CombStruct4Lean: A Formal Combinatorial Benchmark Emphasizing Structures for Automated Theorem Proving

Long Doan

Department of Computer Science George Mason University ldoan5@gmu.edu

ThanhVu Nguyen

Department of Computer Science George Mason University tvn@gmu.edu

Abstract

Formal theorem proving with large language models (LLMs) has demonstrated promising results, yet combinatorial problems remain a notable challenge due to their reliance on intricate, problem-specific structures and definitions. AlphaProof, a notable LLM-based system for automated theorem proving, has shown strong performance in the International Mathematical Olympiad (IMO), obtaining a silvermedalist performance by solving all questions but two combinatorics problems. Existing formal benchmarks have limited combinatorial coverage and often overlook the importance of combinatorial constructions. To address these gaps, we introduce CombStruct4Lean, a novel benchmark composed of 383 combinatorial math-word problems formalized in the Lean4 proof assistant. CombStruct4Lean emphasizes the creation and usage of combinatorial structures, presenting significantly greater complexity and diversity than existing datasets. We evaluate state-of-the-art autoformalization and neural theorem proving methods on our benchmark, revealing substantial room for improvement. Our findings highlight both the difficulties inherent in formalizing combinatorial problems and the need for further research in structured combinatorial reasoning within automated theorem proving.

1 Introduction

Large language models (LLMs) have recently shown remarkable progress in formal theorem proving, achieving strong results on challenging mathematical tasks. Notably, AlphaProof [1] and AlphaGeometry2 [2] obtained a silver-medalist performance at the International Mathematical Olympiad (IMO) 2024 competition. However, both systems failed on two combinatorics problems, which highlight challenges and limitations of LLMs on this domain.

Combinatorics is a branch of mathematics that focuses on reasoning over discrete structures such as graphs, partitions, and permutations with specific constraints, which often require problem-specific definitions and constructions that are difficult to formalize [3]. More broadly, formal theorem proving involves two core tasks: autoformalization—translating a natural language problem into a formal statement—and automated theorem proving—finding a formal proof from that statement. In both cases, the output must be verified by proof assistants like Coq [4], Isabelle [5], or Lean4 [6].

While there have been multiple works tackled on both tasks in both general mathematical domain [7–10] and specific branches [11–13, 2], only a few focused on combinatorics [14, 15]. A significant factor contributing to this limitation is the current state of formal benchmarks, which offer limited coverage of combinatorics. For instances, miniF2F [3], ProofNet [16], and FIMO [17] contain

Table 1: Comparison of combinatorics problems across different benchmarks.

Benchmark	#. combinatorics	Problem Type	Custom Definitions
miniF2F-test [3]	0 (0.0%)	-	-
ProofNet [16]	0 (0.0%)	-	-
PutnamBench [18]	29 (4.4%)	Math-word problem	-
LeanComb-test [15]	100 (100%)	Combinatorial identities	√(shared)
CombStruct4Lean (ours)	383 (100%)	Math-word problem	\checkmark

no combinatorial problems, and PutnamBench [18] includes only a small fraction (29 out of 657) dedicated to this area.

Furthermore, these benchmarks often overlook the aspect of combinatorial constructions. In the formalization of IMO 2024 Problem 5 [19], one of two problems that AlphaProof failed, over 20% of the formalization was focused on defining specific combinatorial objects and structures, with a substantial portion of the remaining code consisting of lemmas directly related to these new constructs. Despite the importance, none of the mentioned benchmarks included any problem-specific definitions dedicated to combinatorics. LeanComb [15], a recent formal benchmark on combinatorics, only focused on combinatorial identities with pre-defined constructions, which limits its ability to evaluate a model's capacity to invent or define new combinatorial structures.

To address this gap, we introduce CombStruct4Lean, a benchmark of formal combinatorial problems with an emphasis on combinatorial structures. CombStruct4Lean consists of 383 combinatorial math-word problems, sourced from high-school olympiad-level competitions and formalized in the Lean4 proof assistant. Our benchmark creation process incorporates a LLM-based feedback-driven formalization pipeline that iteratively refines the formal statement by analyzing compilation failures and retrieving relevant premises. Unlike prior methods that rely on a single-pass generation [7, 10, 16], this process enables the model to define and adapt problem-specific structures, which are essential for combinatorial problems. To ensure quality, we incorporate a two-stage semantic checking strategy that checks the consistency between the informal problem and its formal counterpart, followed by manual review by human experts. We illustrate the differences between our CombStruct4Lean and existing benchmarks in Tab. 1. Our analysis shows CombStruct4Lean posess a significantly higher diversity in terms of formalization length and the number of custom definitions required than other widely used formal benchmarks. Through experiments on both autoformalization and automated theorem proving tasks, we demonstrate limitations of current models on our benchmark.

Contributions This paper makes the following contributions: (i) We introduce CombStruct4Lean, a benchmark consisting of 383 formalized combinatorial problems sourced from high-school Olympiad-level competitions. A key feature of our benchmark is its strong emphasis on the creation and utilization of combinatorial structures. (ii) We describe our benchmark construction process, including the iterative formalization pipeline and the semantic checking strategy, along with an analysis highlighting how CombStruct4Lean differs from existing benchmarks. (iii) We evaluate state-of-theart autoformalization and automated theorem proving methods to demonstrate the complexity and difficulty inherent in CombStruct4Lean, which make our benchmark a suitable testbed for future research on formal combinatorics.

2 Related Work

2.1 Autoformalization

Early LLM-based explorations in autoformalization task adopted in-context learning methods [7] and later incorporated techniques such as back-translation to enrich training sets [16, 20]. More recent work began tackling other aspects of autoformalization, such as fidelity and correctness. RAutoformalizer [21] introduced premise retrieval to ground generated formalization with premises information. Process-Driven Autoformalization [20] included Lean4 compiler's traceback information to verify the quality of a formalization. While both methods focused on checking the correctness of a formal statement, AutoForm4Lean [14] leveraged LLMs to evaluate the formal code based on multiple criteria, whereas Li et al. [22] proposed two self-consistency approaches: symbolic equivalence and semantic equivalence. However, their symbolic approach is primarily designed

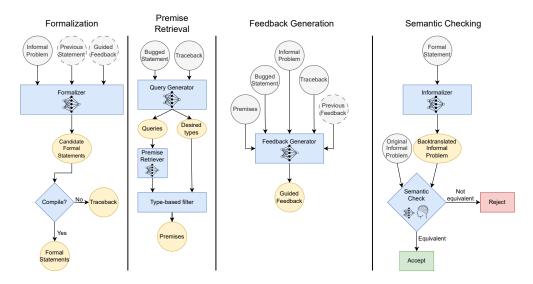


Figure 1: Illustrations of each step in benchmark creation.

for problems involving numerical expressions, making its extension to the combinatorics domain non-trivial.

2.2 Combinatorics in Formal Benchmarks

Current formalization benchmarks, including MiniF2F [3], ProofNet [16], and FIMO [17], largely focus on foundational areas such as algebra, number theory, and analysis, with minimal coverage of combinatorics. For example, MiniF2F, ProofNet and FIMO have no combinatorial problems, while only 29 out of 657 instances in PutnamBench [18] are in combinatorics domain. This underrepresentation occurs because combinatorial problems often require intricate, problem-specific definitions and constructions, making them particularly challenging to formalize [3].

Recent research, such as AutoForm4Lean [14] and LeanComb [15], aim to address this by introducing methods that can synthesize new combinatorial benchmarks. AutoForm4Lean proposed a dataset construction pipeline focused on both syntactically and semantically correctness of the formalization. LeanComb developed a data augmentation approach that can automatically generate new theorems from a complete formal proof and introduced a benchmark dedicated to combinatorial identities. However, these combinatorial identities can be solved by applying algebraic techniques without consideration of combinatorial reasoning or combinatorial structures.

3 Benchmark Creation

In this section, we detail the construction process of CombStruct4Lean, which consists of 383 competition-level combinatorial problems formalized in Lean4 proof assistant [6]. To our knowledge, CombStruct4Lean is the first benchmark dedicated on formalizing math-word problems in combinatorics domain with a focus on problem-specific combinatorial structures.

3.1 Informal Problem Sources

To ensure the quality of CombStruct4Lean, we select informal combinatorial problems from high-school olympiad-level competitions [23]. We avoid problems that require computing a solution (e.g., how many arrangements satisfy a certain constraints) and choose only problems that requires to prove a statement. At the end of this process, we obtained 8608 combinatorial problems. Among those, we randomly sample 1000 problems to create the benchmark.

Table 2: Notations.

Symb	Meaning
p	Informal problem
s	Formal statement candidate
f	Guided feedback
t	Traceback from Lean
P	Retrieved premises

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Algorithm 1: Formalization Process
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Input: Informal combinatorics problem p
Output: A statement s if formalization succeeds

1 f \leftarrow \emptyset, s \leftarrow \emptyset;

2 while not terminated do

3 s \leftarrow \text{FORMALIZATION}(p, s, f);

4 t \leftarrow \text{COMPILE}(s);

5 if t = \emptyset then return s;

6 P \leftarrow \text{RETRIEVEPREMISE}(s, t);

7 f \leftarrow \text{GENERATEFEEDBACK}(p, s, t, f, P)

8 return \emptyset;
```

3.2 Formalization Process

To improve clarity, we introduce the following notations that will be used consistently throughout the benchmark creation pipeline in Tab. 2. The formalization process for each informal combinatorial problem is described in Algorithm 1. Here, we discuss each of the step included in this process, namely *formalization*, *premise retrieval*, *feedback generation*. Fig. 1 also provides an overview on how each step work.

Formalization. Given an informal combinatorics problem p, the formalization step uses the previous formal attempt s and guided feedback f to produce a new candidate statement. This process is handled by the Formalizer module. In the first iteration, both s and f is empty. The Formalizer first determines whether additional definitions or structures are needed and generates them accordingly, then constructs a formal statement based on these elements. In our implementation, the formalization step is performed using Claude-3.5-Sonnet API as the LLM. We generate a single candidate formal statement in each iteration with a temperature of 0.3.

If the generated statement s compiles successfully, it proceeds to semantic checking (Sec. 3.3). Otherwise, the compiler returns a traceback t, which is used in the next phase, *premise retrieval*. Fig. 2 provides an example input to the Formalizer, including the problem p, the previous s, and guided feedback f.

Premise Retrieval. A common errors we found during the formalization is the incorrect usages of existing premises, which can be occurred because of the lack of grounding between the LLM and the Mathlib library. To address this, we use a retrieval-augmented generation approach via the premise retriever module, which provide the LLM's knowledge with relevant premises documentation. Although previous work has applied RAG to the autoformalization task [21], none has used it explicitly to correct buggy formal statements.

Given the bugged statement s and traceback t, the query generator produces queries q and associated desired types T(q). Each query q and Mathlib premise p_i are encoded using Dense Passage Retrieval [24], and their cosine similarity is computed as:

$$\mathrm{sim}(q,p_i) = \frac{f(q) \cdot f(p_i)}{\|f(q)\| \cdot \|f(p_i)\|}$$

We select the top-k entries from the corpus of Mathlib premises with the highest similarity and match with the desired types:

$$P = \{p_i \mid \operatorname{sim}(q, p_i) \text{ among top-} k \land T(q) = T(p_i)\}$$

We forward these retrieved premises P to the next phase for generating feedback. See Fig. 3 for a detailed example. To generate the queries and desired types for each query, we use Claude-3.5-Haiku as the LLM with a temperature of 0.3. We use CodeRankEmbed [25] to embed the query and signatures of each premise in the Mathlib library. For each pair of query and expected type, the retriever returns at most k=5 relevant premises, though there is no restriction on the number of queries or types that can be generated.

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Translate the following problem into a formal theorem in Lean4:
Consider a graph where each vertex is connected to exactly three other
                     vertices (a 3-regular graph). Prove that it is possible to color the
                     edges of such a graph using only three colors in such a way that no two
                      adjacent edges share the same color if the graph is bipartite.
Previous formalization attempt:
structure ThreeRegularGraph {V : Type} where
def EdgeColoring {V : Type} (G : ThreeRegularGraph V)
def IsValidColoring {V : Type} (G : ThreeRegularGraph V) (c : EdgeColoring V
                    G)
def IsBipartite {V : Type} (G : ThreeRegularGraph V)
theorem three_regular_edge_coloring {V : Type} (G : ThreeRegularGraph V) :
           (\exists \ \mathsf{c} \ : \ \mathsf{EdgeColoring} \ \mathsf{V} \ \mathsf{G}, \ \mathsf{IsValidColoring} \ \mathsf{G} \ \mathsf{c}) \ 	o \ \mathsf{IsBipartite} \ \mathsf{G} \ := \ \mathsf{G} \ 
           sorrv
Guided feedback from expert:
                              • The three_regular field in 'ThreeRegularGraph' has multiple problems ...
                              • The EdgeColoring definition has type mismatches ...
                             • IsBipartite definition could be improved ...
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Figure 2: Example of an input prompt to the Formalizer LLM. Detailed feedback and implementations are abbreviated for brevity.

Feedback Generation. The feedback generation module produces guided feedback f using the original problem p, the current formalization s, the traceback t, retrieved premises P, and prior feedback. This guided feedback helps refine s in the next iteration by (i) diagnosing root causes of compilation failure using t; (ii) analyzing whether custom definitions align with p; (iii) demonstrating correct use of retrieved premises P with a code snippet.

We provide an example of a generated feedback in Fig. 2. The feedback f is reused in the next call to *formalization* step, continuing the iterative refinement loop. We use Claude-3.5-Sonnet to generate the feedback, producing one feedback candidate per iteration with a temperature of 0.7.

For each informal problem, we perform the formalization process for a maximum of 5 iterations. At the end, we obtained 634 examples that compile successfully. Among those, we removed 127 examples that contain placeholder sorry in their definitions, resulted in 507 examples to perform semantic checking.

3.3 Semantic Checking

Successfully compiling a formal statement does not guarantee its semantic correctness. We provide an example of this issue in Fig. 4. In the first formalization, the code includes an implementation for valid subsets valid_subsets and compares the output of the function f with the number of valid subsets returned by valid_subsets. This formalization faithfully captures all mathematical objects described in the informal problem, making it semantically correct. In contrast, the second formalization lacks an implementation for valid subsets and does not reference any set S in the theorem's statement. Although it compiles, it fails to reflect the structure of the original problem and is thus semantically incorrect.

To verify the correctness of a formal statement, we adopt a two-stage semantic checking strategy. Similar to semantic equivalence [22], we first informalize the formal statement, then compare the back-

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Bugged Statement:
structure ThreeRegularGraph (V : Type) where
  three_regular : \forall v : V, (({w | (v, w) \in edges}).card = 3)
Traceback:
Text: ((\{w \mid (v, w) \in edges\}).card
Error: invalid field 'card', the environment does not contain 'Set.card'
  \{w \mid (v, w) \in edges\} has type Set V
Step 1: Query Generation
Queries: ["Set.card", "Set to finset"]
Desired types: ["Set", "null"]
Step 2: Premise Retrieval
Premises related to "Set.card":
      • def card : Cardinal
      • def card (\alpha) [Fintype \alpha] : Nat
Premises related to "Set to finset":
      • def toFinset (s : Set \alpha) [Fintype s] : Finset \alpha
      • def toFinset (s : Multiset \alpha) : Finset \alpha
Step 3: Type-Based Filtering
      • "Set.card": Matching premises: N/A
      • "Set to finset": Matching premises:
        def to
Finset (s : Set \alpha) [Fintype s] : Finset \alpha
        def toFinset (s : Multiset \alpha) : Finset \alpha
```

Figure 3: Example of Premise Retrieval step

translated version with original informal problem. However, instead of computing cosine similarity between their sentence embeddings, we leverage LLMs to assess their semantic alignment based on multiple criteria: combinatorial objects and structures, constraints, goals, scope, and equivalence (i.e., can we restate one version by using the other?). This approach also shares similarities with AutoForm4Lean [14], which uses LLMs to compare formal and informal representations. However, our method avoids the challenge of cross-modality comparison by evaluating two informal statements, thereby reducing the complexity introduced by differences in syntax and representation between code and natural language. The entire semantic checking process is supervised by a human experts. We use Claude-3.5-Haiku with a temperature of 1.0 for both informalization and semantic checking. At the end of this stage, we obtained 383 examples for CombStruct4Lean.

3.4 Benchmark Analysis

As mentioned in Sec. 1, a key challenge in formalizing combinatorial problems is the need to define new concepts to support the main theorem. We analyze this issue in our benchmark using two aspects: formalization length in Fig. 5a and number of definitions created in Fig. 5b. For formalization length, we remove all comments and the header block (e.g, import, open) and count only the code related to the theorem statement. For number of definitions, we count code blocks beginning with one of the following keywords def, structure, class, inductive, coinductive, abbrev, instance, mutual, constant, axiom.

From the figures, we observe that CombStruct4Lean is much more diverse than existing benchmarks in both of formalization length and number of custom definitions support each theorem. Over 85% of problems in miniF2F and PutnamBench require fewer than 10 lines of code, whereas CombStruct4Lean shows a broader distribution, with many examples exceeding this range. Notably, only 14% of CombStruct4Lean problems fall within the 0–9 LoC range. A similar pattern

Figure 4: Example of formal statements that are semantically correct and incorrect. Implementations of definitions are abbreviated for brevity.

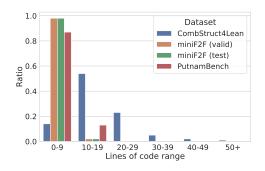
appears in the number of custom definitions: all problems in miniF2F and PutnamBench define no new concepts, while only 2% of examples in CombStruct4Lean exhibit similar behaviors. The rest of CombStruct4Lean require varying numbers of new definitions, with the highest count of definitions reaching 12 in one example. These findings highlight the diversity and complexity of CombStruct4Lean, presenting a realistic and challenging setting for autoformalization and formal reasoning in combinatorics.

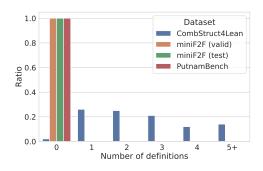
4 Evaluation

We evaluate CombStruct4Lean using two tasks: autoformalization and automated theorem proving. Given the inherent difficulty of combinatorics, even in formalizing statements, we assess how well current models perform the autoformalizing task by using our benchmark as a reference. To demonstrate the significant challenge of the benchmark, we also perform evaluation on the automated theorem proving task with different theorem provers. We conduct all experiments on a machine with 2 A100 80GB GPUs, 32-cores AMD CPU and 100GB of RAM. We public our benchmark and the code for experiments at https://github.com/dynaroars/CombStruct4Lean.

4.1 Autoformalization

Experiment Setting. Due to the lack of existing models for autoformalization, we use Goedel-Formalizer [10] as the main model for this experiment. We consider two versions of the model, one of them is trained on the open Numina dataset [23] annotated with the CLAUDE-3.5-SONNET API, denoted as SONNETANNOTATED, and the other is finetuned on LeanWorkbook [26] dataset, denoted as LEANWORKBOOKANNOTATED. For both models, we sample $n \in \{1,16\}$ formal statement candidates with a temperature of 1.0. We use two metrics for evaluation, one is #.Compiled indicating the number of examples with at least one candidate successfully compile, and the other is Ground-truth Alignment where we use another LLM to check whether each candidate align with the ground truth formalization and the informal problem, and count the number of examples that have an aligned candidate. The alignment is judged based on two criteria: (i) Mathematical equivalence—Does the candidate aim to formalize the same mathematical problem as the ground truth and the informal problem? (ii) Fidelity—Does the candidate accurately represents the mathematical entities, scope, assumptions, and definitions of the informal problem, using the ground truth as a reference? We use Claude-3.5-Haiku with a temperature of 1.0 as the evaluator LLM here. Due to





- (a) Distribution of formalization lengths.
- (b) Distribution of number of custom definitions.

Figure 5: Benchmark Analysis.

the differences in Lean4 environments, we do not include RAutoformalizer model and BEq metric [21] despite being a closely related work.

We also conduct a small ablation study on our formalization process (Sec. 3.2) by removing either the *premise retrieval* step (denoted as No PREMISE) or the *feedback generation* step (denoted as No Guided Feedback) to understand their impact on performance. In particular, in the No Premise setting, we exclude retrieved premises from the inputs to *guided feedback* step. In the No Guided Feedback setting, we directly use the traceback as feedback for the Formalizer LLM. In both settings, we sample a single candidate with a temperature of 0.3.

Results. Tab. 3 presents our experiment results. We observe that the SONNETANNOTATED model obtained a substantial higher compiled rate than the LEANWORKBOOKANNOTATED model: 293 vs. 11 when sampling 1 candidate, and 383 vs. 112 when sampling 16 candidates. However, note that the SONNETANNOTATED model share the same data source and the same foundation LLM as our benchmark, which may introduce some potential data leakage. Nonetheless, despite a high compiled rate, the alignment with the ground-truth formal statement remains relatively low for SONNETANNOTATED, with only 106/293 and 311/383 candidates aligned for n=1 and n=16 settings, respectively. This further reinforce our argument in Sec 3.3 that successful compilation does not necessarily indicate semantic correctness.

Interestingly, the No Premise model obtained a higher compiled rate than the No Guided Feedback model (347 vs. 285). Upon closer inspection, we found that when given with only the compiler traceback, the Formalizer LLM tends to iteratively refine its original formalization to make the code compile. In contrast, the guided feedback in No Premise setting is more likely to suggest radical changes to the formalization, many of which fail to compile due to the lack of grounding with premise documentation from the Mathlib library. However, when considering the percentage of compiled candidates that are semantically aligned with the ground truth formalization, the No Premise model outperforms No Guided Feedback, with 76.8% vs. 71.1% alignment, highlighting the importance of guided feedback in improving semantic correctness. A similar trend is observed when comparing No Premise with Sonnetannotated (n=1): although their compiled rates are similar, No Premise yields more than twice the number of aligned candidates, further demonstrating the impact of guided feedback on formalization quality. These findings show the importance of guided feedback and premise retrieval in producing both syntactically and semantically correct formal statements.

4.2 Automated Theorem Proving

Experiment Setting. We evaluate different theorem provers on our CombStruct4Lean with two types of models, specialized LLMs finetuned on the automated theorem proving task and general-purpose LLMs. For specialized LLMs, we choose DEEPSEEK-PROVER-V1.5 [9] and GOEDEL-PROVER [10]. For general-purpose LLMs, we perform evaluation on standard model CLAUDE-3.5-SONNET and reasoning model O4-MINI. We follow evaluation in ProofNet [16] and use Pass@K as the evaluation metric, with $K \in \{1, 5, 10\}$. Considering the computational cost, we adopt the whole-proof generation approach for all theorem provers. Specifically, we sample K candidate proofs,

Table 3: Evaluation on Autoformalizing task.

Models	#. Compiled	Ground-truth Alignment
Goedel-Formalizer - SonnetAnnotated $(n = 1)$	293	106
- SonnetAnnotated $(n = 16)$ - LeanWorkbookAnnotated $(n = 1)$	383 11	311
$\frac{\text{- LeanWorkbookAnnotated } (n=16)}{\text{Claude-3.5-Sonnet}}$	112	8
No PremiseNo Guided Feedback	285 347	219 247

Table 4: Evaluation on Automated Theorem Proving task.

Models	Pass@1	Pass@5	Pass@10
Deepseek-Prover-V1.5	0	0	0
Goedel-Prover	0	0	0
Claude-3.5-Sonnet	3	7	10
o4-mini	0	0	0

remove all candidates that violates the integrity of the original formal statement and candidates with placeholder proof (i.e., sorry), then check whether each proof compile or not.

Results. Tab. 4 presents the results. We observe that except for CLAUDE-3.5-SONNET, all theorem provers failed to solve any problems in CombStruct4Lean. For two specialized LLMs, this weak performance may be due to the limited exposure to combinatorics during their finetuning. However, in the case of the reasoning model O4-MINI, we found that a majority of responses are either stopped due to excessively long reasoning chains or the model decide that the problem is not solvable. Interestingly, in multiple examples, O4-MINI just flat out decline to generate an answer. In contrast, CLAUDE-3.5-SONNET was able to solve 10 problems in our benchmark. Upon closer inspection, we found that CLAUDE-3.5-SONNET has a tendency of placing a placeholder sorry for tactics that creating new subgoals, such as have or by_cases. If we include such proofs for evaluation, the number of problems solved by Claude increased to 75, or 19.6% of the benchmark, suggesting potential research directions involving subgoal based approaches.

5 Conclusion

We introduced CombStruct4Lean, a benchmark of combinatorial problems formalized in Lean4 proof assistant with a focus on combinatorial structures. We detailed the benchmark construction process, including an iterative formalization pipeline and semantic checking strategy, and showed how CombStruct4Lean differs from existing benchmarks. Our experiments reveal that current autoformalization and theorem proving methods struggle significantly on CombStruct4Lean, especially on the theorem proving task. These results demonstrate the complexity and difficulty inherent in CombStruct4Lean, which make our benchmark a suitable testbed for future research on formal combinatorics.

Broader Impacts CombStruct4Lean improves research in formal reasoning by providing a structured, challenging suite of formalized combinatorial problems. As combinatorial reasoning plays a vital role in areas such as cryptography, algorithm design, and network theory, our work may also support the broader adoption of formal methods in safety-critical and high-assurance domains.

Limitations CombStruct4Lean is built specifically for Lean4, which restricts the applicability to other proof assistants like Coq or Isabelle. Our benchmark is also developed on specific Lean4 and Mathlib versions, giving concerns in incompatibilities unless actively maintained. Finally, our work focuses on formalizing problem statements only and omit informal proofs, which allow us to isolate and evaluate the challenges of translating informal problem into formal statements.

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