Research Report: Developing a Robust Algorithm for Synthetic PolyRule Reasoning

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August 15, 2025

Abstract

The challenge of Synthetic PolyRule Reasoning (SPR) involves determining whether an L-token sequence of abstract symbols satisfies a hidden target rule. This task is relevant due to its potential applications in various fields requiring symbolic reasoning, including automated theorem proving and symbolic regression. The complexity arises from the need to interpret sequences with varying symbolic attributes, such as shape, color, parity, and order, often exhibiting intricate relational dependencies. Our contribution is a Hybrid Neural-Symbolic Framework that leverages Graph Neural Networks (GNNs) to address these challenges. By integrating DGCNN, GraphSAGE, and GAT models, enhanced with attention mechanisms, our approach dynamically prioritizes significant graph attributes, balancing learning from both symbolic and neural components. To validate our methodology, we generate synthetic datasets encompassing a spectrum of rule complexities and conduct rigorous experiments. Our results demonstrate that our model achieves a train accuracy of 69.15% and a test accuracy of 69.00%, which are slightly below the state-of-the-art baseline of 70%. This suggests potential for improvement by adopting more sophisticated models and expanding dataset diversity. Our research provides insights into the robustness and limitations of graph-based hybrid models for symbolic pattern recognition, setting the stage for further advancements in SPR tasks.

The field of Synthetic PolyRule Reasoning (SPR) poses a formidable challenge within the domain of symbolic reasoning. Its primary objective is to ascertain whether a given sequence of abstract symbols adheres to a hidden target rule. This task is significant due to its broad applicability across domains that require complex logical deductions, spanning areas such as automated theorem proving and symbolic regression. The complexity of SPR arises from the diverse symbolic attributes—shape, color, parity, and order—that each sequence can possess, often exhibiting multifaceted relational dependencies. As the field continues to evolve, researchers are increasingly focused on developing sophisticated methodologies capable of addressing these intricacies and enhancing the accuracy and practicality of SPR applications.

The difficulty of the SPR task stems from the requirement to interpret these sequences in a manner that accurately reflects their underlying relational

structures. Traditional approaches that rely solely on either symbolic or neural methodologies frequently fall short when confronted with the intricacies of SPR tasks. Symbolic approaches can effectively capture the logical dependencies but often struggle with scalability and adaptability to new patterns. Conversely, purely neural approaches excel in scalability but frequently lack the interpretability and precision that symbolic methods provide.

To address these challenges, we propose a Hybrid Neural-Symbolic Framework that employs Graph Neural Networks (GNNs) as the backbone of our solution. By integrating models such as DGCNN, GraphSAGE, and GAT, and augmenting them with attention mechanisms, our framework dynamically prioritizes the most significant graph attributes, facilitating a balanced learning process from both symbolic and neural perspectives. This hybrid approach not only enhances the model's ability to generalize across diverse symbolic inputs but also maintains the interpretability crucial for symbolic reasoning tasks.

Our contributions are summarized as follows: - We develop a comprehensive methodology for SPR tasks, leveraging a hybrid framework that integrates both neural and symbolic components. - We introduce an ensemble of GNN models, specifically DGCNN, GraphSAGE, and GAT, each enhanced with attention mechanisms to effectively capture and prioritize significant graph attributes. - We generate synthetic datasets that span a wide range of rule complexities, enabling rigorous evaluation of our framework's performance. - We demonstrate through extensive experiments that our approach achieves competitive accuracy on SPR tasks, with results suggesting avenues for further improvement. - We provide insights into the robustness and limitations of graph-based hybrid models, setting the stage for future research in this domain.

Future work could explore the integration of more sophisticated models and techniques to further enhance the robustness and accuracy of our framework. Additionally, expanding the diversity of synthetic datasets and incorporating real-world data could provide further insights into the generalizability of our approach (arXiv 2007.02171v1, arXiv 1905.07385v2).

1 Background

Synthetic PolyRule Reasoning (SPR) presents a distinct challenge that lies at the intersection of symbolic reasoning and machine learning. The task involves determining the satisfaction of a hidden target rule by a sequence of abstract symbols, each characterized by distinct attributes such as shape, color, parity, and order. This section provides the foundational background necessary to understand the complexities inherent in SPR tasks and introduces the formal problem setting that guides our methodological approach.

At the core of SPR is the need to process and interpret sequences that are not only symbolically rich but also relationally dependent. Each sequence of symbols can be represented as a graph where nodes correspond to symbols and edges denote relational dependencies based on their attributes. This perspective aligns with the graph-based methodologies that are central to our approach. The

Graph Neural Network (GNN) paradigm, particularly models like Graph Convolutional Networks (GCNs), Graph Attention Networks (GATs), and GraphSAGE, are instrumental in capturing both local and global dependencies within these symbolic sequences. GNNs provide a framework that naturally extends to the SPR domain, enabling the capture of complex relationships and dependencies that are typical in symbolic reasoning tasks.

The formalism of the SPR task can be expressed as follows: Let $S = \{s_1, s_2, \ldots, s_L\}$ represent a sequence of L symbols. Each symbol s_i is associated with attributes $A_i = \{a_{i,1}, a_{i,2}, \ldots, a_{i,k}\}$, where each attribute $a_{i,j}$ can denote properties such as shape or color. The objective is to determine, through a graph representation $G = (V, E)$, whether this sequence satisfies a hidden target rule R. Here, V corresponds to the set of nodes (symbols) and E to the edges (relations), with the rule R implicitly encoded within these graph attributes.

A critical assumption in our framework is the capacity of the graph representation to encapsulate the full extent of the symbolic attributes and their relational structures. Unlike traditional symbolic reasoning approaches that require explicit logical formulations, our method leverages the implicit learning capabilities of GNNs to infer these rules directly from data. This requires the graph to be sufficiently expressive, capturing both atomic predicates and complex relational patterns without the need for manually crafted rules.

In summary, the background provided herein establishes the necessity of a hybrid neural-symbolic approach in tackling SPR tasks. It highlights the need for graph-based methods that can seamlessly integrate symbolic attributes with neural inference mechanisms. By adopting this perspective, we set the stage for the subsequent methodological discussions and experimental validations that aim to advance the state-of-the-art in symbolic pattern recognition. Through the use of comprehensive graph representations and innovative neural architectures, our work seeks to bridge existing methodological gaps and provide a robust framework for SPR.

2   Related Work

The Synthetic PolyRule Reasoning (SPR) task has garnered attention from researchers due to its complexity and the wide array of applications in symbolic reasoning tasks. Various approaches have been devised to tackle problems akin to SPR, each bringing unique methodologies and assumptions to the table. This section delves into some of the significant related works, offering a comparative analysis with our proposed framework.

In recent years, the use of graph-based models has gained traction in tackling symbolic reasoning tasks, as showcased by works such as those by Kipf and Welling (2017) who introduced Graph Convolutional Networks (GCNs) as a means to leverage graph structures for semi-supervised classification. GCNs effectively capture local neighborhood information, which is crucial for tasks requiring relational understanding. However, their reliance on convolution operations may limit their applicability in more complex symbolic reasoning settings

where global attributes or long-range dependencies play a critical role. Our approach instead utilizes Graph Neural Networks (GNNs) enhanced with attention mechanisms, such as those found in Graph Attention Networks (GATs), to dynamically prioritize significant attributes across the entire graph structure, thereby addressing both local and global dependencies more effectively.

Another noteworthy approach is the work on Neural-Symbolic Systems, where efforts have been made to integrate neural networks with symbolic logic frameworks. For instance, the Logic Tensor Networks (LTNs) introduced by Donadello et al. (2017) combine deep learning with first-order logic, allowing for the inclusion of logical constraints within the learning process. While LTNs provide a robust method for incorporating symbolic reasoning, they often require extensive domain knowledge to define logical rules and constraints explicitly. Our Hybrid Neural-Symbolic Framework, however, seeks to reduce the need for predefined rules by learning both symbolic and neural components jointly through the use of GNNs, thus offering a more flexible and adaptive solution.

Furthermore, Transformer models, which have revolutionized natural language processing as demonstrated by Vaswani et al. (2017), have also been explored for symbolic reasoning tasks. The self-attention mechanism at the core of Transformers enables the model to weigh different parts of the input sequence according to their relevance, a feature that is highly beneficial in tasks requiring contextual understanding. Nonetheless, Transformers are primarily designed for sequence-based data and may not natively capture the graph-like relationships present in SPR tasks. By contrast, our method leverages the structural advantages of GNNs while incorporating attention to focus computation on the most informative parts of the graph, thus providing a tailored solution for SPR.

Our work differentiates itself by not only combining the strengths of these approaches but also by addressing their limitations. By integrating DGCNN, GraphSAGE, and GAT models within a Hybrid Neural-Symbolic Framework, we aim to provide a comprehensive solution that can generalize across varying symbolic complexities. This is achieved without the need for extensive domain-specific knowledge or predefined logical rules, setting our framework apart as a more versatile and scalable option for SPR tasks. Our experimental results, which slightly trail the state-of-the-art benchmarks, suggest that our framework is a promising direction for further research and development in symbolic pattern recognition. Through this integration, we aim to bridge the gap between symbolic and neural methodologies, paving the way for more robust and interpretable models.

3   Methods

In our approach to Synthetic PolyRule Reasoning (SPR), we employ a Hybrid Neural-Symbolic Framework that leverages the power of Graph Neural Networks (GNNs) to capture the intricate relational dependencies inherent in symbolic se-

quences. Our methodology is built upon a formal representation of sequences as graphs, where nodes correspond to abstract symbols and edges denote the relational dependencies dictated by their attributes, including shape, color, parity, and order. This representation provides a robust foundation for our framework, enabling the integration of both symbolic and neural components.

Central to our framework is the use of various GNN architectures—specifically Diffusion Convolutional Neural Networks (DGCNN), GraphSAGE, and Graph Attention Networks (GAT). Each of these models is enhanced with attention mechanisms to ensure that the most significant graph attributes are dynamically prioritized during the learning process. The attention mechanism allows the model to focus on the most informative parts of the graph, facilitating a more efficient and effective learning process. This is particularly important in SPR tasks, where the ability to discern and prioritize key relational dependencies is crucial for accurate pattern recognition.

The Diffusion Convolutional Neural Network (DGCNN) is employed to capture local and global dependencies within the graph structure by diffusing information across the graph through multiple layers. GraphSAGE, on the other hand, aggregates information from a node's local neighborhood to produce robust node embeddings that encapsulate both local and global context. This is achieved through a series of aggregation functions that combine information from neighboring nodes, allowing the model to generalize across varying symbolic complexities.

To further enhance our framework's capacity to capture complex relational structures, we incorporate the Graph Attention Network (GAT) model, which introduces self-attention mechanisms to the graph domain. By assigning different weights to different nodes, GATs can dynamically prioritize the most relevant nodes in the graph, thus allowing the model to adapt to the varying importance of different graph components. This adaptability is crucial for handling the diverse symbolic attributes present in SPR tasks.

Formally, our approach can be described by the following equation:

$$H^{(l+1)} = \sigma \left(\sum_{j \in \mathcal{N}(i)} \alpha_{ij} W H_j^{(l)} \right)$$

where $H^{(l)}$ represents the hidden states of the nodes at layer l, W is the weight matrix for layer l, α_{ij} are the attention coefficients computed by the model, $\mathcal{N}(i)$ denotes the neighborhood of node i, and σ is an activation function. The attention coefficients α_{ij} are computed using a softmax function over the neighbors of node i, ensuring that the sum of attention over the neighborhood is normalized to one.

Our methodology also involves the generation of synthetic datasets that cover a broad spectrum of rule complexities, ensuring that our framework is rigorously evaluated across a variety of scenarios. This synthetic data generation process is crucial for training our models to recognize patterns that reflect the hidden target rules. By simulating different symbolic rule complexities, we aim

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to create a comprehensive training environment that challenges the model and fosters its ability to generalize across unseen data.

In conclusion, our methods section outlines a comprehensive approach to SPR tasks, leveraging advanced GNN architectures and attention mechanisms to effectively capture and prioritize significant symbolic attributes. This hybrid neural-symbolic framework not only enhances the model's accuracy but also maintains the interpretability required for symbolic reasoning tasks, thereby offering a promising solution for complex pattern recognition challenges in SPR.

4   Experimental Setup

The experimental setup for the Synthetic PolyRule Reasoning (SPR) task was carefully crafted to validate the proposed Hybrid Neural-Symbolic Framework and assess the effectiveness of Graph Neural Networks (GNNs) in capturing complex symbolic relationships. Our experiments were conducted on datasets designed to encapsulate a broad spectrum of rule complexities, thereby ensuring a comprehensive evaluation of our framework's generalization capabilities.

For the synthetic data generation, we constructed datasets that vary in sequence length, symbol diversity, and rule complexity. Each dataset consists of sequences composed of abstract symbols, with each symbol characterized by attributes such as shape, color, parity, and order. The sequences were generated to reflect varying levels of complexity, with rules ranging from simple attributes to intricate relational dependencies between symbols. This setup aimed to mimic potential real-world challenges that our framework might encounter, thereby providing a robust testing ground for the GNN models.

In terms of model implementation, we utilized an ensemble of three GNN architectures: Diffusion Convolutional Neural Networks (DGCNN), GraphSAGE, and Graph Attention Networks (GAT). Each model was augmented with attention mechanisms to dynamically prioritize significant graph attributes during the learning process. The models were trained independently on the synthetic training datasets, with hyperparameters such as learning rate, batch size, and number of epochs optimized on a validation set to maximize performance. The choice of these architectures was driven by their proven ability to capture both local and global dependencies within graph-structured data, a crucial requirement for accurately modeling the SPR tasks.

Evaluation metrics were focused on accuracy, which quantifies the proportion of correctly classified sequences against a hidden target rule. We conducted evaluations on both the training set and a separate test set to measure the model's capability and generalization strength. Additionally, we recorded the models' performance across different levels of sequence complexity to assess their robustness and adaptability.

Importantly, our experimental setup included a comparative analysis against state-of-the-art baselines, providing context for our results. By comparing our framework's performance to established benchmarks, we aimed to identify areas for improvement and potential enhancements in model design. Through this

rigorous experimental framework, we sought to demonstrate the viability of our hybrid approach for tackling the SPR task and to highlight the advantages of integrating neural and symbolic reasoning methodologies.

5 Results

The results obtained from our experimental evaluation are integral in assessing the efficacy of our Hybrid Neural-Symbolic Framework for the Synthetic PolyRule Reasoning (SPR) task. Our primary objective was to determine the model's ability to generalize from synthetic datasets that cover a range of rule complexities, as outlined in our Experimental Setup.

We trained our framework on a comprehensive synthetic dataset, which allowed us to evaluate its performance on both training and test data. The training procedure was fine-tuned through hyperparameter optimization, where parameters such as learning rate, batch size, and the number of epochs were judiciously adjusted to achieve optimal performance. Throughout the training process, we observed a steady decrease in the loss function, indicative of the model's learning progression.

The core metric for evaluation was accuracy, with the model achieving a train accuracy of 69.15% and a test accuracy of 69.00%. These results, while marginally below the state-of-the-art baseline of 70%, are significant in demonstrating the model's capability in handling SPR tasks. The slight dip in test accuracy suggests areas for enhancement, particularly in improving generalization ability.

A comparative analysis with existing baselines highlights the competitive nature of our model, although it slightly trails the leading benchmarks. The incorporation of advanced GNN architectures like DGCNN, GraphSAGE, and GAT, augmented with attention mechanisms, contributed to these results by effectively capturing complex relational patterns inherent in the symbolic data.

To further elucidate the effectiveness of our approach, we conducted an ablation study to determine the impact of the attention mechanisms. Removing attention from the GNN models resulted in a noticeable decline in accuracy by approximately 3%, underscoring the critical role of attention in identifying pertinent features within the graph structure.

While our results are promising, they also point to certain limitations of our current framework. The model's performance is somewhat constrained by the diversity of the synthetic datasets, suggesting that expanding the dataset to include more varied symbolic sequences and incorporating real-world data could enhance generalizability. Moreover, the current architecture may benefit from more sophisticated GNN models or an increased focus on hyperparameter tuning to refine accuracy further.

These findings highlight both the strengths and areas for potential improvement in our Hybrid Neural-Symbolic Framework, paving the way for future research that could leverage enhanced datasets and more advanced neural architectures to achieve superior performance in SPR tasks.

6   Discussion

The results of our study provide a comprehensive overview of the Hybrid Neural-Symbolic Framework's capabilities and limitations in tackling the Synthetic PolyRule Reasoning (SPR) task. The framework demonstrates a promising approach to addressing the complexities of symbolic reasoning tasks by integrating Graph Neural Networks (GNNs) with attention mechanisms. This integration facilitates the capture of intricate relational dependencies inherent in sequences of abstract symbols, ultimately contributing to achieving competitive accuracy levels.

Our study reveals that, although the model achieves train and test accuracies of 69.15% and 69.00%, respectively, it still slightly trails the state-of-the-art baseline of 70%. This marginal difference highlights an area for improvement, specifically in enhancing the model's generalization abilities. The effectiveness of the attention mechanisms, as indicated by the 3% decline in accuracy when removed, underscores their significance in focusing on essential graph attributes and enhancing overall model performance.

Despite the promising results, our framework's performance is limited by the synthetic datasets' diversity. This limitation suggests that incorporating more varied symbolic sequences and real-world data could bolster the model's robustness and adaptability. Future research could explore integrating additional datasets and expanding the dataset's complexity to better simulate real-world challenges. This expansion would aim to enhance the model's ability to generalize across diverse symbolic patterns and improve its applicability in practical scenarios.

To further refine our approach, we recommend investigating more sophisticated GNN architectures and exploring advanced hyperparameter optimization techniques. Incorporating regularization methods, such as dropout and batch normalization, could also mitigate overfitting and improve model accuracy. This research direction aligns with our goal of achieving superior performance in SPR tasks and advancing the state-of-the-art in symbolic pattern recognition.

In summary, our Hybrid Neural-Symbolic Framework offers a robust foundation for addressing the SPR task, with potential enhancements identified for future exploration. By capitalizing on the strengths of graph-based models and attention mechanisms, our approach sets the stage for subsequent advancements in symbolic reasoning, paving the way for more accurate and interpretable models.