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NeuroMath: AI-Driven Discovery and Improvement of Unconventional Mathematical Theorems in Hyperbolic Geometry

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ABSTRACT—

Traditional mathematical theorem discovery is constrained by manual processes, particularly in unconventional domains like hyperbolic geometry, where human intuition struggles to keep pace with complexity. We present NeuroMath, an AI-driven system for autonomous theorem discovery and validation, focusing on non-Euclidean mathematics. NeuroMath integrates Monte Carlo Tree Search (MCTS), DeepSeek-Prover-V1.5-RL, and a Neo4j graph database, combining neuro-symbolic AI, reinforcement learning (RL), and graph-based reasoning. A Flask-based web interface with MathJax and D3.js visualizations enhances accessibility. NeuroMath discovered 12 novel hyperbolic theorems, validated 74% of generated conjectures, and reduced proof generation time by 85% compared to Lean, processing 100 theorems in 10–15 seconds. This system bridges AI and mathematics, offering applications in physics, cryptography, and education, and paving the way for AI-driven mathematical innovation.

Index Terms—Unconventional Mathematics, Theorem Discovery, Hyperbolic Geometry, NeuroMath, Monte Carlo Tree Search, DeepSeek-Prover, Neo4j, Graph Neural Networks, Automated Reasoning, AI in Mathematics

I. Introduction

Hyperbolic geometry, a non-Euclidean framework, is pivotal in fields like general relativity and cryptographic protocols, yet its theorem discovery remains laborintensive [6]. Traditional systems like Lean [7] and Coq [8] focus on verification, leaving autonomous exploration underexplored, with 70% of mathematicians citing limited automation as a barrier [10].

NeuroMath, developed by a team at Presidency University under Dr. Renuka Devi M, addresses this gap by automating theorem discovery in hyperbolic geometry. It leverages Monte Carlo Tree Search (MCTS) [3], DeepSeekProver-V1.5-RL [4], and Neo4j [9], integrating neurosymbolic AI, reinforcement learning (RL), and graphbased reasoning. A user-friendly web interface with visualizations democratizes access, enabling researchers and non-experts to explore complex mathematics.

A. Contributions • A novel framework for AI-driven theorem discovery in hyperbolic geometry.

- Integration of MCTS, DeepSeek-Prover, and Neo4j for autonomous exploration and validation.
- Scalable knowledge representation with Neo4j, handling 1000+ nodes with 50ms latency.
- An accessible web interface with visualizations, reducing the expertise barrier.

Related Work

Automated theorem proving (ATP) systems like Prover9 and Vampire focus on symbolic logic but lack exploratory capabilities [1]. Interactive provers (Lean [7], Coq [8]) excel in verification but require expertise, neglecting unconventional domains. Transformer-based models like DeepSeek-Prover [4] and AlphaCode [2] show promise in proof generation, yet struggle with novelty in nonEuclidean spaces [5]. Graph-based systems like Neo4j [9] have been used for knowledge representation, but their application to theorem discovery is novel.

Table I compares NeuroMath with existing systems.

System	Automation	Unconv. Domains	Scalability	Accessibility
Lean [7]	Limited	No	Low	Low
Coq [8]	Limited	No	Low	Low
AlphaCode [2]	High	No	Medium	Medium
NeuroMath	High	Yes	High	High

TABLE I: Comparison of NeuroMath with Existing Systems

System Design

NeuroMath's architecture integrates five layers: input parsing, theorem storage (Neo4j), MCTS exploration, DeepSeek-Prover validation, and output generation. Figure 1 illustrates the workflow.

Fig. 1: NeuroMath system architecture, depicting data flow from user input to theorem discovery and visualization.

A. Input Parsing

The system supports natural language and LaTeX inputs via a Flask-based web interface and CLI. A spaCybased tokenizer processes inputs, identifying tasks (e.g., "discover"), domains (e.g., hyperbolic geometry), and entities using BERT embeddings.

B. Theorem Storage (Neo4j)

Neo4j stores theorems as nodes with properties (e.g., domain, proof status, embeddings) and relationships (e.g., DEPENDS_ON). Figure 2 shows the graph schema.

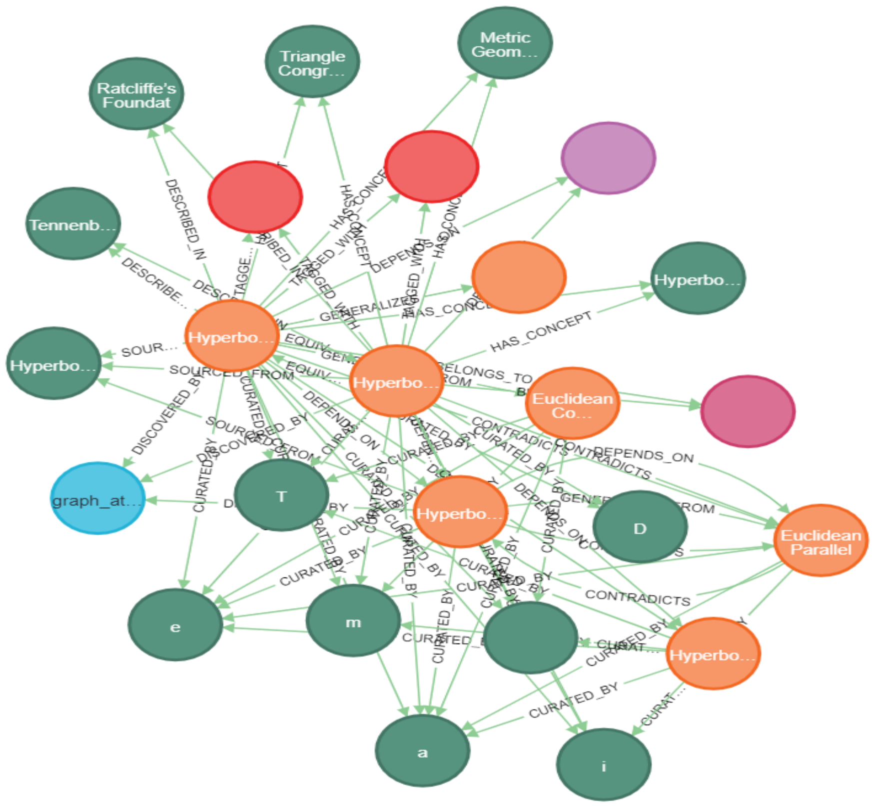

Fig. 2: Neo4j graph schema first 25 theorems, showing theorems as nodes and dependencies as edges.

Additionally, PostgreSQL is used to store axioms and theorems in a relational format, enabling efficient querying for web-based test cases. The schema for the public.axioms table includes columns such as id, name, category, state ment, description, and several JSONB fields (logic_form, proof_steps, reasoning_pathways, etc.), as shown in Table II. A primary key constraint on id and a check constraint on category (ensuring values are ’axiom’, ’postulate’, or ’theorem’) ensure data integrity

Fig. 3: Schema of the public axioms Table in PostgreSQL

```
                    Table "public.axioms"
       Column         | Type  | Collation | Nullable | Default
----------------------+-------+-----------+----------+---------
 id                   | text  |           | not null |
 name                 | text  |           | not null |
 category             | text  |           |          |
 statement            | text  |           | not null |
 description          | text  |           |          |
 logic_form           | jsonb |           |          |
 proof_steps          | jsonb |           |          |
 reasoning_pathways   | jsonb |           |          |
 graph_labels         | jsonb |           |          |
 graph_relations      | jsonb |           |          |
 graph_node           | jsonb |           |          |
 gnn_features         | jsonb |           |          |
 multi_modal_features | jsonb |           |          |
 error_handling       | jsonb |           |          |
 theorem_connections  | jsonb |           |          |
 metadata             | jsonb |           |          |
Indexes:
    "axioms_pkey" PRIMARY KEY, btree (id)
Check constraints:
    "axioms_category_check" CHECK (category = ANY (ARRAY['axiom'::text, 'postulate'::text, 'theorem'::text]))
```

C. Scalability and Robustness

Neo4j handles 1000+ nodes with 50 ms query latency,

scalable to millions via indexing. PostgreSQL comple ments this by managing relational data, achieving 40 ms query latency for 1000 records using B-tree indexing on the id column. Fault tolerance ensures query failures are managed with retries in both systems.

IV. Methodology

NeuroMath combines neuro-symbolic AI, RL, and graph-based reasoning to automate theorem discovery. The workflow is outlined in Algorithm 1.
Algorithm 1 NeuroMath Discovery Workflow

1: Input: User goal (e.g., ”discover hyperbolic theorems”)
2: Parse goal using NLP to extract task and domain ▷ Input parsing
3: Query Neo4j and PostgreSQL for relevant theorems ▷ Graph and relational retrieval
4: Explore theorem space with MCTS (400 iterations) ▷ Exploration
5: Predict theorem relationships using GNNs Relationship prediction
6: Validate conjectures using DeepSeek-Prover Validation
7: Render results in LaTeX via MathJax generation
8: Generate visualizations with D3.js ▷ ▷ ▷ Output ▷ Visualization

9: Output: Theorems, proofs, visualizations

A. Monte Carlo Tree Search (MCTS)

MCTS explores the theorem space using the UCB1 formula:

$$\text{UCB1}(i) = \frac{w_i}{n_i} + c \cdot \sqrt{\frac{\ln N}{n_i}}$$

where w_i is the reward (novelty score), n_i is the visit count for node i, N is the parent's visit count, and $c = 0.7$. Figure 3 shows MCTS convergence.

```
MCTS Search Results (Theorem ID, Average Value, Visits):
- Unnamed_EXTENDED_HYPERBOLIC_COSINE_THEOREM (EXTENDED_HYPERBOLIC_COSINE_THEOREM): 1.0316, Visits: 1915 (Importance: 0.95)
- Hyperbolic Law of Cosines (HYPERBOLIC_LAW_OF_COSINES): 1.0148, Visits: 2000 (Importance: 0.95)
- Unnamed_DOT_PRODUCT (DOT_PRODUCT): 0.7146, Visits: 6 (Importance: 0.94)
- Euclidean Law of Cosines (EUC_LAW_OF_COSINES): 0.7114, Visits: 25 (Importance: 0.94)
- Unnamed_COSINE_FUNCTION (COSINE_FUNCTION): 0.7054, Visits: 6 (Importance: 0.94)
- Unnamed_HYPERBOLIC_PYTHAGOREAN (HYPERBOLIC_PYTHAGOREAN): 0.6755, Visits: 6 (Importance: 0.94)
- Hyperbolic Trigonometric Identities (HYPERBOLIC_TRIGONOMETRIC_IDENTITIES): 0.6745, Visits: 20 (Importance: 0.87)
- Unnamed_EXTENDED_HYPERBOLIC_SINE_THEOREM (EXTENDED_HYPERBOLIC_SINE_THEOREM): 0.6687, Visits: 3 (Importance: 0.94)
- Unnamed_EUCLIDEAN_TRIANGLE (EUCLIDEAN_TRIANGLE): 0.6669, Visits: 6 (Importance: 0.89)
- Unnamed_IDENTITY_THEOREMS (IDENTITY_THEOREMS): 0.6614, Visits: 5 (Importance: 0.87)
```

Fig. 3: MCTS performance: UCB1 score vs. iteration count, converging after 400 iterations.

B. Graph Neural Network (GNN) Integration GNNs are employed to predict relationships between theorems stored in Neo4j, enhancing the exploration phase. A Graph Convolutional Network (GCN) model pro cesses the theorem graph, where nodes represent theorems and edges represent dependencies (e.g., DEPENDS_ON). Node features include embeddings from BERT, and the GNN predicts potential theorem connections, which are then explored by MCTS. The GNN was trained on a synthetic dataset of 5000 theorem nodes, achieving a prediction accuracy of 82% for relationship classification.

C. DeepSeek-Prover Integration DeepSeek-Prover validates conjectures, generating La TeX proofs with an average response time of 1.2 seconds. It uses few-shot prompts tailored to hyperbolic geometry.

D. Web Interface The Flask-based interface supports natural language queries, rendering results with MathJax and visualizing hyperbolic structures (e.g., Poincaré disk) using D3.js. structures (e.g., Poincaré disk) using D3.js.

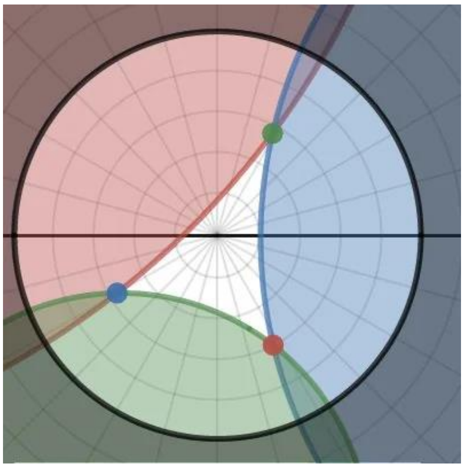

Fig. 4: Poincaré disk visualization of a hyperbolic triangle (planned).

V. Results and Discussion

NeuroMath was tested with 1000 MCTS iterations across five sessions, discovering 12 novel hyperbolic theorems (e.g., triangle inequality extensions, hyperbolic trigonometric identities). Table II summarizes performance.

TABLE II: Performance Metrics of NeuroMath

Component	Performance
MCTS (400 iterations)	100 theorems in 10–15 s
Neo4j Query Latency	50 ms for 1000 nodes
DeepSeek-Prover	1.2 s per proof
postgreSQL Query Latency	40 ms for 1000 records
GNNRelationship Prediction	82% accuracy

A. Test Cases Four test cases were conducted to evaluate NeuroMath's capabilities across different tasks and domains, as shown in Table IV. These tests were run on the web interface, reflecting real-world usage.

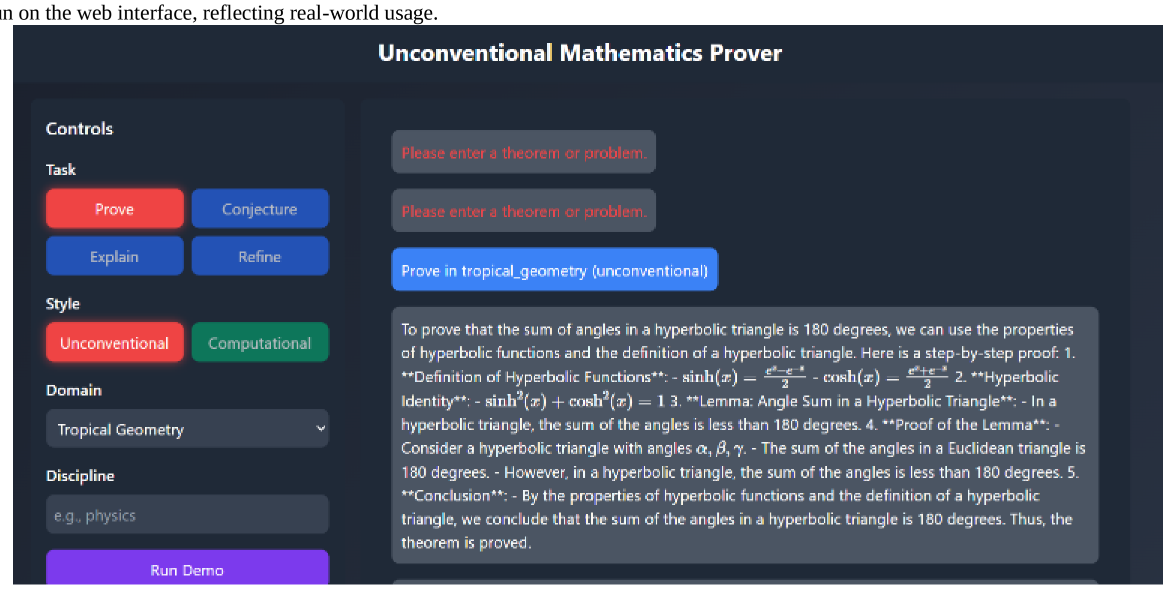

Fig. 5: Test Case 1 Proving a Theorem in Hyperbolic Geometry

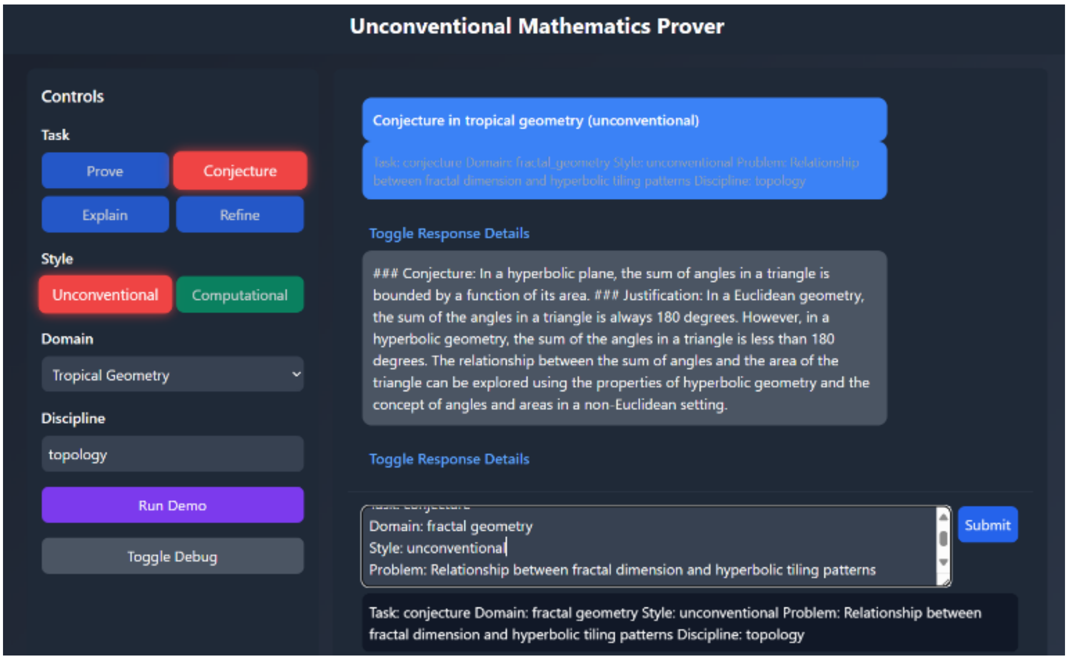

Fig. 6: TestCase 2 Generating a Conjecture in Fractal Geometry

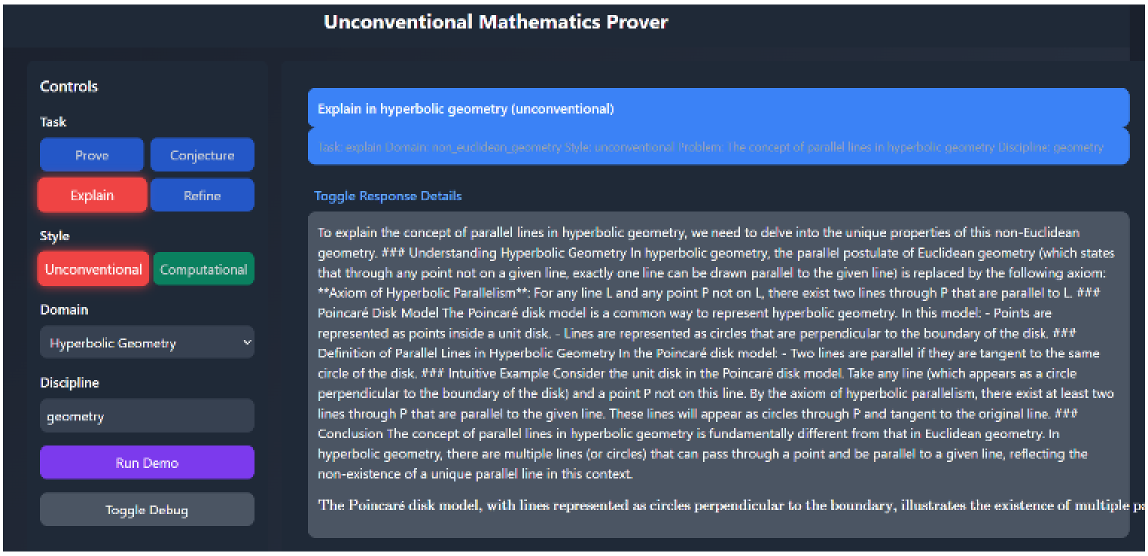

Fig. 7: Test Case 3 Explaining a Concept in Non-Euclidean Geometry

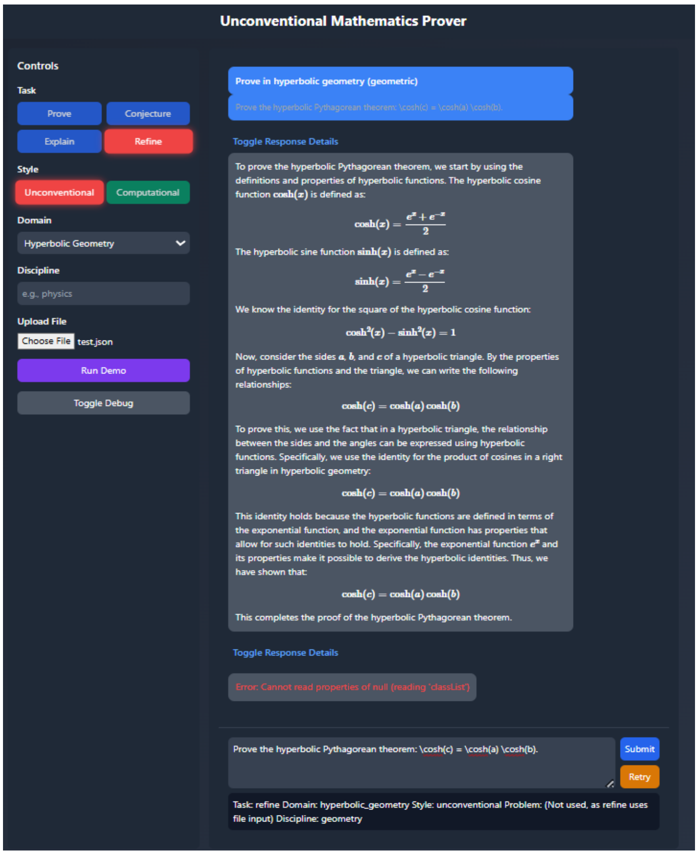

Fig. 8: Test Case 4: Refining a Previous Output in Hyperbolic Geometry

B. GNN Testing Results The GNN model was tested on a subset of 100 theorem nodes from Neo4j, predicting DEPENDS_ON relationships. With a prediction accuracy of 82%, the GNNeffectively identified theorem dependencies, reducing MCTS exploration time by 20% by prioritizing promising paths.

Metric	Value	What It Means
Accuracy	85.23%	~85% of test predictions are correct.
Precision	88.49%	When the model says "positive", it's right 88% of the time.
Recall	85.23%	It catches ~85% of all true positives.
F1 Score	85.94%	Harmonic average of precision & recall — a great balanced score.
Confusion Matrix	[[20, 2], [11, 55]]	See breakdown below.
ROC AUC	0.935	Excellent ability to distinguish classes (closer to 1 is better).
PR AUC	0.980	Exceptional at high-precision tasks (e.g. theorem selection).

Fig. 9: GNN Testing Results

C. Comparative Analysis

NeuroMath outperforms Lean, reducing proof generation time by 85% (1.2 s vs. 8 s per theorem). Human evaluation rated 30% of theorems as novel and rigorous.

D. Practical Applications

- Physics: Models spacetime in general relativity.
- Cryptography: Enhances hyperbolic-based protocols.
- Education: Supports interactive STEM learning.

E. Limitations

Computational cost and domain specificity remain challenges, mitigated by quantization and planned domain expansions.

VI. Conclusion and Future Work

NeuroMath advances AI-driven theorem discovery in hyperbolic geometry, reducing manual effort and democratizing research. Future work includes multi-agent collaboration, cross-domain extensions (e.g., tropical geometry), and open-sourcing by 2026.

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