lean environment, yet, expanding evaluation to various general-purpose LLMs. Our key contributions include:

- FunEq Dataset: We created the FunEq dataset <sup>1</sup>, a curated collection of functional equation problems formalized in Lean. This dataset spans three difficulty levels (simple, intermediate, hard), providing a rigorous benchmark for evaluating automated theorem provers in this domain. Hard problems are drawn from shortlisted IMO problems.
- FEAS Agent: We introduce the FEAS agent<sup>2</sup>, which refines COPRA's prompt generation and response parsing mechanisms. FEAS instructs a LLM to produce high-level proof strategies in natural language, followed by their formalization and translation into Lean proofs. It adopts a robust block-based parsing strategy for error handling and backtracking.
- Heuristic Integration: To enhance and stabilize FEAS's performance, we explicitly incorporate domain-specific functional equation heuristics [3] directly into the agent's prompts.

#### 2 Related Work

Deep learning has emerged as a promising approach to tackle the combinatorial explosion of the search space in automated theorem proving (ATP) [24] [2] [4] [23]. The advent of Transformer-based language models revolutionized automated theorem proving by eliminating the need to explicitly hardcode the syntax of interactive theorem provers (ITPs). GPT-f [17] pioneered this approach, utilizing language models to generate novel proofs accepted into the Metamath [12] library. PACT [5], a follow-up project, utilized self-supervised data to improve tactic prediction in the Lean proof assistant. Further enhancements with expert iteration [16] enabled autonomous curriculum learning, achieving state-of-the-art

 $<sup>^{1}\; \</sup>mathtt{https://github.com/bio-ontology-research-group/FunEq.git}$ 

https://github.com/bio-ontology-research-group/FEAS.git

performance on the miniF2F benchmark [26], a dataset of formal Olympiad-style problems.

Subsequently, Thor [10] integrated language models with Isabelle's Sledghammers [15] for premise selection, alleviating the need for explicit specification of every proof step. Other work [9] leveraged this integration, employing in-context learning for autoformalization and expert iteration to achieve improved results on the MiniF2F benchmark. Concurrently, HTPS [11] explored the integration of reinforcement learning with LLMs for guided proof search.

Recent advances have sought to address the computational cost of LLM pretraining. LLEMMA [1] continued pretraining Code Llama on mathematical data, demonstrating capability in formal theorem proving. ReProver [25] focused on premise selection using a retrieval-augmented approach, achieving success with relatively modest computational resources.

However, the computational burden of fine-tuning LLMs remained a concern. COPRA [19] addressed this by employing general-purpose LLMs within an incontext learning framework. This approach repeatedly queries a LLM to propose tactics, leveraging feedback from the proof environment and retrieved lemmas to refine subsequent queries. While COPRA outperformed several baselines, it, like most prior works, generates proofs one tactic at a time, focusing on low-level proof steps in comparison to human-like informal reasoning. Additionally, previous work primarily developed general solvers without leveraging domain-specific knowledge, limiting their efficacy in specialized areas like functional equations.

# 3 The FunEq Dataset

We developed the FunEq dataset, a manually curated collection of functional equation problems formalized in Lean. Our focus on functional equations is motivated by the fact that, while a specialized domain, their solutions necessitate a diverse array of proof techniques. These range from basic algebraic manipulations to sophisticated reasoning about concepts like continuity [21], providing a rich testing ground for automated theorem provers.

To accommodate varying levels of difficulty,  $\mathit{FunEq}$  is structured into three categories:

Simple Dataset This dataset introduces 18 problems which require only fundamental functional equation reasoning steps. Proofs primarily involve simple substitutions, linear arithmetic, the use of involutions, straightforward induction, and basic case analysis.

Intermediate Dataset This dataset contains 15 problems which focuse on proving intermediate lemmas often encountered in the solution process of more complex functional equations such as establishing injectivity and surjectivity. Problems are sourced primarily from Evan Chen's article [3] and the book "Functional Equations: A Problem-Solving Approach" by Venkatachala [21].

Hard Dataset This dataset consists of most of the International Mathematical Olympiad (IMO) shortlisted functional equation problems since 2002

[8]. These problems, originally posed in the context of finding all functions satisfying given hypotheses, have been reformulated for Lean 3 by explicitly stating the solutions as the goal state. This modification simplifies the problem representation compared to their original form in the competition.

### 4 The FEAS Agent

```
Function FEAS(O, \alpha):
    PUSH(st, O)
    for j \leftarrow 1 to t do
         if \alpha = \{\} then
             p \leftarrow \text{PROMPTIFY}(st, \text{Bad}(O))
             \alpha \leftarrow \text{PARSETACTIC}(\text{LLM}(p))
         end
         a \leftarrow POP(\alpha)
         O' \leftarrow T(O, a)
         if O' = QED then
             terminate successfully
         else if O' \in Err \ or \ \exists O'' \ s.t. \ O' \equiv O'' \ then
             add a to Bad(O)
             \alpha \leftarrow \{\}
         else
            FEAS(O', \alpha)
         end
    end
    POP(st)
```

Algorithm 1: Given an initial proof state  $(O_{in})$  and an empty queue of tactics  $(\alpha)$ , FEAS aims to find a sequence of tactics that transforms  $(O_{in})$  into the goal state (QED). Each proof state is either a set of obligations (goal-hypothesis pairs) or an error state. The agent utilizes a stack (st) to manage proof states, a failure dictionary (Bad(O)) to track unproductive tactics, and functions PROMPTIFY and PARSETACTIC to interact with an LLM. The algorithm proceeds by iteratively querying the LLM for tactics, applying them to the current proof state, and adjusting its search based on success, errors, or lack of progress as determined by a symbolic checker and the transition function (T(O, a)).

The FEAS (Functional Equation Automated Solver) agent (Algorithm 1) builds upon the foundation of the COPRA framework [19], specializing in the domain of functional equations.

**Prompt Engineering.** FEAS introduces a key refinement in the system prompt structure. Rather than directly soliciting a Lean proof step, FEAS guides a LLM through a multi-stage response generation process. It prompts the LLM to first articulate a high-level proof strategy in natural language, then formalize and translate this strategy into a Lean-compatible proof.

```
Algebraic Manipulation: Derive algebraic expression that simplify an existing
\hookrightarrow expression or help derive new ones. You can usually prove the new derivation
\hookrightarrow simply by 'nlinarith' which immediately prove any simple linear or non-linear
\hookrightarrow derivation without the need of using complicated 'rw' tactics. For example, if we
\leftrightarrow know that \forall x f(x)^3 = f(x), then we obtain f(x) (f(x) - 1) (f(x) + 1) = 0. Here
\rightarrow is the example and its proof in LEAN syntax: given 'h1 : \forall x: R, f(x)^3 = f(x)'
\hookrightarrow then 'intro x,\n have hx:= h1 x,\n have h2: f(x) * (f(x) - 1) * (f(x) +1) = 0 :=

→ by linarith, '.

b)
The goal is to derive a contradiction from the
                                                          have h3 : f 0 \neq 0, {

→ given hypotheses. 'h0 : f 0 = f 0 ^ 2'

                                                             intro h4,
→ suggests that 'f 0' must be a fixed point
                                                             rw h4 at h0,
                                                                                      - Block 1
\hookrightarrow of the function 'x x^2', which are '0'
                                                             simp at h0,
→ and '1'. Since both '0' and '1' are ruled
                                                             contradiction,

→ out by 'h1' and 'h', we have a

                                                          },

→ contradiction.

                                                          have h5 : f 0 = 1, {
To proceed, we can use the fact that 'h0 : f 0
                                                             rw ←h0,
\rightarrow = f 0 ^ 2' and 'h1 : f 0 ^ 2 = 0' to show
                                                                                       Block 2
                                                             exact h3.
\hookrightarrow that 'f 0' must be nonzero. Then, we can
                                                          }.
\rightarrow use 'h : f 0 = 1' to derive the
                                                          contradiction,
contradiction.
                                                                                     → Block 3
```

Fig. 1: Example of FEAS's Prompting and Response Generation for a Functional Equation Problem. (a) An example of domain-specific heuristic included in the system prompt. (b) Natural language proof steps generated by the LLM in response to the current proof state. (c) The corresponding Lean proof generated by the LLM, segmented into blocks for error handling and parsing.

Multi-Block Parsing and Error Handling. FEAS adopts a dynamic block-based parsing strategy to manage the multi-line Lean proofs generated by a LLM. This strategy enhances robustness by dividing the generated proof into logical blocks based on the underlying structure of Lean proofs. By processing each block independently, FEAS can effectively isolate and recover from errors in specific parts of the proof, potentially salvaging and utilizing valid proof segments even if the overall proof generated by the LLM is not entirely correct.

Automatic Tactic Application. After either successful parsing of all blocks or encountering an error, FEAS attempts the automatic application of the nlinarith tactic — which can simplify proofs by automatically handling complex algebraic manipulations that would otherwise need to be done manually. Successful application incorporates this step into the proof, otherwise, it is omitted. This provides automation and taps into the power of Lean's built-in tactics.

**Domain-Specific Heuristics.** FEAS integrates functional equation heuristics [3] directly into the system prompt alongside Lean syntax examples. These heuristics encompass substitution-based simplification, techniques for proving

Algorithm	Few Shots	COPRA	FEAS	FEAS+Heuristics
$\operatorname{GPT}$	50.0% (50.0%)	77.78% (77.78%)	80.56% (83.33%)	86.11% (94.44%)
Gemini	33.34% (38.89%)	52.78%~(61.11%)	80.56% ( <b>88.89</b> %)	$\mathbf{88.89\%}\ (\mathbf{88.89\%})$
Claude	0% (0%)	83.33% (83.33%)	$91.67\% \ (100\%)$	86.11% (88.89%)
Llama3	0% (0%)	50.0%~(50.0%)	<b>75.0</b> % ( <b>77.78</b> %)	$63.89\% \ (66.67\%)$

Table 1: Performance comparison of pass@1 (pass@2) on the simple tier of FunEq dataset

Algorithm	Few Shots	COPRA	FEAS	FEAS+Heuristics
GPT	0% (0%)	0% (0%)	$6.67\% \ (\mathbf{13.33\%})$	10.0%~(13.33%)
Gemini	0% (0%)	$6.67\% \ (6.67\%)$	10.0%~(13.33%)	3.33%~(6.67%)
Claude	0% (0%)	6.67%~(6.67%)	<b>13.33</b> % ( <b>13.33</b> %)	$13.33\%\ (13.33\%)$
Llama3	0% (0%)	0% (0%)	0% (0%)	$6.67\%\ (6.67\%)$

Table 2: Performance comparison of pass@1 (pass@2) on the intermediate tier of FunEq dataset

bijectivity, exploitation of symmetry and involution, and the utilization of induction over natural and rational numbers. This integration aims to guide the LLM towards generating more relevant and successful proof strategies within this specific problem domain.

#### 5 Evaluation

We conduct a series of experiments to evaluate the performance of the FEAS agent and the impact of incorporating domain-specific heuristics. Our evaluation includes comparisons across four different LLMs: GPT-4 Turbo, Gemini-1.5-Pro, Claude-3.5-Sonnet, and Llama3 70b. We evaluate FEAS agents against two baselines: Few-Shots and COPRA, the original in-context learning agent, which serves as points of comparison. We assess FEAS in two distinct configurations: one with the integrated domain-specific functional equation heuristics and one without.

The experiments are performed on the simple and intermediate tiers of the FunEq dataset. To gauge performance on more complex problems, we further evaluate all agents on the A1 subset of the hard dataset, which consists of the easiest shortlisted algebra problems from each corresponding IMO year. To control for potential variability in LLM responses, we execute each experiment twice on the simple and intermediate datasets. Due to computational resource constraints, we limit our evaluation to a single run on the A1 subset.

In all experiments, we impose a maximum limit of 60 LLM queries and a timeout of 720 seconds. The LLMs are used with a temperature setting of 0, prioritizing deterministic responses. Performance is assessed using Pass@1 and Pass@2 metrics, representing success on the first and second attempts, respectively. For the simple and intermediate datasets, Pass@1 is calculated as an average of the results of the two runs.

#### 5.1 Results

Tables 1 and 2 show our evaluation across the Simple and Intermediate tiers of FunEq. All combinations of agents and LLMs fail to generate proofs on the Hard tier of FunEq. On the Simple dataset, FEAS agents consistently achieves the highest success rates across all evaluated LLMs. FEAS with integrated heuristics on GPT and Gemini achieves the highest performance, demonstrating the efficacy of domain-specific knowledge. However, Claude and Llama3, without heuristics, shows superior performance on this dataset, suggesting that in certain LLM configurations, heuristics may misguide proof search.

On the more challenging Intermediate dataset, the challenge increases substantially, with all approaches showing lower success rates. However, FEAS agents again consistently ranks highest in performance, highlighting its ability to navigate more complex functional equation proofs. Again, in some cases, Gemini, FEAS performs better without heuristics. Furthermore, all methods fail to generate proofs on the Hard tier of FunEq, indicating that significant challenges remain in automated theorem proving for functional equations.

#### 6 Conclusion

Our experiments establish the FEAS agent as an advancement in automated theorem proving for functional equations. FEAS refines prompting, parsing, and integration of domain-specific heuristics demonstrate improvement over baselines. While results on the Simple dataset are encouraging, performance on the Intermediate and Hard datasets highlights the ongoing challenges in this complex domain.

Specifically, the challenges revealed by our evaluation can be decomposed into two distinct sub-problems: (1) proposing mathematically useful proof steps, and (2) accurately translating these high-level steps into the formal language of the theorem prover. Each of these sub-problems poses its own complexities, requiring distinct approaches for further improvement.

Several avenues present themselves for future research. The development of agents tailored to specific sub-tasks within the framework. Incorporating a broader repertoire of high-level proof tactics within the LLM's prompting could improve the performance of generating Lean proof steps. Investigating search algorithms beyond the currently employed depth-first search has the potential to improve efficiency and solution discovery. Finally, designing efficient self-learning mechanisms for FEAS would enable it to continuously refine its strategies based on both successful and unsuccessful proof attempts.

#### References

- Azerbayev, Z., Schoelkopf, H., Paster, K., Santos, M.D., McAleer, S., Jiang, A.Q., Deng, J., Biderman, S., Welleck, S.: Llemma: An open language model for mathematics. arXiv preprint arXiv:2310.10631 (2023)
- Blaauwbroek, L., Urban, J., Geuvers, H.: The tactician: A seamless, interactive tactic learner and prover for coq. In: International Conference on Intelligent Computer Mathematics. pp. 271–277. Springer (2020)
- Chen, E.: Introduction to functional equations (2016), https://web.evanchen.cc/ handouts/FuncEq-Intro/FuncEq-Intro.pdf, accessed on: 08 May 2024
- 4. Gauthier, T., Kaliszyk, C., Urban, J., Kumar, R., Norrish, M.: Tactictoe: learning to prove with tactics. Journal of Automated Reasoning 65(2), 257–286 (2021)
- 5. Han, J.M., Rute, J., Wu, Y., Ayers, E.W., Polu, S.: Proof artifact co-training for theorem proving with language models (2022)
- Harrison, J., Urban, J., Wiedijk, F.: History of Interactive Theorem Proving, vol. 9, pp. 135–214. North Holland (12 2014). https://doi.org/10.1016/B978-0-444-51624-4.50004-6
- 7. Huet, G., Kahn, G., Paulin-Mohring, C.: The Coq Proof Assistant: A Tutorial: Version 7.2. Research Report RT-0256, INRIA (Feb 2002), https://inria.hal.science/inria-00069918, projet COQ
- IMO: International mathematical olympiad official website, https://www.imo-official.org/, accessed: 08 May 2024
- 9. Jiang, A., Staats, C.E., Szegedy, C., Rabe, M., Jamnik, M., Li, W., Wu, Y.T.: Autoformalization with large language models. NeurIPS (2022)
- 10. Jiang, A.Q., Li, W., Tworkowski, S., Czechowski, K., Odrzygóźdź, T., Miłoś, P., Wu, Y., Jamnik, M.: Thor: Wielding hammers to integrate language models and automated theorem provers. Advances in Neural Information Processing Systems 35, 8360–8373 (2022)
- 11. Lample, G., Lacroix, T., Lachaux, M.A., Rodriguez, A., Hayat, A., Lavril, T., Ebner, G., Martinet, X.: Hypertree proof search for neural theorem proving. Advances in neural information processing systems **35**, 26337–26349 (2022)
- 12. Megill, N., Wheeler, D.: Metamath: A Computer Language for Mathematical Proofs. Lulu.com (2019), https://books.google.com.sa/books?id=dxqeDwAAQBAJ
- de Moura, L., Kong, S., Avigad, J., van Doorn, F., von Raumer, J.: The lean theorem prover (system description). In: Felty, A.P., Middeldorp, A. (eds.) Automated Deduction CADE-25. pp. 378–388. Springer International Publishing (2015)
- 14. OpenAI: Gpt-4 and gpt-4 turbo, https://platform.openai.com/docs/models/gpt-4-and-gpt-4-turbo
- 15. Paulsson, L.C., Blanchette, J.C.: Three years of experience with sledgehammer, a practical link between automatic and interactive theorem provers. In: Proceedings of the 8th International Workshop on the Implementation of Logics (IWIL-2010), Yogyakarta, Indonesia. EPiC. vol. 2 (2012)
- Polu, S., Han, J.M., Zheng, K., Baksys, M., Babuschkin, I., Sutskever, I.: Formal mathematics statement curriculum learning (2022)
- 17. Polu, S., Sutskever, I.: Generative language modeling for automated theorem proving (2020)
- Slind, K., Norrish, M.: A brief overview of hold. In: Mohamed, O.A., Muñoz, C., Tahar, S. (eds.) Theorem Proving in Higher Order Logics. pp. 28–32. Springer Berlin Heidelberg, Berlin, Heidelberg (2008)

- 19. Thakur, A., Tsoukalas, G., Wen, Y., Xin, J., Chaudhuri, S.: An in-context learning agent for formal theorem-proving (2024)
- Trinh, T., Wu, Y., Le, Q., et al.: Solving olympiad geometry without human demonstrations. Nature 625, 476–482 (2024). https://doi.org/10.1038/s41586-023-06747-5, https://doi.org/10.1038/s41586-023-06747-5
- 21. Venkatachala, B.: Functional Equations A Problem Solving Approach. Prism (2002)
- 22. Wenzel, M., Paulson, L.C., Nipkow, T.: The isabelle framework. In: Mohamed, O.A., Muñoz, C., Tahar, S. (eds.) Theorem Proving in Higher Order Logics. pp. 33–38. Springer Berlin Heidelberg, Berlin, Heidelberg (2008)
- Wu, M., Norrish, M., Walder, C., Dezfouli, A.: Tacticzero: Learning to prove theorems from scratch with deep reinforcement learning. Advances in Neural Information Processing Systems 34, 9330–9342 (2021)
- 24. Yang, K., Deng, J.: Learning to prove theorems via interacting with proof assistants. In: International Conference on Machine Learning. pp. 6984–6994. PMLR (2019)
- Yang, K., Swope, A., Gu, A., Chalamala, R., Song, P., Yu, S., Godil, S., Prenger, R.J., Anandkumar, A.: Leandojo: Theorem proving with retrieval-augmented language models. Advances in Neural Information Processing Systems 36 (2024)
- Zheng, K., Han, J.M., Polu, S.: Minif2f: a cross-system benchmark for formal olympiad-level mathematics. arXiv preprint arXiv:2109.00110 (2021)

end

## 7 Appendix

#### 7.1 Qualitative Analysis

```
theorem intermediate_funeq_2
(f : \mathbb{R} \to \mathbb{R})
(h_0 : \forall x, f(x + 1) = f(x) + 1)
(h_1 : \forall x, x \neq 0 \rightarrow f(1/x) = f(x)/x^2) :
\forall x, x \neq 0 \rightarrow f(1 + 1/x) = 1 + f(x)/x^2 :=
begin
    intro x,
    intro hx,
    have h_2: f(1/x+1) = f(1/x) + 1 := h_0(1/x),
    have h_3 : f(1 / x) = f x / x^2 := h_1 x hx,
    rw h_3 at h_2,
    rw add_comm at h_2,
    nlinarith,
end
                           Listing 1.1: FEAS Proof
theorem intermediate_funeq_2
(f : \mathbb{R} \to \mathbb{R})
(h_0 : \forall x, f(x + 1) = f(x) + 1)
(h_1 : \forall x, x \neq 0 \rightarrow f(1/x) = f(x)/x^2) :
\forall x, x \neq 0 \rightarrow f(1 + 1/x) = 1 + f(x)/x^2 :=
begin
    intro x, intro hx,
    rw [h_0 (1 / x), h_1 x hx] at *,
    field_simp [hx],
    rw mul_comm at *,
    rw [\leftarrowh_0 (1 / x), h_1 x hx] at *,
    rw [\leftarrowh_0 (1 / x), h_1 x hx] at *,
    ring_nf,
```

Listing 1.2: COPRA Incomplete Proof

To illustrate the distinct strengths of FEAS, we examine a specific functional equation problem (intermediate\_funeq\_2) where it succeeds while COPRA does not. FEAS' solution demonstrates its ability to generate high-level intermediate proof steps using the have tactic, mirroring a human's approach. This contrasts with COPRA, which focuses solely on lower-level Lean tactics. FEAS' strategy, guided by the system prompt instruction to first generate a natural language proof sketch, leads to a more human-readable and strategically structured proof.

Furthermore, FEAS' block-by-block parsing successfully handles errors within individual proof blocks. While all three lines generated by the LLM contained

incorrect tactic applications, FEAS was able to isolate and utilize the correct proof concepts within each block. This error recovery mechanism showcases the robustness of FEAS' parsing strategy.

Interestingly, despite the LLM failing to suggest the final correct tactic (erroneously proposing exact h\_2), FEAS' automated application of the nlinarith tactic successfully concludes the proof. This demonstrates the complementary nature of FEAS' high-level reasoning and the underlying theorem prover's automated capabilities.