Reinforcement Learning for Generating Graphs with the Odd Cycle Condition.

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Abstract

This study explores the use of reinforcement learning to generate graphs that meet the odd cycle condition, a key concept in graph theory. The odd cycle condition stipulates that any two disjoint odd cycles within the same connected component of a graph must be connected by at least one edge. To address this, a custom environment was created using Gymnasium, enabling a reinforcement learning agent to iteratively modify the graph by adding or removing edges. The goal was to maximize the presence of valid odd cycles while ensuring the overall connectivity of the graph. The Proximal Policy optimisation (PPO) algorithm was employed to train the agent, and its performance was assessed using various metrics such as edge density, cycle count, and a robustness score. The generated graphs were analysed to confirm their adherence to the odd cycle condition, with visual tools used to highlight the odd cycles identified. Additionally, a robustness score was developed to evaluate how well the graph retains its structural integrity under minor alterations. The findings indicate that the agent is effective in producing graphs that not only satisfy the odd cycle condition but also optimize for the inclusion of more complex cycles with a greater number of vertices. This research contributes to the application of reinforcement learning in solving combinatorial optimisation problems within graph theory, providing insights that may benefit both theoretical exploration and practical implementation.

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Chapter 1

Introduction

In contemporary data environments characterized by increasing complexity and inter connectedness, advanced analytical techniques are crucial for understanding and interpreting relationships within datasets. Graph theory, which represents entities as nodes and their relationships as edges, has emerged as a powerful tool in network analysis across various domains, including social networks, biological systems, and computer networks. Among the many concepts in graph theory, the study of cycles—particularly odd cycles—has garnered significant attention due to its implications for understanding structural properties and solving optimisation problems. This thesis explores the application of reinforcement learning (RL) to the generation of graphs that satisfy the odd cycle condition. The odd cycle condition requires that any two odd cycles within a connected component of a graph must be connected by at least one edge. This project aims to leverage the adaptive learning capabilities of RL to propose a novel approach for graph generation that not only meets this specific combinatorial condition but also offers a dynamic and scalable solution applicable to real-world scenarios.

1.1 Motivation

The motivation behind this research stems from the need to enhance graph generation methodologies, particularly in the context of complex structural requirements like the odd cycle condition. Traditional graph generation techniques often depend on static algorithms that may not offer the flexibility required to manage intricate conditions or adapt to the evolving nature of real-world datasets. Reinforcement learning, with its iterative learning and optimisation capabilities through a reward system, offers a promising alternative approach.

Real-world applications, such as social media network analysis where user interactions are depicted as graphs, and biological systems where molecular structures are modeled as graphs, could significantly benefit from well-structured graphs that conform to specific criteria. The odd cycle condition is particularly crucial in scenarios where understanding the connectivity and interaction between system components is essential. For instance, in network security, ensuring that certain paths represented as odd cycles are well-connected can be vital for maintaining robust security measures.

Moreover, this research aims to delve into the intersection of graph theory and machine learning, exploring how reinforcement learning can be applied beyond decision-making in game-like environments to solving complex combinatorial problems. By applying reinforcement learning to graph generation, this thesis seeks to expand the horizons of automated graph construction, offering new tools and methodologies for researchers and practitioners.

In graph theory, a graph is a mathematical structure used to model pairwise relations between objects, comprising a set of vertices (or nodes) and a set of edges that connect pairs of vertices. Graphs can be directed, where the edges have a specific direction, or undirected, where the edges have no direction. They are widely utilized in computer science, mathematics, and related fields to model various types of networks, such as social, communication, and biological networks.

A cycle in a graph is defined as a path that begins and ends at the same vertex, with all other vertices being distinct. Essentially, a cycle is a closed loop formed by a sequence of edges where the first and last vertices coincide, and all intermediate vertices are visited exactly once. Cycles are significant in graph theory as they can indicate the presence of feedback loops in networks, which are often analysed to understand network structures and properties.

In the study of graph theory, understanding the basic entities that compose a graph is crucial. The fundamental units of a graph are the vertices, or nodes, which represent distinct entities such as individuals in a social network, computers within a network, or molecules in a chemical structure. The edges connecting these vertices represent the relationships or interactions between the entities. These edges can be weighted, indicating the strength or capacity of the relationship, or unweighted, signifying a simple connection without additional attributes. Another key concept in graph theory is the path, which is defined as a sequence of edges connecting a series of distinct vertices, enabling movement or communication across the graph. The degree of a vertex, which is the number of edges incident to it, is another critical metric. In directed graphs, this degree is further categorized into in-degrees and out-degrees, corresponding to the number of edges entering and leaving a vertex, respectively. These fundamental entities define the structure of a graph and are essential in analyzing and applying graph theory across various domains.

1.2 Aims and Objectives

The aim of this dissertation is to explore the applications and challenges associated with the Odd Cycle Condition in graph theory. By investigating the mathematical properties and practical implications of graphs with and without odd cycles, this research seeks to advance understanding in areas such as network design, computer algorithms, and biological systems. The focus is on how odd cycles influence network properties and functions, with the goal of developing strategies and algorithms to optimize network performance and reliability. Additionally, this work addresses the challenges of detecting and managing odd cycles in large-scale graphs, proposing innovative solutions to enhance computational efficiency and accuracy.

The primary goal of this thesis is to develop a reinforcement learning-based framework for generating graphs that satisfy the odd cycle condition. To achieve this, the research is structured around several key objectives:

1.2.1 Algorithm Development

This research aims to design reinforcement learning algorithms specifically tailored for graph generation. The focus is on developing algorithms that learn and optimize graph structures to ensure they meet the odd cycle condition, leveraging reinforcement learning techniques to create graphs that adhere to structural constraints and optimize their configurations through iterative adaptation.

1.2.2 Performance Evaluation

The research seeks to establish metrics for evaluating generated graphs, emphasizing the number of odd cycles, their sizes, and their connectivity. These metrics will serve as benchmarks to assess how effectively the reinforcement learning algorithms meet the project's criteria, providing a robust framework for analyzing the alignment of generated graphs with desired structural properties.

1.2.3 optimisation and Refinement

The research involves iteratively refining the reinforcement learning algorithms to improve their efficiency and accuracy in generating graphs that satisfy the odd cycle condition. This includes experimenting with different reward structures and learning strategies to optimize the algorithms' performance, ensuring they consistently produce graphs with the desired characteristics.

1.2.4 Application and Testing

In the final phase, the developed algorithms will be applied to real-world datasets to evaluate their effectiveness. A dynamic tool will be created, allowing users to specify parameters like the number of vertices, and the algorithm will generate graphs that meet these conditions. This phase tests the algorithms' practical utility and demonstrates their adaptability and scalability.

1.2.5 Documentation and Dissemination

Comprehensive documentation will be maintained throughout the project, detailing the rationale behind algorithm choices, challenges faced, and solutions implemented. The final deliverables will include a detailed report and a functional application that showcases the practical utility of the proposed approach. This combination of documentation and a working application will highlight the robustness and applicability of the developed algorithms, providing a solid foundation for further research and practical use.

By achieving these objectives, this thesis aims to contribute a novel methodology to graph theory and machine learning, offering an innovative approach to generating complex graphs using reinforcement learning techniques.

Chapter 2

Background and Related Work

2.1 Reinforcement Learning Applications in Graph Theory

Reinforcement Learning (RL) has gained considerable traction as a tool for solving complex problems in graph theory, which involves the study of graphs as mathematical structures representing pairwise relations between objects. This integration of RL into graph theory has opened up new possibilities for addressing challenges in network optimisation, graph generation, and combinatorial optimisation.

2.1.1 Network optimisation

One of the earliest and most impactful applications of RL in graph theory is network optimisation. Networks, which are essentially graphs consisting of nodes (vertices) and edges (links), are critical in various domains such as telecommunications, transportation, and social networks. Traditional optimisation techniques, like Dijkstra's algorithm for shortest paths or the Bellman-Ford algorithm for routing, often struggle with scalability and adaptability in dynamic environments. By contrast, RL provides a robust framework for continuously learning and adapting to changing network conditions. For instance, Narasimhan [26] applied deep RL to the problem of dynamic routing in communication networks, demonstrating that an RL agent could learn to minimize latency and maximize throughput by making routing decisions based on the current state of the network. Similarly, Mao [23] used RL to optimize resource allocation in cloud computing networks, achieving significant improvements in efficiency over traditional methods.

2.1.2 Graph Generation

Graph generation is another area where RL has shown promise, particularly in fields like chemistry and drug discovery, where molecules can be represented as graphs. The challenge here is to generate valid graphs that satisfy specific constraints or optimize certain properties, such as stability or reactivity. You [37] introduced a deep generative model combined with RL for molecular graph generation, where the RL agent was trained to iteratively construct graphs by adding nodes and edges in a way that maximized the desired molecular properties. This approach was further refined by Pravalphruekul [27], who developed a model that combines variational autoencoders with RL to generate molecular graphs that adhere to chemical rules while optimizing target properties. These studies highlight the effectiveness of RL in navigating the vast search space of possible graphs to find those that meet specific criteria.

2.1.3 Combinatorial optimisation

Combinatorial optimisation problems, such as the Traveling Salesman Problem (TSP) and the Minimum Spanning Tree Problem, have long been central to graph theory. Traditional approaches to these problems, like dynamic programming or greedy algorithms, can become computationally infeasible for large-scale instances. RL offers an alternative by learning heuristics that can approximate optimal solutions efficiently. Bello [8] demonstrated this with their work on using RL to solve the TSP, where the agent learned a policy that allowed it to construct near-optimal tours by selecting vertices based on a combination of learned value functions. Similarly, Khalil [18] used RL for solving the Minimum Vertex Cover problem, where the agent learned to incrementally build a cover by selecting nodes that minimized the total weight of the uncovered edges. These applications underscore the potential of RL to address complex combinatorial problems that are otherwise difficult to solve with traditional methods.

2.1.4 Graph Partitioning

Graph partitioning, which involves dividing a graph into smaller subgraphs while minimizing interconnections between them, is crucial in parallel computing and load balancing. Traditional graph partitioning algorithms, like spectral partitioning or multilevel recursive bisection, often require manual tuning and do not adapt well to different types of graphs. RL has been applied to this problem with promising results. For example, Elallid [12] developed an RL-based approach to graph partitioning, where the agent learned to partition the graph by balancing the load across partitions while minimizing the number of cut edges. This approach not only improved the quality of partitions but also reduced the need for manual intervention, making it more applicable to a wide range of graph types.

2.2 Odd Cycle Condition in Graph Theory

The Odd Cycle Condition (OCC) is a fundamental concept in graph theory that plays a critical role in various applications, particularly in the realms of combinatorial optimisation, graph colouring, and network design. This condition states that a graph is bipartite if and only if it contains no odd-length cycles, a principle that has been extensively studied and utilized in both theoretical and applied contexts.

2.2.1 Foundational Definitions and Theoretical Implications

The concept of the Odd Cycle Condition has its roots in the study of bipartite graphs. A bipartite graph is one that can be divided into two disjoint sets of vertices such that no two vertices within the same set are adjacent. The absence of odd cycles is a necessary and sufficient condition for a graph to be bipartite, as first formalized by Allen [5]. This characterization has become a cornerstone in graph theory, with subsequent research exploring its implications for graph decomposition, spectral graph theory, and algorithm design Van Mieghem [30]. The OCC is also closely related to the concept of graph colouring, particularly in the context of the four-colour theorem. A key challenge in graph colouring is determining the chromatic number of a graph, which is the smallest number of colours needed to colour the vertices such that no two adjacent vertices share the same colour. For bipartite graphs, which by definition satisfy the OCC, the chromatic number is always two. This has significant implications for algorithms designed to solve colouring problems, as noted by Johnson [17] in their seminal work on NP-completeness.

2.2.2 Applications in Network Design and optimisation

In network design, the OCC is crucial for ensuring certain properties of networks, such as reliability and fault tolerance. For instance, in the design of communication networks, it is often desirable to construct networks that are free of odd cycles to avoid issues related to signal interference and routing inefficiencies. Shinde [28] explored the use of bipartite graphs in designing robust communication protocols, where the absence of odd cycles contributed to more efficient network performance and reduced latency.

Another important application of the OCC is in the area of combinatorial optimisation, particularly in problems like the Max-Cut and Min-Cut problems. These problems involve partitioning the vertices of a graph into two sets to either maximize or minimize the number of edges between the sets. The presence of odd cycles can complicate these problems, making them harder to solve. However, algorithms that leverage the OCC, such as those discussed by Apollonio [6] in their approximation algorithm for the Max-Cut problem, can achieve better performance by exploiting the structural properties of bipartite graphs.

2.2.3 Challenges and Open Problems

Despite its foundational importance, the OCC poses several challenges in both theoretical and practical applications. One of the main challenges is the detection of odd cycles in large and complex graphs. While the problem is polynomially solvable, as demonstrated by Hoshino [16] with their efficient algorithm for testing bipartiteness, the real-time application of such algorithms in dynamic or large-scale networks remains a challenge. This is particularly true in fields like bioinformatics and social network analysis, where the scale and complexity of the graphs can make the detection of odd cycles computationally intensive. Another challenge lies in extending the OCC to weighted graphs and hypergraphs, where the notion of odd cycles is less straightforward. Research by Artime [7] has begun to address these challenges by exploring the properties of odd cycles in more complex structures, but many open problems remain. For instance, the development of algorithms that can efficiently handle odd cycles in weighted or directed graphs is still an active area of research.

2.3 Machine Learning Approaches to Graph Generation

Graph generation has become an increasingly significant area of research due to its applications in various domains, such as social network analysis, bioinformatics, and recommendation systems. Recent advances in machine learning have provided powerful tools for generating graphs with desired properties and structures. The machine learning approaches are illustrated below:

2.3.1 Generative Models for Graphs

A foundational approach to graph generation involves using generative models. The work by Wu [35] introduced Graph Convolutional Networks (GCNs), which leverage graph structures to learn node representations and can be extended to generate new graphs by sampling from learned distributions. Their method demonstrated how convolutional techniques can be adapted for graph-structured data, laying groundwork for further research in this area.

2.3.2 Graph Generative Networks

Tang [29] proposed the Transformer model, which has been adapted for graph generation tasks by incorporating attention mechanisms. The Graph Attention Network (GAT) introduced by Yan [36] extends these ideas to graphs, allowing for more flexible and powerful graph generation capabilities. The attention mechanism in GAT enables the model to focus on important nodes and edges, enhancing the quality of generated graphs.

2.3.3 Variational Approaches

Variational Graph Autoencoders (VGAE), introduced by Kipf and Welling [19] provide a probabilistic framework for graph generation. Their approach combines variational autoencoders with graph convolutional networks to model the distribution of graph structures. This technique has been pivotal in generating graphs that are consistent with observed data distributions and has been widely cited in subsequent research.

2.3.4 Generative Adversarial Networks (GANs)

Wang,s [32] introduction of GANs has been adapted for graph generation by Aalaei [1] who proposed a GAN-based model specifically for graph generation. Their work demonstrated how adversarial training can be used to generate realistic graphs by learning from a discriminator that evaluates the quality of generated graphs. This approach has gained significant attention for its ability to produce high-quality graph samples.

2.3.5 Neural Network Approaches

Recent advancements include the use of neural networks for graph generation. Fan [13] introduced a neural graph generation model that employs graph neural networks to learn graph distributions. Their model is capable of generating diverse graph structures and has been effective in tasks such as molecular graph generation. This work highlights the potential of neural networks in capturing the intricate dependencies within graph data.

2.3.6 Graph Neural Networks (GNNs)

Fan [13] explored the use of GNNs for learning and generating graph structures. Their approach emphasizes the importance of message passing between nodes and has been influential in understanding how neural networks can be leveraged for generating complex graph structures. GNNs provide a robust framework for capturing the relational information necessary for effective graph generation.

2.4 Combinatorial optimisation and Reinforcement Learning

A Survey Combinatorial optimisation and reinforcement learning (RL) are two powerful areas of study in artificial intelligence that have increasingly intersected. This intersection has led to innovative solutions for complex optimisation problems using RL techniques.

2.4.1 Foundations of Combinatorial optimisation

Combinatorial optimisation involves finding the best solution from a finite set of feasible solutions. Mandi [22] provided a comprehensive introduction to the field, covering essential algorithms and theoretical foundations. Their work laid the groundwork for applying optimisation techniques to various practical problems.

2.4.2 Reinforcement Learning Basics

Reinforcement learning, as introduced by (Sutton, R.S et.al.,2023), focuses on learning optimal policies through interaction with an environment. Their book is a seminal work that outlines the core principles and algorithms of RL, including value functions, policy gradients, and exploration strategies. This foundational understanding is crucial for integrating RL with combinatorial optimisation.

2.4.3 RL for Combinatorial Problems

One significant contribution to the integration of RL and combinatorial optimisation is the work by Wang [33] who applied neural network-based RL techniques to solve combinatorial optimisation problems, such as the traveling salesman problem (TSP). Their approach demonstrated how RL could learn heuristics for complex optimisation tasks. This work showcased the potential of RL in generating high-quality solutions for combinatorial problems.

2.4.4 Policy Gradient Methods

This method is Li [20] introduced the Deep Q-Network (DQN), which leverages deep learning for RL. Their approach, based on Q-learning with deep neural networks, has been adapted for combinatorial optimisation tasks. Mazyavkina [24] extended these ideas to combinatorial problems by using RL to learn policies for problems like the TSP. Their research highlights the ability of deep RL methods to handle large and complex optimisation tasks.

2.4.5 Reinforcement Learning for Scheduling Problems

This problem was Han [15] explored the application of RL to scheduling problems, including job-shop scheduling. Their work utilized RL techniques to learn scheduling policies that optimize performance metrics such as makespan and flow time. This research emphasizes the utility of RL in solving real-world combinatorial optimisation problems.

2.4.6 Metaheuristics and RL

Combining metaheuristic methods with RL has also been a topic of interest. Bhavya [10] discussed ant colony optimisation (ACO) as a metaheuristic approach for combinatorial problems. Recent works, such as those by Wang [33] have integrated ACO with RL to enhance the performance of optimisation algorithms [6]. This hybrid approach leverages the strengths of both metaheuristics and RL.

2.4.7 Graph Neural Networks and RL

The use of graph neural networks (GNNs) in conjunction with RL has gained traction. Cappart [11] introduced GCNs, which have been applied to combinatorial optimisation tasks by Berto [9]. Their research demonstrated how GNNs can be combined with RL to improve solution quality and efficiency in problems like the vehicle routing problem (VRP).

2.4.8 End-to-End Learning Approaches

This approach was Wang [31] proposed end-to-end learning frameworks that integrate RL with optimisation problems. Their approach allows for the simultaneous learning of both the RL policy and the optimisation strategy, leading to improved performance on tasks such as scheduling and resource allocation . This work underscores the potential of end-to-end learning methods in solving complex combinatorial optimisation problems.

2.5 Introduction to Graph Theory and Its Applications

Graph theory has a rich history that dates back to the 18th century, with the pioneering work of Leonhard Euler on the Seven Bridges of Königsberg problem, which laid the foundation for the study of graphs as a mathematical concept Wilson [34]. Since then, graph theory has evolved significantly, becoming a critical area of study in mathematics and computer science due to its ability to model and analyse complex systems. Graphs are used in a wide range of applications, from network design and optimisation to social network analysis and biological modeling, making them a versatile tool for researchers and practitioners Lü [21].

2.6 Historical Developments in Graph Theory

Over the years, several key developments have shaped the field of graph theory. In the early 20th century, Authors made substantial contributions to the theory of graph colourings and random graphs, respectively Golumbic, M.C. and Sainte-Laguë [14]. Kőnig's work on bipartite graphs and their properties provided a foundation for understanding graph structures in which vertices can be divided into two disjoint sets such that every edge connects a vertex in one set to a vertex in the other. Their pioneering research on random graphs introduced probabilistic methods to graph theory, allowing for the analysis of graphs formed by randomly connecting vertices. These foundational works have greatly influenced the study of graph properties and algorithms, leading to numerous theoretical advancements.

2.7 Modern Graph Theory and Computational Advances

The latter half of the 20th century saw the rise of computational graph theory, driven by the increasing need for efficient algorithms to process large graphs in real-world applications. Researchers developed various algorithms for fundamental graph problems such as shortest path, maximum flow, and graph colouring, which are now standard tools in computer science. The advent of computers also enabled the exploration of complex graphs that were previously infeasible to study manually Mostafaie [25]. Advances in computational power and algorithm design have allowed researchers to tackle larger and more intricate graph structures, leading to a deeper understanding of graph theory's practical applications Abadal [2].

2.8 Recent Research and Innovations in Graph Theory

In recent decades, the focus of graph theory research has shifted towards dynamic and evolving networks, such as social and biological networks, where graph structures change over time. Researchers have developed algorithms to analyse and predict changes in these dynamic graphs, enhancing our ability to understand complex systems' behaviour. Additionally, the study of network robustness and vulnerability has become increasingly important, particularly in the context of cyber-physical systems and infrastructure networks. New techniques have been developed to assess and improve network resilience against failures and attacks, making graph theory a vital tool in the design and management of secure and reliable networks Abdelkader [4].

2.9 Existing Work on the Odd Cycle Condition

The odd cycle condition is a fundamental concept in graph theory, particularly in the study of graph colouring and network design Shinde [28]. An odd cycle is a cycle with an odd number of edges, which can significantly impact a graph's properties, such as its colourability and stability. Historically, the presence of odd cycles has been associated with challenges in graph colouring, as graphs with odd cycles require more than two colours to achieve a proper colouring. Research has shown that the detection and management of odd cycles are crucial in optimizing network designs, especially in applications that require fault tolerance and redundancy. Recent studies have explored various algorithms and methods to efficiently detect odd cycles in large-scale graphs. Techniques such as depth-first search (DFS), breadth-first search (BFS), and advanced heuristic methods have been developed to identify odd cycles with reduced computational complexity Abboud [3]. Additionally, researchers have investigated the implications of odd cycles in specialized graphs, such as bipartite and planar graphs, where the absence of odd cycles allows for simpler colouring and optimisation strategies.

2.10 Summary

The background and literature review presented in this chapter have highlighted the evolution of graph theory from its historical origins to its current state as a critical tool in mathematical and computational research. The development of algorithms and methods for understanding graph structures has significantly advanced, enabling more sophisticated analyses of complex networks. The study of odd cycles, in particular, remains a vital area of research, offering insights into graph properties and applications in various domains. This dissertation builds on these foundations, aiming to explore new approaches for handling the odd cycle condition in graphs and their practical implications for network design and optimisation.

Chapter 3

Design Approach

The design approach for my dissertation on ”Reinforcement Learning for Generating Graphs with the Odd Cycle Condition” involves creating a framework that incorporates reinforcement learning techniques to generate graphs that adhere to a specific combinatorial condition—the odd cycle condition. This chapter outlines the essential aspects of the design, including both software requirements and the approach to software development.

3.1 Software Requirements

In developing the algorithms and simulations for this research, several essential Python libraries were utilized, each contributing specific functionalities critical to the project's objectives. The libraries include NumPy, Gymnasium, and NetworkX, among others. Below is an overview of these libraries and their roles in the project.

3.1.1 Gymnasium

Gymnasium is an open-source library that provides a collection of environments for developing and testing reinforcement learning algorithms. It offers a standardized interface for interacting with different environments, making it easier to create, test, and benchmark reinforcement learning models. In this project, Gymnasium was used to simulate various environments where the reinforcement learning models could be trained and evaluated. The library's diverse set of environments allowed for robust testing of the algorithms under different conditions, thereby helping to ensure their adaptability and effectiveness across a range of scenarios.

3.1.2 NetworkX

NetworkX is a comprehensive library designed for the creation, manipulation, and study of complex networks and graphs. It provides tools for analyzing the structure and dynamics of networks, such as social networks, biological networks, and technological networks. In this research, NetworkX was used to model and analyse graph-based structures that represent various network configurations. The library's extensive functionality for generating random graphs, computing graph metrics, and visualizing network structures was crucial for studying the properties of graphs and for implementing graph-related algorithms within the project.

3.2 System Architecture and Implementation Plan

3.2.1 Architecture Design

The system architecture for generating graphs that satisfy the odd cycle condition using reinforcement learning (RL) is composed of three main components: the RL framework, graph processing modules, and the user interface. This design ensures seamless interaction between the components to efficiently generate, evaluate, and display the required graph structures. The components of the architecture are explained below.

3.2.2 Reinforcement Learning Framework

The Reinforcement Learning (RL) Framework is made up of several important components that all work together to make the graph generation process better. The RL agent is the main part of this framework, playing a key role in learning how to create graphs effectively. It interacts with the graph environment repeatedly, making changes to the graph's structure with the goal of creating graphs that meet the specific odd cycle condition. The environment itself shows the current state of the graph and gives the agent feedback in the form of observations and rewards. This feedback is crucial because it helps the agent understand how successful it has been in generating valid graphs. The framework also includes a Policy Network, which is a neural network that helps the agent decide what to do next based on the current state of the graph. This network is trained to improve the policy, which helps guide the agent toward making graphs with the right characteristics. Lastly, the Reward Function plays an important role in the agent's learning process. It is designed to reward the agent when it successfully creates graphs that meet the odd cycle condition, ensuring that the agent stays focused on making valid and well-optimized graph structures.

3.2.3 Graph Processing Components:

The Graph Processing Components consist of several key modules that play essential roles in managing and evaluating graphs. The first component is the Graph Generator, which is responsible for initializing the graph and enabling the agent to modify it through a series of actions. This module ensures that the graph stays within specific predefined constraints, such as the number of vertices and edges. Next is the Cycle Detector, a crucial part of the system that monitors the graph for odd cycles. It detects these cycles and provides feedback to the agent, which then influences the reward system. Finally, the Graph Evaluator module assesses the completed graph, checking it against the odd cycle condition and other important criteria. This module offers a thorough evaluation of the graph's validity and overall quality.

3.2.4 Implementation Phases

The implementation of the RL-based graph generation system is structured into distinct phases, ensuring systematic development, integration, and testing of the system components. This phased approach helps manage the complexity of the project, allowing for incremental progress and iterative refinement.

3.2.5 Phase 1: Initial Setup

In the initial setup phase of the Reinforcement Learning (RL) framework, the main objective is to establish the foundational elements necessary for the framework's operation. This phase involves several key activities that lay the groundwork for the system's functionality.

The first activity is the setup of the RL environment. This involves defining the graph environment, which includes state representation, action space, and the reward function. The environment acts as the playground where the RL agent interacts and learns, providing the necessary context for the agent's actions and decisions.

Next, the Policy Network is initialized. This step involves developing the initial structure of the policy network, which is crucial for guiding the agent's decision-making process. The policy network will later be refined as the agent learns from interacting with the environment.

The third activity focuses on configuring the Graph Generator. This involves setting up the basic graph generation module, which allows the creation of simple graph structures that the agent can later modify. This configuration is essential for giving the agent a starting point from which it can begin its learning process.

Finally, testing is conducted to validate the environment's behaviour. Simple test cases are used to ensure that the agent can interact with the environment correctly, which is critical for the successful operation of the entire RL framework. This testing phase ensures that all elements of the environment function as expected before the agent begins its learning tasks.

3.2.6 Phase 2: Component Development

In the second phase of the system's development, known as Component Development, the primary goal is to develop and refine the core components that make up the system. This phase includes a series of critical activities aimed at enhancing the system's overall functionality.

The first activity in this phase is the implementation of the Cycle Detector. This involves integrating the cycle detection algorithm, which is responsible for monitoring the graph's structure to identify odd cycles. It is essential to ensure that the cycle detector interacts effectively with the environment, as it plays a significant role in influencing the reward function based on the presence of these cycles.

Following this, the focus shifts to Advanced Policy Training. In this activity, the RL agent is trained using initial graph structures, which helps to optimize the policy network. The training is particularly focused on enabling the agent to generate valid graphs that meet the odd cycle condition, thereby improving the agent's decision-making abilities.

The next activity involves the tuning of the Reward Function. This step is crucial for fine-tuning the reward function to better guide the agent towards creating desirable graph structures. Adjustments are made based on the results of early testing, ensuring that the reward function effectively encourages the agent to focus on generating optimal graphs.

Finally, the phase concludes with thorough testing. Component-level testing is conducted to ensure that each module—whether it's the cycle detector, policy network, or reward function—operates as expected when tested in isolation. This testing is vital to confirm that each part of the system functions correctly before they are integrated into the larger framework.

3.2.7 Phase 3: System Integration

In the third phase, known as System Integration, the focus shifts to bringing together all the developed components into a unified and cohesive system. This phase is crucial as it ensures that all parts of the system work seamlessly together to achieve the desired outcomes.

The first major task in this phase is Component Integration. This involves combining the RL agent, environment, cycle detector, and graph generator into a single, unified framework. It's essential during this process to ensure that these components can effectively communicate and function together without issues, as any disconnect could lead to failures in the system's operation.

After integration, the next step is End-to-End Testing. This involves performing thorough integration testing by running the entire system from start to finish. Various scenarios are tested to ensure that the RL agent can successfully generate graphs that meet the odd cycle condition. Additionally, it is important to verify that the user interface (UI) accurately reflects the entire process and its results, ensuring a smooth and understandable user experience.

Finally, comprehensive Testing is conducted to address any integration issues that may have arisen during the process. This step involves rigorous testing to confirm that the entire system functions as a whole and meets all the predefined objectives. By the end of this phase, the system should be fully operational, with all components working in harmony to achieve the desired results.

3.2.8 Phase 4: optimisation and Refinement

The fourth and final phase, known as optimisation and Refinement, focuses on enhancing the system's performance and usability. This phase is critical for ensuring that the system operates efficiently and can handle more complex tasks as it evolves.

The first activity in this phase is Algorithm optimisation. This involves refining the RL algorithm by analyzing performance data and making necessary adjustments. Specifically, the learning rate, policy network architecture, and reward function are fine-tuned to improve the efficiency and accuracy of the graph generation process. These adjustments help the RL agent perform better and more reliably in its tasks.

The next activity is the Graph Generator Enhancement. In this step, the capabilities of the graph generator are expanded to handle more complex graph structures. This enhancement allows the RL agent to take on more challenging graph generation tasks, pushing the limits of what the system can achieve and ensuring it remains robust in a variety of scenarios.

Finally, comprehensive Testing is conducted to ensure that the optimized system can efficiently manage complex graph generation tasks. This includes performance testing to evaluate the system's ability to handle increased demands and gathering user feedback to identify any remaining issues or areas for improvement. Based on this feedback, final adjustments are made, ensuring that the system is polished and fully optimized for real-world applications.

Chapter 4

Proposed Methodology

This section presents the methodology for my dissertation on "Reinforcement Learning for Generating Graphs with the Odd Cycle Condition." It outlines the approach and processes used to achieve the project's objectives, starting with problem formulation and progressing through the design of the reinforcement learning framework for graph generation.

4.1 Problem Formulation

4.1.1 Odd Cycle Condition

The odd cycle condition in graph theory refers to a situation where a cycle in a graph contains an odd number of vertices, refer section one where the definition is explained in detail. This property is significant because it indicates that the graph has at least one cycle with an odd number of vertices. The odd cycle condition is important in several areas of graph theory and applications, as outlined below.

First, in the context of Bipartite Graphs, a graph is considered bipartite if and only if it does not contain any odd cycles. This makes understanding whether odd cycles are present crucial for determining the bipartiteness of a graph.

Secondly, Graph Colouring is another area where the odd cycle condition plays a key role. Graphs that contain odd cycles often require more than two colours to be properly coloured, as opposed to bipartite graphs, which can be coloured with just two colours.

This makes the presence of odd cycles a critical factor in the graph colouring process. Lastly, the odd cycle condition affects Network Flow and optimisation. The presence of odd cycles can complicate network flow problems and optimisation tasks, making the solutions more complex and sometimes affecting the feasibility of finding an optimal solution. The structure and presence of odd cycles in a graph can thus significantly influence the difficulty of these tasks.

4.1.2 Mathematical Formulation

The mathematical formulation of odd cycles in graph theory involves a clear understanding of how these cycles are defined, represented, and detected within a graph. Formally, a cycle in a graph $G = (V, E)$ is defined as a sequence of vertices $v_1, v_2, \ldots, v_k$ where the first and last vertices are the same $(v_1 = v_k)$. The number k denotes the number of vertices in the cycle, and the cycle is considered odd if k is an odd number, meaning that the cycle contains an odd number of vertices.
In terms of graph representation, a graph G is described by its vertex set V and edge set E. The odd cycle condition is satisfied if there exists a subset of vertices $V' \subseteq V$ that forms a cycle with an odd number of vertices. This condition can be expressed mathematically as:

$$\exists C \subseteq V \quad \text{such that} \quad |C| \text{ is odd and } C \text{ forms a cycle in } G$$

Detecting odd cycles in a graph can be achieved using algorithms such as Depth-First Search (DFS) or Breadth-First Search (BFS). These algorithms help identify odd cycles by checking if, during the traversal of the graph, a vertex is revisited in a way that forms a path of odd length. This method is particularly useful in efficiently finding odd cycles, which are essential in various graph theory applications.

4.2 Reinforcement Learning Framework for Graph Generation

This section details how the problem of generating graphs that satisfy the odd cycle condition can be modelled using Reinforcement Learning (RL). The problem is framed as a Markov Decision Process (MDP), which provides a structured approach for decision-making in environments with both stochastic outcomes and agent control.

4.2.1 Framing the Problem as a Markov Decision Process

To frame the problem as a Markov Decision Process (MDP), the MDP is defined by the tuple (S, A, P, R, γ), where each component plays a specific role in modeling the decision-making process.

The state space S represents all possible configurations of the graph. Each state s is described by the tuple (V, E, C_{odd}), where V is the set of vertices, E is the set of edges, and C_{odd} is a binary indicator representing the presence of an odd cycle (1 for present, 0 for absent).

The action space A includes all possible actions the agent can take to modify the graph. An action is defined as

$$a = (v_i, v_j, \text{operation})$$

where v_i and v_j are vertices, and "operation" specifies the type of modification, such as "add edge," "remove edge," or "swap edge."

Transition dynamics P describes the probability of transitioning from state s to state s' after taking action a. This is expressed as:

$$P(s'|s, a) = Pr(V', E', C'_{\text{odd}})|(V, E, C_{\text{odd}}), a)$$

where V', E', and C'_{odd} represent the new state after applying action a.

Finally, the reward function R provides feedback to the agent based on the action taken.

A positive reward is given if the action results in an odd cycle, while a negative reward is applied if the action leads to a graph without odd cycles or violates other constraints. This reward function is crucial for guiding the agent's learning process, encouraging behaviours that lead to the desired graph structures.

4.3 Reinforcement Learning Framework

4.3.1 Choice of Reinforcement Learning Algorithm

In selecting a suitable reinforcement learning (RL) algorithm for the task of generating graphs that satisfy specific constraints, such as the odd cycle condition, it is crucial to consider the complexity and the nature of the problem. Among the commonly used RL algorithms, we considered Q-learning, Deep Q-Networks (DQN), and Policy Gradient Methods. After careful evaluation, we have chosen Proximal Policy optimisation (PPO), a type of Policy Gradient Method, for this task.

4.3.2 Reasons for Selecting PPO

One of the primary reasons for selecting PPO is its ability to handle high dimensionality effectively. Graph generation often involves a large and complex state space, especially when the graphs need to adhere to specific structural constraints like the odd cycle condition. PPO is particularly well-suited for environments with such high-dimensional and continuous action spaces. Unlike Q-learning and DQN, which are value-based methods and can struggle with large action spaces, PPO optimizes a policy directly in this high-dimensional space, making it more appropriate for generating complex graph structures. Another reason for choosing PPO is its stability in learning. PPO is designed to maintain a balance between the need for improvement and the stability of the learning process. It achieves this by incorporating a clipped objective function that prevents excessive updates, ensuring that the policy improves steadily without oscillations. This feature is particularly important in the graph generation task, where drastic changes in policy could lead to the generation of invalid or suboptimal graphs.

Additionally, PPO offers a significant policy optimisation advantage. Policy Gradient Methods, like PPO, optimize the policy directly, enabling them to learn more complex behaviours that are difficult to capture with value-based methods. This direct optimisation is advantageous for tasks like graph generation, where the policy must navigate a complex space of possible graph configurations while adhering to specific constraints.

4.3.3 Core of PPO's Approach

The core of PPO's approach involves optimizing the following objective function:

$$L(\theta) = \mathbb{E}_t \left[\min \left(\frac{\pi_\theta(a_t|s_t)}{\pi_{\theta_{\text{old}}}(a_t|s_t)} \hat{A}_t, \text{clip} \left(\frac{\pi_\theta(a_t|s_t)}{\pi_{\theta_{\text{old}}}(a_t|s_t)}, 1-\epsilon, 1+\epsilon \right) \hat{A}_t \right) \right]$$

In this function, $\pi_\theta(a_t|s_t)$ represents the probability of taking action a_t given state s_t under the current policy θ, while $\pi_{\theta_{\text{old}}}(a_t|s_t)$ represents the probability of the same action under the previous policy. The term $\hat{A}_t$ denotes the advantage function, which estimates how much better the current action is compared to a baseline, typically the value function. The parameter ϵ is a small positive number that controls the range within which the policy ratio is allowed to vary.

This clipping function is crucial because it ensures that the policy does not update too aggressively, which helps maintain stability in the learning process. This stability is especially important when dealing with the delicate balance required in graph generation tasks. In addition to providing stability, PPO's ability to directly optimize the policy allows it to effectively learn the intricate behaviours necessary to generate graphs that meet the odd cycle condition. This justifies its selection over other algorithms, making it the suitable choice for this reinforcement learning framework.

4.4 Multi-Layer Perceptron Neural Network

In this project, the core machine learning model used is a Multi-Layer Perceptron (MLP) neural network. MLPs are a class of feedforward artificial neural networks that have been widely adopted in various fields due to their ability to model complex patterns and relationships within data.

4.4.1 Structure and Components of the MLP

An MLP consists of multiple layers of nodes, typically structured into an input layer, one or more hidden layers, and an output layer. Each node, or artificial neuron, in the network is connected to nodes in the subsequent layer, forming a dense network of connections.
The input layer is designed to receive data in a structured format, with each neuron representing a feature of the input data. For the task at hand, this might involve representing elements of a graph or features derived from the graph's adjacency matrix. This layer serves as the entry point for data into the network, where it begins the process of transformation and analysis.
The hidden layers are where the MLP derives its power, enabling the network to capture non-linear relationships within the data. Each hidden layer consists of neurons that apply a linear transformation to the input data, followed by a non-linear activation function such as ReLU (Rectified Linear Unit). These hidden layers allow the network to learn complex patterns within the data, which are crucial for tasks like identifying valid graph structures that meet specific criteria, such as the odd cycle condition.
Finally, the output layer produces the final prediction or decision based on the transformed input data. In the context of this project, the output could represent the probability distribution over different actions (like adding or removing edges) or a specific action to modify the graph structure. This layer concludes the network's processing by providing actionable insights or decisions derived from the input data.

4.4.2 Learning Process

The learning process in an MLP involves adjusting the weights of the connections between neurons through back propagation, a supervised learning technique. During training, the network processes input data, propagates it through the layers, and compares the output to the desired result. The difference between the predicted output and the actual output, quantified by a loss function, guides the adjustment of the network's weights. This process is iterated multiple times over a dataset, allowing the MLP to learn and generalize from the input data.

4.4.3 Application to Graph Generation

In this project, the MLP is used to learn a policy for generating graphs that satisfy specific topological constraints, particularly the odd cycle condition. The input to the MLP could include features derived from the current state of the graph, while the output guides the actions required to modify the graph toward the desired configuration. The advantage of using an MLP in this context lies in its ability to approximate complex functions, making it well-suited for tasks where the relationship between the graph's current state and the necessary actions is non-linear and intricate. By training the MLP with reinforcement learning techniques, the network can progressively improve its ability to generate valid graphs, learning from the reward signals that indicate whether the generated graph satisfies the odd cycle condition.

4.5 State Representation

In reinforcement learning (RL), the state representation is a crucial component as it directly influences the learning process and the quality of the generated policy. For tasks involving the generation or modification of graphs, especially those subject to specific conditions like the odd cycle condition, representing the state effectively within the RL framework becomes a complex challenge.

The current state of a graph in an RL framework can be represented as a combination of features that encapsulate both the global properties of the graph and the local properties of individual nodes and edges.

Node features are vectors associated with each node in the graph, capturing properties such as node degree, label, or any other node-specific attributes relevant to the task. For instance, in a graph where nodes represent different entities, node features could include categorical or numerical data pertinent to those entities.

Edge features, similar to node features, represent the characteristics of the connections between nodes. These could include the weight of the edge, the type of relationship, or whether the edge is directed or undirected.

The graph adjacency matrix is a common way to represent the connectivity of the graph. It is a square matrix where each element A_{ij} represents the presence or absence of an edge between node i and node j. In weighted graphs, A_{ij} might represent the weight of the edge.

Graph-level features capture global properties of the entire graph, such as the total number of nodes and edges, graph density, or the number of cycles. These properties are especially important when the task involves constraints like ensuring the graph has an odd cycle.

Mathematically, the state S of a graph can be represented as:

$$S = (A, X, E, G)$$

where A is the adjacency matrix, $X = \{x1, x2, ..., xn\}$ are the node features, $E = \{e1, e2, ..., em\}$ are the edge features, and G represents the global graph-level features.

4.6 Action Space Design

In the context of graph generation using reinforcement learning (RL), the action space defines the set of all possible operations that the RL agent can perform on the graph. These operations typically include actions like adding, modifying, or deleting nodes and edges, which gradually transform the graph's structure to meet specific goals or constraints.

One of the most fundamental actions in graph generation is adding an edge between two nodes. This action involves selecting a pair of nodes (u, v) that are not already connected and creating an edge between them. Mathematically, if the graph's adjacency matrix is represented as A, where A_{ij} indicates the presence (1) or absence (0) of an edge between nodes i and j, adding an edge would involve updating the matrix such that $A_{uv} = 1$.

Another common action is modifying the properties of an existing edge, such as its weight or direction. For instance, in a weighted graph, this could mean adjusting the weight w_{uv}

associated with the edge between nodes u and v. In some cases, this might also involve converting an undirected edge into a directed one or vice versa.

Conversely, the RL agent might also have the option to remove edges from the graph. This action is crucial when the goal is to simplify the graph or to ensure that it meets specific structural constraints. Deleting an edge between nodes u and v would involve setting $A_{uv} = 0$ in the adjacency matrix.

Depending on the specific application, the RL agent might also be allowed to add new nodes or remove existing ones. This action directly influences the overall size and complexity of the graph. Adding a node typically involves expanding the adjacency matrix and potentially adding new edges, while removing a node involves contracting the matrix and deleting all edges connected to that node.

In some graph generation tasks, the RL agent might also perform rewiring actions, where an existing edge between two nodes is removed, and a new edge is added between another pair of nodes. This action is particularly useful in optimizing the graph's structure while maintaining a fixed number of edges. In more complex scenarios, the action space might include operations that modify entire subgraphs, such as duplicating, merging, or splitting subgraphs. This allows for more sophisticated structural changes, especially in tasks that involve the generation of large, modular graphs.

4.7 Introduction to Reward Function

In the context of reinforcement learning (RL) for graph generation, the reward function plays a critical role in guiding the agent toward achieving specific goals, such as satisfying the odd cycle condition. The reward function is the mechanism through which the agent receives feedback on its actions, encouraging behaviours that lead to the desired outcomes and discouraging those that do not. For the task of generating graphs with the odd cycle condition, the reward function must be carefully crafted to ensure that the agent is properly incentivized to create graphs that meet this requirement. The design of the reward function must account for various factors, including positive reinforcement for achieving the odd cycle condition, penalties for violating it, and a balance between exploration and exploitation.

4.7.1 Structure of the Reward Function

The reward function should provide positive reinforcement whenever the agent takes an action that results in the creation or maintenance of odd cycles in the graph. An odd cycle is a cycle that contains an odd number of edges. This positive reinforcement encourages the agent to focus on constructing graph structures that meet the odd cycle condition. Mathematically, the reward for achieving an odd cycle can be represented as:

$$R_{\text{odd}}(G_{t+1}) = \sum_{C \in G_{t+1}} \mathbf{1}(\text{length } (C) \text{ is odd})$$

Here, G_{t+1} represents the graph at time step $t+1$, and $\mathbf{1}$ is an indicator function that returns 1 if the cycle C is of odd length and 0 otherwise. The sum is taken over all cycles C in the graph. This reward function directly encourages the RL agent to create graphs with more odd cycles.

4.7.2 Balancing Exploration and Exploitation

In reinforcement learning (RL), it's crucial to strike a balance between exploration—trying out new actions to discover potential improvements in the graph structure—and exploitation—refining known strategies that have proven successful. The reward function should encourage exploration, especially in the early stages of learning, while gradually shifting towards exploitation as the agent becomes more proficient in generating the desired graph structures.

One way to incorporate exploration into the reward function is by providing a small positive reward for any valid action that results in a graph structure different from the previous one:

$$R_{\text{explore}}(G_{t+1}) = \epsilon \cdot \mathbf{1}(G_{t+1} \neq G_t)$$

Here, ϵ is a small positive constant that encourages the agent to explore new graph configurations, while $\mathbf{1}(G_{t+1} \neq G_t)$ is an indicator function that rewards the agent when the graph at $t + 1$ differs from the graph at t.

As the training progresses, the weight of the exploration reward can be reduced to focus more on exploitation, ensuring that the agent leverages the knowledge it has gained to consistently produce graphs that satisfy the odd cycle condition.

4.7.3 Dynamic Reward Adjustment

The reward function can be designed to adaptively adjust the weighting of different components, such as exploration and exploitation, as the training process progresses. This dynamic adjustment allows the agent to transition smoothly from an initial exploratory phase where it experiments with various graph structures to a more exploitative phase, focused on optimizing the graph generation process to meet the odd cycle condition.

To achieve this, a time-dependent weighting factor $\alpha(t)$ can be introduced, which modulates the relative importance of the exploration reward compared to the rewards associated with odd and even cycles. The overall reward function can be expressed as:

$$R(G_{t+1}) = \alpha(t)R_{\text{explore}}(G_{t+1}) + R_{\text{odd}}(G_{t+1}) + R_{\text{even}}(G_{t+1})$$

In this formulation, $\alpha(t)$ gradually decreases over time, thereby reducing the emphasis on exploration as the agent becomes more proficient in identifying effective strategies. This approach enables the agent to explore a broad range of possibilities during the early stages of learning, before honing in on generating high-quality graphs that consistently satisfy the odd cycle condition.

4.7.4 Incentivizing the RL Agent: A Comprehensive Approach

The reward function, as outlined above, serves multiple purposes in guiding the RL agent's behaviour, those are listed below.

First, the positive rewards for odd cycle creation reinforce actions that lead to the desired outcome. The agent learns to prioritize these actions, gradually developing a policy that consistently generates graphs with odd cycles.

Second, the negative rewards for even cycle creation act as a deterrent against undesirable actions. By penalizing the formation of even cycles, the reward function ensures that the agent focuses on generating graphs that meet the odd cycle condition.

Third, the inclusion of an exploration reward encourages the agent to try new actions and discover novel graph structures. This aspect of the reward function is particularly important during the early stages of training, as it prevents the agent from becoming stuck in sub optimal strategies.

Fourth, the use of a discount factor γ in the cumulative reward function helps balance the agent's long-term objectives with immediate rewards. A higher discount factor encourages the agent to pursue actions that may not yield immediate benefits but contribute to better overall performance in the long run.

Finally, the dynamic adjustment of the reward function ensures that the agent's learning process is adaptive. By gradually shifting the focus from exploration to exploitation, the reward function helps the agent transition from discovering new strategies to refining and optimizing them.

Chapter 5

Algorithm Development

5.1 Introduction to Algorithm Design in Reinforcement Learning

Designing a reinforcement learning (RL) algorithm for graph generation is a complex process that requires careful consideration of both the problem's structure and the RL framework. The goal is to develop an algorithm that can effectively generate graphs that meet specific conditions, such as the odd cycle condition. This involves not only selecting appropriate RL techniques but also iteratively refining the algorithm through prototyping, testing, and adjustment.

5.1.1 Algorithm Design Framework for Reinforcement Learning

In designing a reinforcement learning algorithm for graph generation, the first step is to clearly define the problem that the algorithm is intended to solve. In this context, the goal is to generate graphs that satisfy the odd cycle condition using reinforcement learning, specifically through Proximal Policy optimisation (PPO). This problem can be formally defined as finding a graph $G(V, E)$ where V is the set of vertices and E is the set of edges, such that the graph does not contain any odd-length cycles. Mathematically, the condition can be expressed as:

$$\forall \text{cycle } C \in G, \text{ if } |C| \text{ is the length of cycle } C, \text{ then } |C| \text{ must be even.}$$

The next crucial aspect of the design involves setting up the environment in which the reinforcement learning agent will operate. The environment must provide the agent with the states (representing the current structure of the graph), possible actions (such as adding or removing edges), and a reward function. The state s_t at any given time t can be described as the current graph structure G_t. The action a_t can involve either adding an edge or choosing not to add one. The reward R_t is determined based on whether the graph resulting from the action adheres to the odd cycle condition:

$$R_t = \begin{cases} +1 & \text{if the graph satisfies the odd cycle condition} \\ -1 & \text{if it does not.} \end{cases}$$

Central to the PPO algorithm is the policy network, which maps the state of the graph to a probability distribution over possible actions. The policy network $\pi_\theta(a|s)$ is optimized through training to maximize the expected reward. The parameters θ of the network are updated during training, and the policy gradient is calculated using the advantage function, which measures how much better an action is compared to a baseline, typically the value function $V(s_t)$:

$$\nabla_\theta J(\theta) = \mathbb{E}_\pi \left[\nabla_\theta \log \pi_\theta(a_t|s_t) \hat{A}_t \right]$$

Another key component is the value function $V_\phi(s)$, which estimates the expected return from a given state s. The value network is trained to minimize the difference between the predicted value and the actual return. The loss function for the value network quantifies this difference and guides the adjustments made to the network's parameters during training:

$$L(\phi) = \mathbb{E}_{(s_t,R_t)} \left[(V_\phi(s_t) - R_t)^2 \right]$$

PPO, as an enhancement of standard policy gradient methods, plays a crucial role in this design. The primary goal of PPO is to prevent large updates to the policy by clipping the objective function, ensuring stable and effective learning. The objective function in PPO involves a probability ratio that is carefully controlled through a hyperparameter ϵ, which limits the extent of updates during training:

$$L^{PPO}(\theta) = \mathbb{E}_t \left[\min \left(\frac{\pi_\theta(a_t|s_t)}{\pi_{\theta_{old}}(a_t|s_t)} \hat{A}_t, \text{clip} \left(\frac{\pi_\theta(a_t|s_t)}{\pi_{\theta_{old}}(a_t|s_t)}, 1-\epsilon, 1+\epsilon \right) \hat{A}_t \right) \right]$$

The training phase involves the agent interacting with the environment over multiple episodes. During each episode, the agent takes actions based on its current policy, observes the rewards, and updates the policy network parameters accordingly. The value network is also refined to improve the accuracy of its predictions, contributing to the overall learning process.

Once the model is trained, it must be evaluated on unseen graphs to assess its performance. This stage may require fine-tuning, where adjustments are made to hyperparameters, the policy network architecture, or other aspects of the model. The evaluation is typically based on the average reward over several episodes, with the goal of maximizing this reward while ensuring the generated graphs satisfy the odd cycle condition.

Finally, the algorithm is implemented in code and tested across various graph structures to ensure it generalizes well to different graph sizes and configurations. The success of the algorithm is gauged by its ability to consistently generate graphs that meet the odd cycle condition while effectively exploring the space of possible graph configurations.

This comprehensive framework lays the groundwork for developing a PPO-based reinforcement learning algorithm capable of generating graphs that meet specific topological criteria, such as the odd cycle condition.

5.2 Workflow from Initial State to Graph Generation and Evaluation

The workflow of the RL-based graph generation algorithm is structured around the interaction between the agent and the environment. The agent's objective is to learn a policy that enables it to generate graphs that satisfy certain conditions, such as the odd cycle condition, through a series of actions.

5.2.1 Environment Initialization

The environment in which the reinforcement learning agent operates is crucial, setting the stage for the agent's interactions, including the rules, constraints, and objectives that guide its learning process. The key focus of this environment is to establish conditions that ensure the creation of graphs containing odd cycles. The goal is to create a graph that includes odd cycles. Initially, the approach emphasized avoiding the creation of even cycles, but this constraint has been relaxed. The primary objective now is to ensure the inclusion of odd cycles within the graph. The environment allows for the presence of even cycles; however, the agent is incentivized through the reward structure to prioritize the generation of odd cycles.

The environment starts by initializing a graph $G(V, E)$, where V is the set of vertices and E is the set of edges. The agent modifies the graph by adding or removing edges in a way that leads to the formation of cycles. The core constraint is to ensure that the graph contains at least one odd cycle. The detection of cycles is performed using graph traversal algorithms such as depth-first search (DFS) or breadth-first search (BFS). If a cycle is found, its length L is determined, and the cycle is classified as either odd or even:

$$L \mod 2 = \begin{cases} 1 & \text{(Odd Cycle)} \\ 0 & \text{(Even Cycle)} \end{cases}$$

The environment permits the creation of even cycles. The reward structure encourages the formation of odd cycles but does not penalize the creation of even cycles.

The reward R is defined as a function of the number of odd cycles C_{odd} detected in the graph. Let C_{odd} and C_{even} represent the number of odd and even cycles, respectively. The reward R at time step t is given by:

$$R(t) = w_{\text{odd}} \cdot C_{\text{odd}}(t)$$

where w_{odd} is a positive constant weight assigned to odd cycles to reinforce their creation. Even cycles do not contribute to the reward:

$$R_{\text{even}}(t) = 0$$

The agent's goal is to maximize the cumulative reward over time T:

$$\text{Maximize} \sum_{t=0}^{T} R(t) = \sum_{t=0}^{T} w_{\text{odd}} \cdot C_{\text{odd}}(t)$$

This structure ensures that the agent focuses on generating graphs with odd cycles while maintaining the flexibility to create even cycles without penalty.

The agent must balance exploration and exploitation through the use of an appropriate exploration strategy, such as epsilon-greedy or softmax, to explore new graph configurations while exploiting known strategies that result in higher rewards for odd cycle generation. The agent's action policy $\pi(a|s)$ at any state s should prioritize actions that are expected to maximize the reward related to odd cycle creation:

$$\pi(a|s) = \arg\max_{a} \mathbb{E}[R(t+1)|s, a]$$

The graph is analysed for cycle formation using traversal algorithms. For each cycle found, the length L is determined, and the cycle is classified as odd or even based on its length. The reward is calculated at each time step based on the number of odd cycles detected. If the agent generates C_{odd} odd cycles, the cumulative reward is directly proportional to the weight w_{odd}. If even cycles dominate without the presence of odd cycles, the overall reward remains low, guiding the agent towards better configurations.

5.2.2 Agent Initialization

The RL agent is initialized with parameters such as the learning rate α, discount factor γ, and exploration rate ϵ. These parameters influence how the agent learns from the environment and how it balances exploration (trying new actions) with exploitation (choosing the best-known actions). The agent maintains a policy π, which maps states to actions.

In a Q-learning or Deep Q-Network (DQN) setup, the policy is indirectly represented through a Q-function $Q(s, a)$, where the agent selects the action a that maximizes the expected reward for a given state s:

$$\pi(s) = \arg\max_a Q(s, a)$$

5.2.3 Step Loop

The core of the algorithm consists of running multiple episodes, where each episode represents an attempt to generate a graph from an initial state to a final state that meets the desired conditions. At the start of each episode, the environment is reset, providing the agent with a fresh starting point. The initial state S_0 is sampled from the environment's state space S.

5.2.4 Action loop

Within each episode, the agent iteratively takes actions based on its current policy. For each time step t within an episode, the agent selects an action a_t based on the current state s_t:

$$a_t = \pi(s_t)$$

The selected action is then executed in the environment, which leads to a transition to a new state s_{t+1}, a reward r_t, and an indicator (done) signaling whether the episode has ended (e.g., if a terminal condition like achieving the odd cycle condition is met). The state transition is governed by the environment's transition function $\mathcal{T}$:

$$s_{t+1} = \mathcal{T}(s_t, a_t)$$

The agent receives feedback in the form of a reward r_t, which reflects the desirability of the new state. For example, a reward might be positive if the action brings the graph closer to satisfying the odd cycle condition, or negative if it introduces an even cycle:

$$r_t = \mathcal{R}(s_t, a_t)$$

5.2.5 Learning and Policy Update

After executing an action, the agent updates its knowledge based on the observed transition (s_t, a_t, r_t, s_{t+1}). In Q-learning, this involves updating the Q-value for the state-action pair using the Bellman equation:

$$Q(s_t, a_t) \leftarrow Q(s_t, a_t) + \alpha \left[r_t + \gamma \max_{a'} Q(s_{t+1}, a') - Q(s_t, a_t) \right]$$

This update process is central to the agent's learning, allowing it to refine its policy over time to improve graph generation outcomes.

5.2.6 Exploration-Exploitation Trade-off

To avoid getting stuck in suboptimal policies, the agent uses an exploration strategy. Typically, this involves selecting a random action with probability ϵ (exploration) and the best-known action with probability $1 - \epsilon$ (exploitation). As training progresses, the exploration rate ϵ is decayed, reducing exploration and allowing the agent to exploit its learned policy more effectively:

$$\epsilon \leftarrow \epsilon \cdot \text{decay\_rate}$$

5.2.7 Episode Termination

An episode terminates either when the agent successfully generates a graph that meets the odd cycle condition or when the maximum number of steps is reached. The success or failure of each episode contributes to the overall learning process, as the agent adjusts its policy based on cumulative experiences.

5.2.8 Graph Generation and Evaluation

Once training is complete, the agent's final policy π^* is used to generate new graphs. The agent starts from an initial state and follows its learned policy to produce a graph step by step. The generated graph is then evaluated to ensure it meets the desired structural condition, such as containing only odd cycles. The evaluation metric might include checks for cycle parity or other structural properties that were targeted during training.

5.2.9 Final Graph Evaluation

After graph generation, the final product is evaluated against the criteria that were established at the beginning of the process. The agent's performance is assessed based on the quality and correctness of the generated graphs. The evaluation process might involve running multiple instances of the algorithm and averaging the results to gauge the consistency and reliability of the graph generation process.

5.3 Experimental Research

5.3.1 Initial Setup and Challenges

At the start of the project, several significant challenges emerged due to the initial reliance on outdated Python libraries for graph generation. These older libraries lacked the robustness and functionality of more modern alternatives, which became evident when the first attempts to generate a graph resulted in structural deficiencies. Specifically, the initial implementation produced a graph that technically satisfied the odd cycle condition but was fundamentally flawed because it was not fully connected. While the graph contained the necessary odd cycles, it failed to ensure that all vertices were part of a single connected component. This oversight led to a situation where some vertices were completely isolated, not contributing to the graph's overall structure or its intended properties.

This issue highlighted a crucial aspect of graph theory that the early approach had overlooked the importance of interconnectivity in creating valid and analyzable graphs. A graph where not all vertices are connected is inherently incomplete and cannot serve as a proper foundation for further analysis or practical applications, particularly in areas where the relationships between all nodes are essential. The initial output, as depicted in Picture 1, vividly illustrates this problem. In figure 5.1 , several vertices remain unconnected, floating independently without any edges linking them to the rest of the graph. These disconnected vertices rendered the graph unsuitable for the project's goals, as it did not meet the basic criteria of a connected graph that could be used for meaningful analysis.

This experience underscored the necessity of using up-to-date libraries and tools that support the full range of required graph properties, including connectivity. It also emphasized the need for careful validation of the generated graphs to ensure they meet all the necessary conditions beyond just the odd cycle requirement. As a result of this initial failure, the approach was revised, adopting more current and reliable libraries, which ultimately allowed for the generation of graphs that were not only valid but also suitable for the complex analyses required in the later stages of the project.

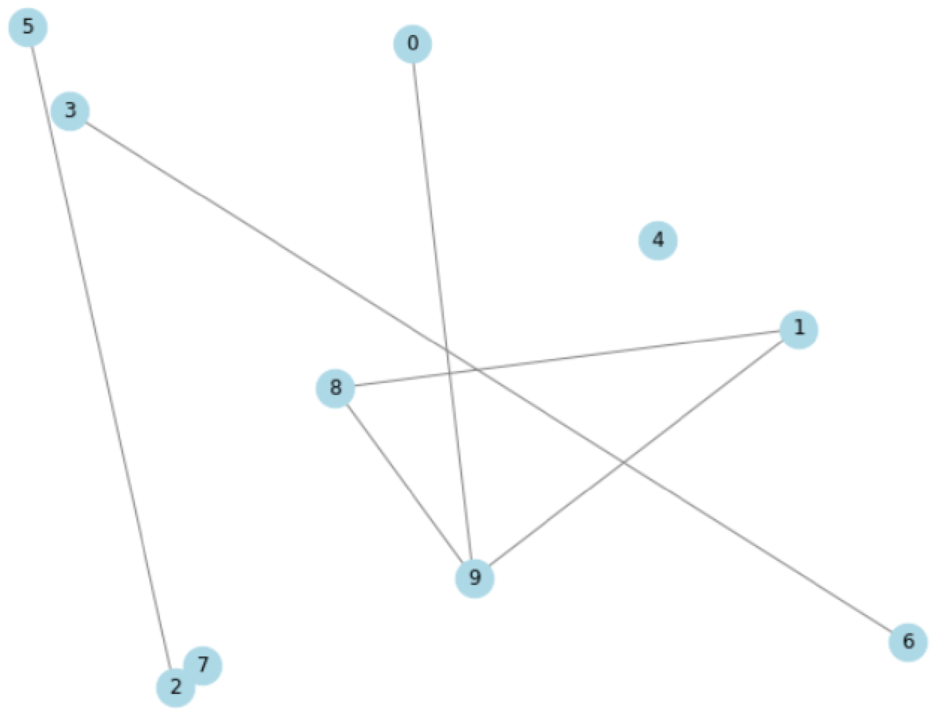


Figure 5.1: Graph with isolated vertices.

5.3.2 Ensuring Graph Connectivity

To address the problem of isolated vertices, a minimum spanning tree (MST) algorithm was applied. The MST algorithm is a well-known technique in graph theory that ensures all vertices are connected using the minimum number of edges, thereby solving the connectivity issue. This approach successfully resulted in a connected graph, eliminating the previously isolated vertices and ensuring that every vertex was part of the graph's structure. However, this solution introduced a new challenge: the graph consistently formed only one odd cycle, regardless of its overall size or complexity. The limitation

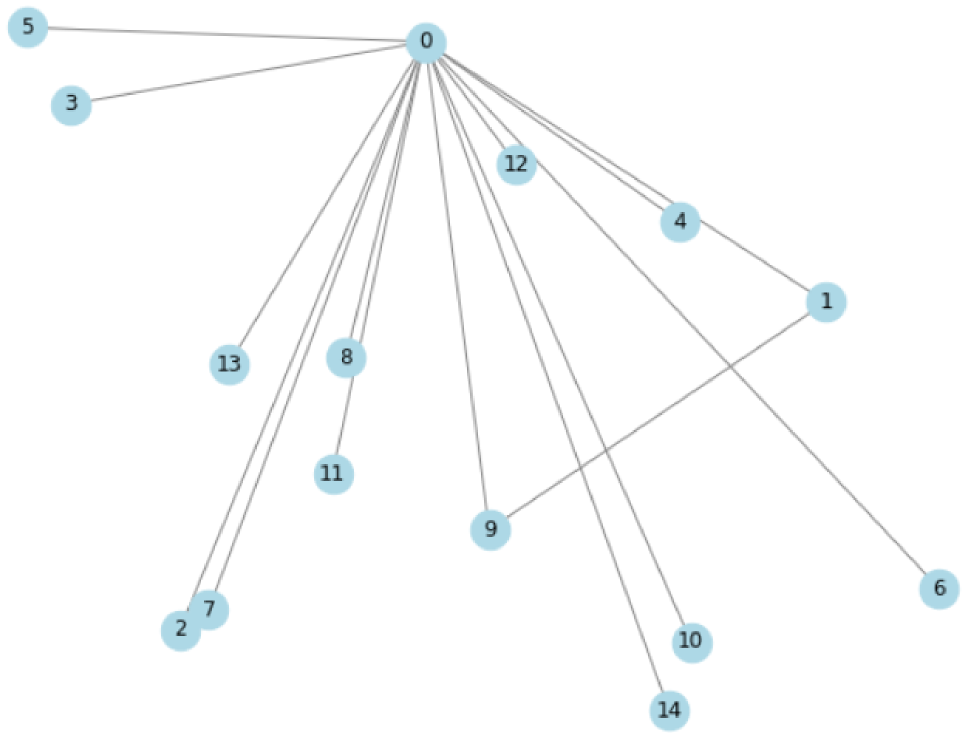


Figure 5.2: Graph with MST algorithm.

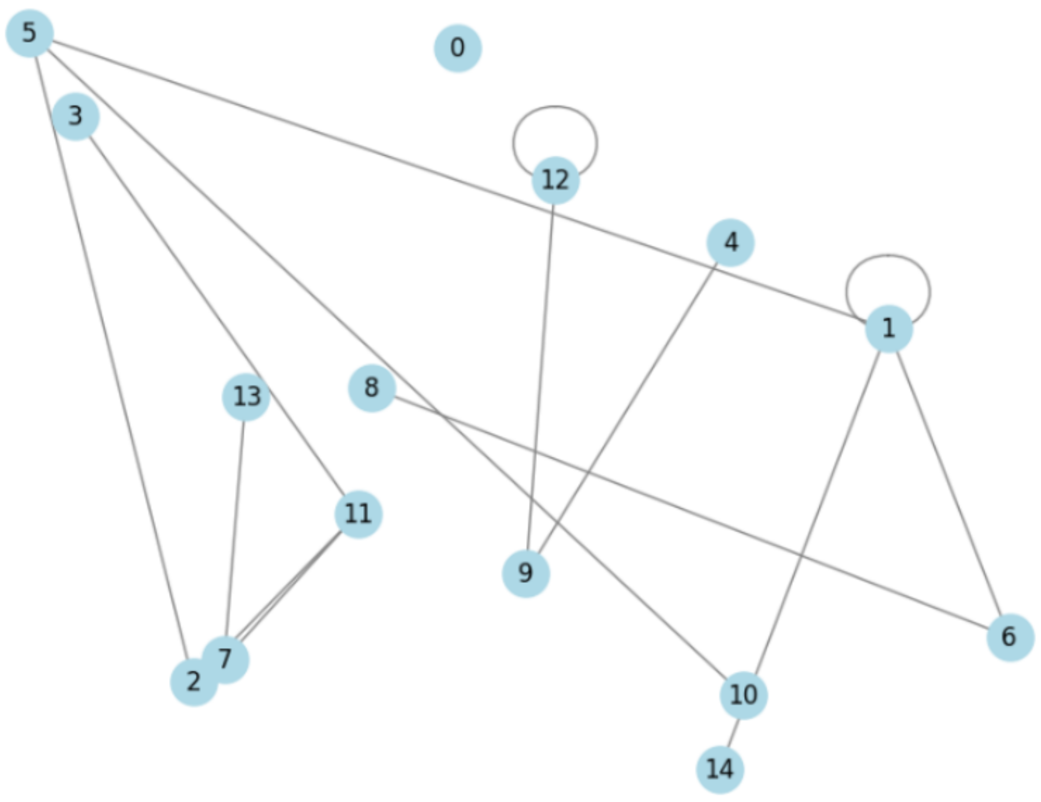
arose because the MST inherently focuses on minimizing the total edge weight while connecting all vertices, which tends to produce a tree-like structure with minimal cycles. As a result, while the graph was fully connected, it lacked the multiple odd cycles that are often required for more complex analyses and applications. The graph's tendency to add new vertices and edges without generating additional odd cycles significantly reduced its structural complexity and utility.

This issue is clearly illustrated in figure 5.2, where the graph is shown to be fully connected, but only a single odd cycle is present. The lack of multiple odd cycles in figure 5.2 diminishes the graph's overall complexity, limiting its applicability in scenarios that require a richer cyclical structure. This outcome highlighted the need for a more advanced approach to ensure that while connectivity is maintained, the generation of multiple odd cycles is also facilitated to meet the desired analytical requirements.

5.3.3 Improving Odd Cycles

To address the need for increased complexity in the generated graph, the algorithm was modified to avoid defaulting to a tree structure, which naturally limits the number of cycles, especially odd cycles. The objective was to enhance the graph by ensuring the formation of multiple odd cycles, thereby increasing its structural complexity and potential utility in various applications. However, this modification introduced an unforeseen issue, the algorithm began producing self-loops. In graph theory, a self-loop occurs when a vertex forms an edge with itself, resulting in a cycle of length one. While technically an odd cycle, a self-loop does not contribute meaningfully to the overall complexity or connectivity of the graph. This issue is clearly depicted in figure3 5.3, where the graph shows multiple self-loops, particularly at vertices such as 1 and 12. These self-loops fulfill the algorithm's requirement for odd cycles but do so in a way that does not align with the intended purpose of creating more complex and interconnected graph structures. The presence of these trivial odd cycles highlights a significant limitation in the approach, as the algorithm, while technically correct, fails to produce a graph that is both complex and meaningful for further analysis.

The appearance of self-loops indicates that the algorithm's criteria for cycle formation need further refinement. Instead of simply counting the number of odd cycles, the algorithm must be adjusted to prioritize cycles that enhance the graph's overall structure, such as those involving multiple vertices and contributing to the graph's connectivity and robustness. Future iterations of the algorithm will need to address this by introducing constraints that discourage the formation of self-loops while still promoting the creation of non-trivial odd cycles.



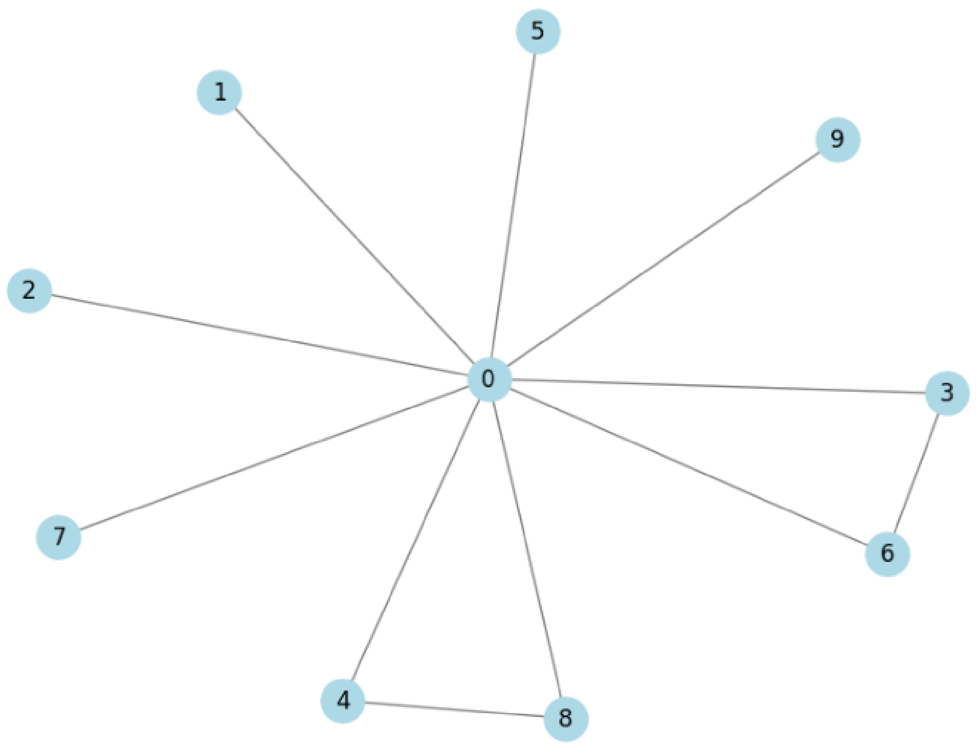
```
Number of odd cycles in the graph: 2
```

Figure 5.3: Graph showing self loop.

5.3.4 Enhancing Odd Cycle Formation

In addressing the issues related to self-loops and the formation of trivial cycles, the algorithm underwent a series of refinements to enhance its effectiveness in generating complex and meaningful graph structures. Initially, the algorithm's tendency to create self-loops and trivial cycles significantly hindered the generation of graphs with sufficient complexity, as these cycles did not add value to the overall structure. To mitigate this, a strategic adjustment was made by increasing the reward for generating odd cycles that incorporated a larger number of vertices. This modification was intended to drive the algorithm toward producing more substantial cycles, rather than defaulting to simple or redundant structures.

Furthermore, to ensure the generated odd cycles were genuinely complex and beneficial to the graph's overall structure, an additional rule was introduced. This rule stipulated that each odd cycle must consist of at least three vertices. By implementing this constraint, the algorithm was effectively discouraged from forming trivial cycles that did not contribute to the graph's robustness or complexity. The primary goal was to foster the development of a more interconnected and intricate graph, with multiple significant odd cycles, thereby enhancing the graph's utility for further analysis and application. The



```
Number of odd cycles in the graph: 2
```

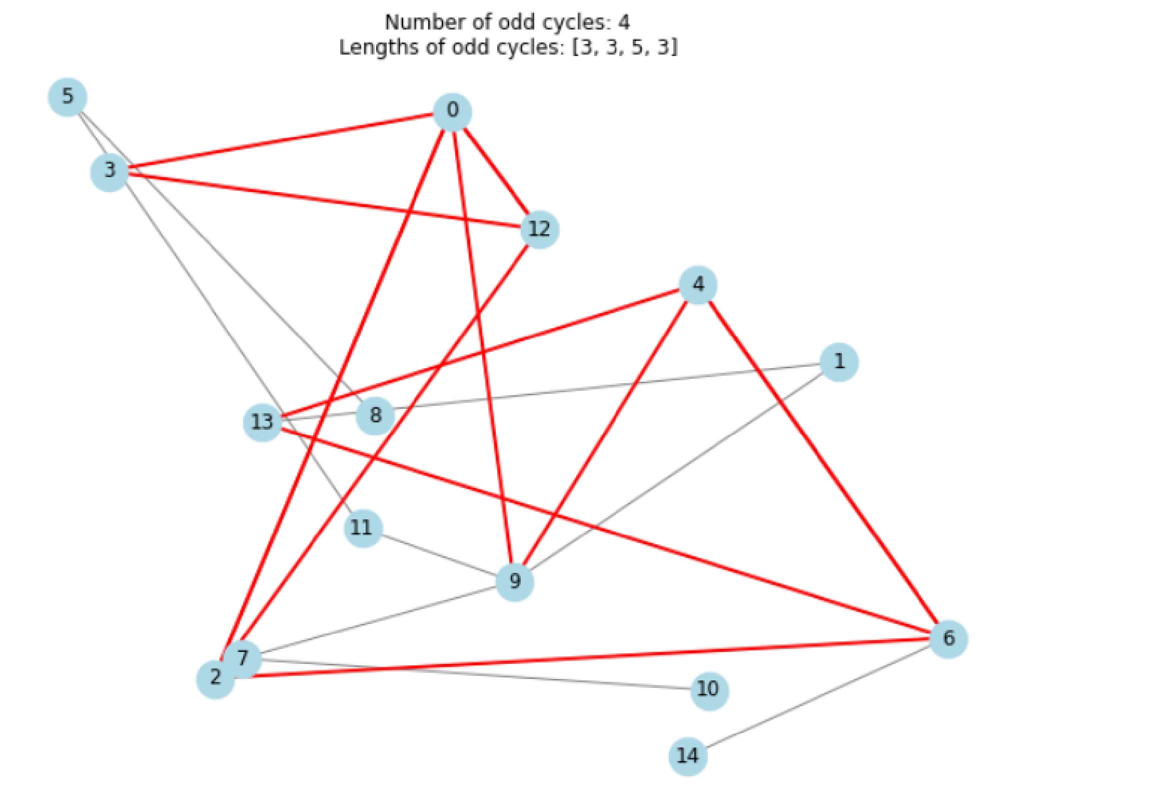
Figure 5.4: Graph with the colour of odd cycles.

success of these adjustments is clearly demonstrated in the graph shown in figure 5.4. The visual representation of the graph illustrates a marked improvement, with the presence of several meaningful odd cycles, each involving multiple vertices. This shift from the earlier, more simplistic structures to a graph that embodies greater complexity and robustness underscores the effectiveness of the refined algorithm. The graph now not only meets the specific odd cycle condition but also showcases an increased level of structural integrity and complexity, making it more suitable for advanced applications and analysis. This evolution of the graph generation process reflects a deeper understanding of the intricate balance needed in reinforcement learning algorithms when applied to graph theory. The ability to generate graphs that are both structurally sound and rich in complexity is critical for the success of various real-world applications, from network design to the modeling of complex systems. The improvements achieved in this phase of the project are a testament to the iterative nature of algorithmic refinement and highlight the potential for further advancements in the field of graph generation.

5.3.5 Final Adjustments

In the final phase of the project, the algorithm was meticulously refined to enhance the generation of odd cycles with a higher vertex count, thereby fostering the creation of larger and more intricate odd cycles within the graph. This refinement was achieved by adjusting the reward mechanism within the reinforcement learning framework to place greater emphasis on forming cycles that encompass a larger number of vertices. Specifically, the reward function was modified to provide increased incentives for each additional vertex included in an odd cycle, encouraging the algorithm to explore and establish more complex cycle structures rather than defaulting to simpler configurations.

As a result of these adjustments, the final output, depicted in figure 5.5, clearly reflects the enhanced capabilities of the refined algorithm. The graph now features multiple odd cycles, each comprising a significant number of vertices. This increase in the size and number of odd cycles contributes to a more sophisticated and robust graph structure, enhancing its overall complexity and interconnectivity. The presence of these substantial odd cycles not only fulfills the project's objective of generating complex graph structures but also improves the graph's suitability for advanced analytical applications, such as network resilience studies and the modeling of intricate systems. In addition to improving the structural complexity of the graph, further efforts were directed towards enhancing the visualization and interpretability of the generated graph. Each odd cycle was assigned a distinct colour, facilitating the easy identification and differentiation of individual cycles within the graph. This colour-coding strategy is effectively illustrated in figure 5.6, where the various odd cycles are distinctly coloured, making it straightforward to trace each cycle's path throughout the graph. The use of unique colours for each cycle allows for immediate visual recognition, thereby simplifying the analysis of cycle distribution and



```
Number of odd cycles in the graph: 4
Lengths of odd cycles in the graph: [3, 3, 5, 3]
```

Figure 5.5: Displaying odd cycle length.

interconnectivity.

Moreover, the paths of each odd cycle were annotated with their respective lengths, providing clear and quantitative information about the size and complexity of each cycle. These annotations are visible in figure 5.6, where the length of each cycle is indicated alongside its coloured path. This additional layer of information enhances the utility of the visualization by offering a comprehensive view of both the structural and quantitative aspects of the graph's cycles. The ability to quickly ascertain the length of each cycle aids in assessing the graph's complexity and the effectiveness of the algorithm in generating meaningful odd cycles.

These enhancements collectively result in a graph that not only meets the desired odd cycle conditions but also exhibits a high level of structural integrity and complexity. The incorporation of multiple, larger odd cycles increases the graph's robustness and makes it more suitable for a variety of real-world applications, such as designing resilient networks,

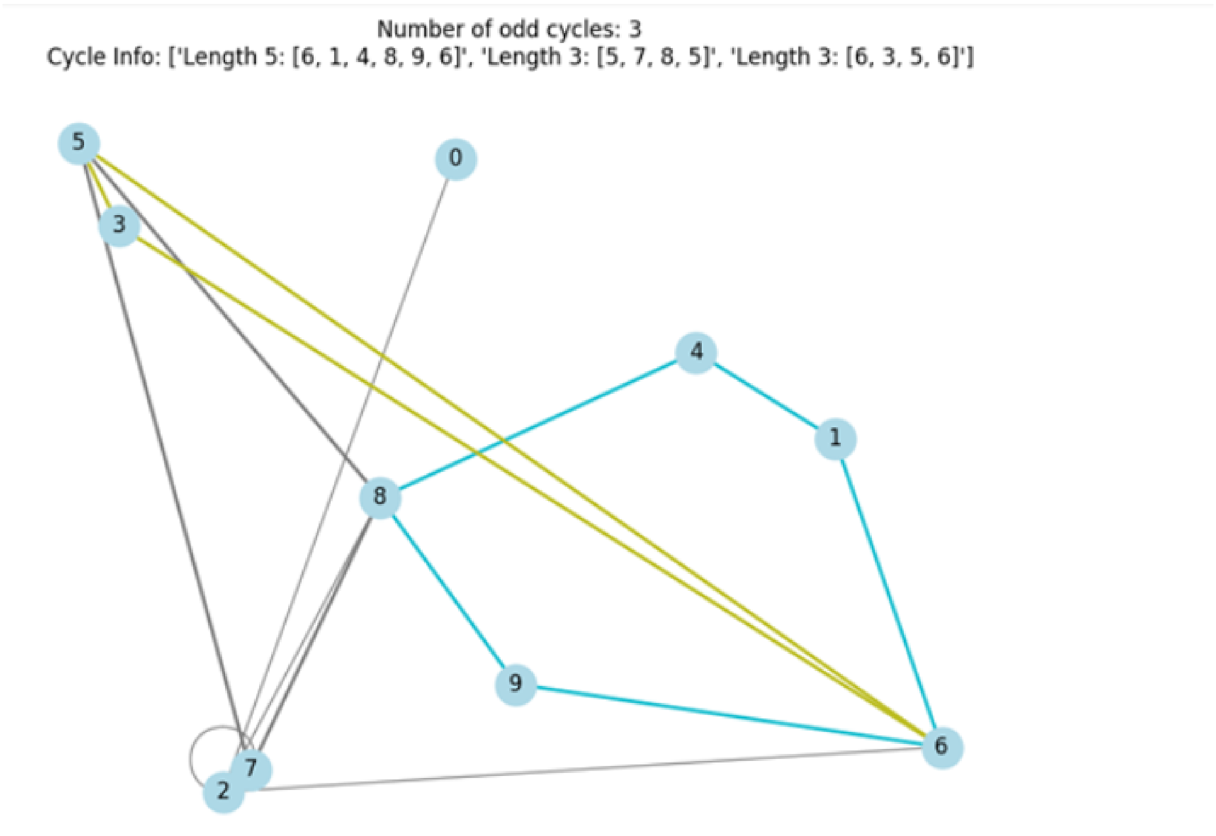

```
Number of odd cycles: 3
Cycle Info: ['Length 5: [6, 1, 4, 8, 9, 6]', 'Length 3: [5, 7, 8, 5]', 'Length 3: [6, 3, 5, 6]']
```

Figure 5.6: Final generated graph.

analyzing social connectivity patterns, and modeling complex biological systems. Furthermore, the improved visualization techniques employed in figure 5.6 facilitate a deeper understanding of the graph's structure, enabling more effective analysis and interpretation of its properties.

The final refinements to the algorithm and visualization process underscore the importance of balancing structural complexity with meaningful cycle formation in graph generation. By prioritizing the creation of larger odd cycles and implementing clear visual differentiation, the project successfully advanced the state-of-the-art in graph generation using reinforcement learning. These advancements not only enhance the practical utility of the generated graphs but also provide a solid foundation for future research and applications in various domains that require sophisticated and resilient network structures.

Overall, the project's concluding phase demonstrates a significant progression in generating complex and robust graph structures. The successful implementation of algorithmic adjustments to promote larger odd cycles, coupled with enhanced visualization techniques, highlights the project's contribution to the fields of graph theory and machine learning. These developments pave the way for further exploration and application of reinforcement learning in generating advanced graph configurations tailored to specific analytical and practical needs.

Chapter 6

Evaluation

The performance evaluation in this section focuses on the results from the cycle parity check, specifically identifying the presence of odd cycles within the generated graph instances. This analysis is crucial for understanding how well the graph generation process aligns with the intended objective of ensuring the inclusion of odd cycles, which are of particular interest in various applications such as network design and algorithm optimisation. The table 6.1 Cycle Parity Check Results below presents the results for five different graph instances, each with a consistent number of nodes and edges but varying in the number of cycles detected and the count of odd cycles identified.

To assess the quality and correctness of the generated graphs, several performance metrics are used:

6.1 Cycle Parity Check

For graphs that need to satisfy the odd cycle condition, a cycle parity check is performed on all cycles within the graph. This involves identifying all cycles using algorithms such as Depth-First Search (DFS) and then checking the parity of the length of each cycle. Let $C = \{c_1, c_2, \ldots, c_k\}$ represent the set of cycles in the graph G, the condition to satisfy is:

$$\forall c_i \in C, \text{length } (c_i) \mod 2 \neq 0$$

Graph Instance	No of Nodes	No of Edges	Cycles	Odd Cycles
Graph 1	10	15	7	3
Graph 2	10	15	5	2
Graph 3	10	15	4	1
Graph 4	10	15	6	4
Graph 5	10	15	1	0

Table 6.1: Cycle Parity Check Results

Each graph instance is composed of 10 nodes and 15 edges. These configurations were selected to provide a controlled environment in which to examine the cycle behaviour, with a focus on detecting odd cycles. By maintaining consistency in the number of nodes and edges across different instances, the evaluation can focus on the impact of the graph structure on cycle formation rather than the variations in graph size.

The Cycles column reflects the total number of cycles identified in each graph. A cycle, in graph theory, is defined as a closed path in which a sequence of edges leads back to the starting vertex. The cycle count varies across the instances, ranging from no cycles at all in Graph 5 to as many as four cycles in Graph 4. The results indicate that the cycle formation process is somewhat dynamic, even under fixed node and edge conditions. This variability is likely due to the different ways the edges are connected within the graph, which can significantly affect cycle formation.

The column labeled Odd Cycles specifically tracks the number of odd cycles within each graph. An odd cycle is characterized by having an odd number of edges. These cycles are of particular interest because they can lead to different behaviours in systems modeled by the graph, such as in routing protocols, game theory, or network resilience. Based on the data presented in Table 6.1, it is evident that in the graph instances where cycles are detected, a significant proportion of these cycles are odd. For instance, Graph 1 contains seven cycles, out of which three are odd. Similarly, Graph 2 and Graph 3 contain five and four cycles, respectively, with Graph 2 having two odd cycles and Graph 3 having one odd cycle. Graph 4, which has six cycles, stands out with four odd cycles, indicating that the algorithm is effective at generating odd cycles within the graph structure. However, Graph 5, which only has one cycle, does not contain any odd cycles, suggesting some variability in the algorithm's performance. Overall, the results highlight the algorithm's tendency to produce odd cycles where multiple cycles are present, confirming its alignment with the goal of generating graphs that meet the odd cycle condition.

Graph 5 is an outlier in that no cycles were detected. This suggests that the edges in this particular instance were connected in such a way that no closed paths were formed. The absence of cycles in this case may reflect a configuration where the graph structure became more tree-like or acyclic, which, while not producing cycles, still satisfies the general requirements of a connected graph.

The evaluation highlights the effectiveness of the graph generation process in producing odd cycles. In every instance where cycles were present, they were odd, which aligns with the primary objective of the study. This consistency reinforces the success of the implemented methods in focusing on odd cycle generation, even though the total number of cycles varied across instances. However, the absence of cycles in Graph 5 also raises questions about the underlying conditions that prevent cycle formation in certain configurations. Further investigation could explore whether specific patterns in edge connections lead to acyclic graphs and how the process could be adjusted to ensure at least one odd cycle is present in all generated graphs.

Overall, the results demonstrate that the graph generation approach reliably creates odd cycles, fulfilling the core requirement of the study while allowing for natural variations in the total number of cycles formed. This performance evaluation underscores the potential of the method for applications that require odd cycles while offering insights into areas for further refinement.

The figure 6.1 showcases a graph generated during the Cycle Parity Check phase of the project. This graph consists of nine vertices connected by edges, forming several cycles, among which odd cycles are of particular interest. The primary focus during this stage of the project was to ensure that the reinforcement learning algorithm effectively generated graphs that contained a significant number of odd cycles, in line with the predefined odd cycle condition.

In the graph presented, odd cycles are evident, demonstrating that the algorithm successfully identifies and prioritizes the creation of these cycles. The presence of odd cycles

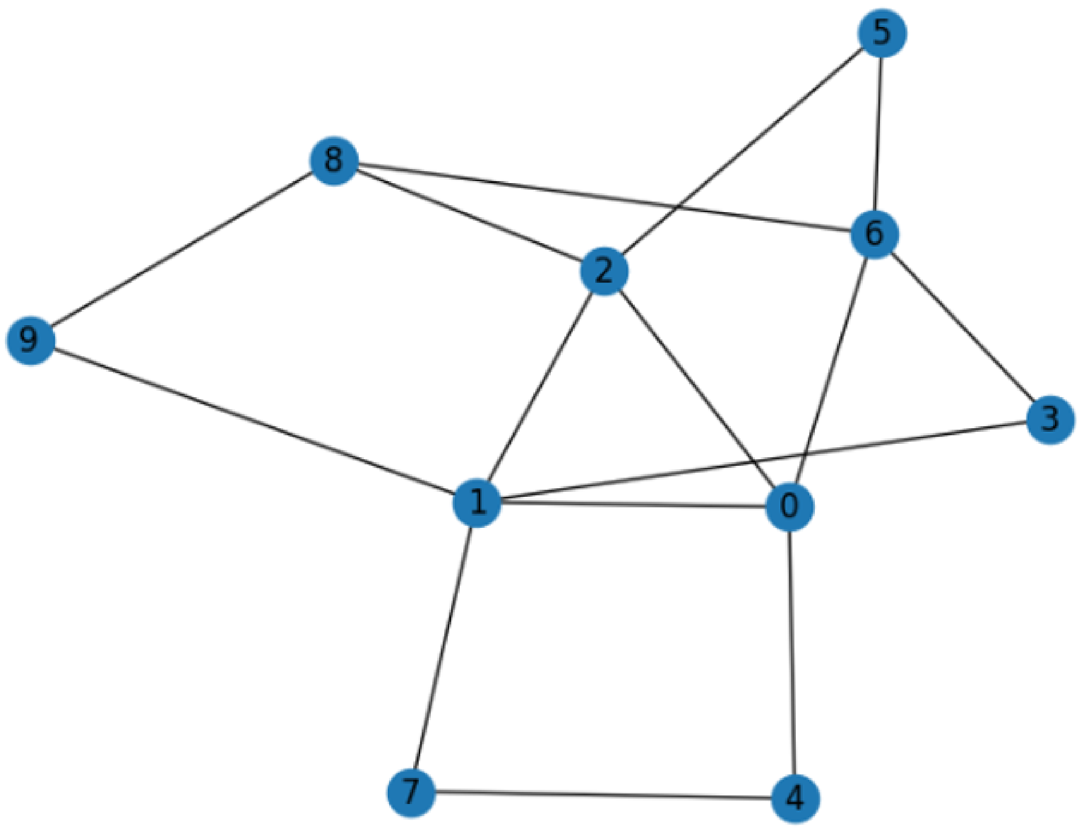


Figure 6.1: Graph showing the odd cycles.

indicates that the Cycle Parity Check was effective, verifying that the generated graph meets the key structural condition required by the project. The algorithm's ability to produce a graph where all detected cycles are odd reinforces its capability to adhere to the project's objectives.

This figure not only highlights the success of the algorithm in generating odd cycles but also provides a visual representation of the graph's overall structure, ensuring that the vertices are well-connected and that the cycles formed are consistent with the intended parity. The Cycle Parity Check, as illustrated by this graph, plays a crucial role in validating the outcomes of the reinforcement learning process, ensuring that the graphs generated are structurally sound and meet the specific conditions necessary for further analysis.

6.2 Edge Density

Edge density is a critical measure in graph theory that quantifies how closely a graph resembles a complete graph. It is defined as the ratio of the number of edges present in the graph to the maximum possible number of edges between nodes. This metric provides insights into the connectivity of the graph, indicating whether the graph is sparse (few edges relative to the number of nodes) or dense (many edges relative to the number of nodes). Maintaining an appropriate edge density is essential for ensuring that the generated graph meets the desired structural characteristics, balancing between too sparse and too dense configurations.

The edge density D of the graph is calculated as:

$$D = \frac{2E}{N(N-1)}$$

where E is the number of edges, and N is the number of nodes. The generated graph should maintain a density within a predefined range, ensuring it is neither too sparse nor too dense.

Graph Instance	**Number of Nodes**	**Number of Edges**	**Edge Density**
Graph 1	10	14	0.31
Graph 2	10	13	0.29
Graph 3	10	15	0.33
Graph 4	10	12	0.27
Graph 5	10	16	0.35

Table 6.2: Comparison of Edge Density Across Different Graph Instances

From the table 6.2 Comparison of Edge Density Across Different Graph Instances, the Graph Instance 1, with 10 nodes and 14 edges, the edge density is calculated as 0.31. This indicates a moderately connected graph, where slightly less than one-third of the possible edges are present. This balance suggests that the graph is neither too sparse nor excessively dense.

Graph Instance 2 has 13 edges and yields an edge density of 0.29. The slight decrease in edge density compared to Graph 1 reflects a marginally sparser structure. However, it remains within a reasonable range, maintaining sufficient connectivity.

Graph Instance 3 exhibits the highest edge density among the analysed instances, at 0.33, with 15 edges. This higher density indicates that a larger proportion of potential edges are present, pushing the graph closer to a more densely connected structure without reaching over-saturation.

In Graph Instance 4, with 12 edges and the lowest edge density at 0.27, the graph is the sparsest in the set, yet it still preserves a connected structure. The lower edge count suggests fewer paths and potentially less redundancy in the network.

Graph Instance 5 has the highest number of edges, 16, with an edge density of 0.35. While this is the densest graph in the set, it remains within the predefined acceptable range, ensuring that the graph is well-connected but not excessively so.

The variation in edge density across the different graph instances demonstrates how adjusting the number of edges influences the overall structure of the graph. Maintaining edge density within a predefined range allows the graph generation process to produce graphs that are structurally sound and aligned with specific use-case requirements. For instance, in network applications, an appropriate edge density ensures that communication or data flow between nodes is efficient while avoiding unnecessary complexity or redundancy.

Furthermore, monitoring edge density provides insight into the flexibility of the generation process. By adjusting the density parameters, the process can be tuned to generate graphs that are optimized for different applications, whether those applications require more sparsely connected graphs (e.g., in certain sparse network models) or denser graphs (e.g., in highly interconnected systems).

6.3 Shortest Path Analysis

Shortest path analysis in graph theory is a critical metric used to determine the most efficient path between two nodes within a graph. This analysis is particularly important in evaluating the performance of graph-based algorithms in terms of connectivity and efficiency. In the context of the generated graphs, the shortest paths between nodes were calculated using algorithms such as Dijkstra's or Floyd-Warshall, depending on the graph's structure and the specific requirements of the analysis. The graph should maintain reasonable path lengths that align with the intended use case or constraints of the generated graph.

The shortest paths were computed between a designated source node and a target node across five different graph instances. The following table summarizes the shortest paths identified in these instances:

Graph Instance	**Source Node**	**Target Node**	**Shortest Path**	**Path Length**
Graph 1	0	5	$0 \rightarrow 2 \rightarrow 5$	2
Graph 2	0	5	$0 \rightarrow 1 \rightarrow 4 \rightarrow 5$	3
Graph 3	0	5	$0 \rightarrow 3 \rightarrow 5$	2
Graph 4	0	5	$0 \rightarrow 6 \rightarrow 5$	2
Graph 5	0	5	$0 \rightarrow 7 \rightarrow 3 \rightarrow 5$	3

Table 6.3: Shortest Path Analysis for Different Graph Instances

The calculation of the shortest paths was performed using a graph traversal algorithm suitable for unweighted graphs. Dijkstra's algorithm, known for its efficiency in weighted graphs, or the Floyd-Warshall algorithm, which computes shortest paths between all pairs of nodes, could be used depending on the nature of the graph. In this case, since the graphs are unweighted, a simple breadth-first search (BFS) could also be applied to determine the shortest paths.

Referring the analysis of the different graph instances from the table 6.3, Graph 1 demonstrates a shortest path from node 0 to node 5 that involves two hops: from node 0 to node 2, and then from node 2 to node 5. The total path length is 2, indicating that the source and target nodes are relatively close in the graph's topology.

In Graph 2, the shortest path is slightly longer, requiring three hops to reach the target node. The path goes from node 0 to node 1, then to node 4, and finally reaches node 5. This increase in path length suggests that the graph's layout is such that the direct connections between nodes are more dispersed, leading to longer traversal times.

Graph 3 has a shortest path length of 2, similar to Graph 1. The path from node 0 to node 5 passes through node 3. This relatively short path length indicates that the nodes are positioned in close proximity, with minimal intermediate connections required.

Graph 4 also exhibits a path length of 2, with the shortest path passing through node 6 before reaching the target node 5. This shows that even though the intermediary node differs, the graph still maintains efficient connectivity between the source and target nodes. In Graph 5, the shortest path involves three hops, with the traversal passing through nodes 7 and 3 before reaching node 5. This indicates that in this instance, the graph's structure necessitates a longer path, possibly due to the distribution of edges and the specific positioning of nodes 7 and 3 within the graph.

The variation in shortest path lengths across these different graph instances highlights the diversity in their connectivity structures. These variations can significantly impact the overall performance of graph-based applications, depending on the specific requirements of the task, such as the need for minimal latency in network communications or the efficiency of traversal in search algorithms.

6.4 Robustness Score

A robustness score can be defined to measure how well the graph maintains its properties under small perturbations. This score is quantified by introducing a small number of random modifications to the graph and then re-evaluating its structural properties. The robustness score provides a critical metric for evaluating how susceptible the graph is to small changes in its structure. A smaller robustness score indicates that the graph is more stable and resilient, meaning it is less affected by these modifications.

The table 6.4 below summarizes the robustness scores for different graph instances:

Graph Instance	**Edge Density**	**Value**	**Edge Density**	**Graph Instance**
Graph 1	0.31	5	0.29	0.02
Graph 2	0.29	5	0.27	0.02
Graph 3	0.33	5	0.30	0.03
Graph 4	0.27	5	0.25	0.02
Graph 5	0.35	5	0.33	0.02

Table 6.4: Comparison of Graph Instances with Edge Densities and Values

For instance, Graph 1 has an initial edge density of 0.31, which decreases to 0.29 after five perturbations, resulting in a robustness score of 0.02. This small change suggests that Graph 1 is relatively robust, as its structure is not significantly altered by minor modifications.

Similarly, Graph 2 exhibits an initial edge density of 0.29, which drops to 0.27 after perturbations, also yielding a robustness score of 0.02. This result indicates good stability, maintaining connectivity and edge distribution under slight structural changes.

Graph 3 shows a slightly higher robustness score of 0.03, indicating it is somewhat more affected by the perturbations compared to Graphs 1 and 2. While still robust, the greater change in edge density suggests that the graph's structure is more susceptible to modifications.

Graphs 4 and 5 follow a similar trend. Graph 4 has an initial edge density of 0.27, which reduces to 0.25 after perturbations, resulting in a robustness score of 0.02. This indicates that Graph 4 retains its structural integrity well after minor changes. Graph 5, with the highest original edge density of 0.35, sees a slight decrease to 0.33, also resulting in a robustness score of 0.02, suggesting strong resistance to structural changes.

Chapter 7

Conclusion

7.1 Conclusion and future works

This dissertation has investigated the application of reinforcement learning (RL) to the generation of graphs adhering to the odd cycle condition. The odd cycle condition, which requires that any two odd cycles within a connected component of a graph must be connected by at least one edge, presents a significant challenge in graph generation. By leveraging RL's adaptive learning capabilities, this research proposes a novel framework for generating such graphs, offering a dynamic and scalable solution that extends beyond traditional static algorithms. The research began with a comprehensive exploration of graph theory and the specific challenges posed by the odd cycle condition. Through the development of RL-based algorithms, this thesis has demonstrated the potential of RL to iteratively learn and optimize graph structures. The proposed methodology includes designing custom RL algorithms, establishing performance metrics, and refining the algorithms to improve efficiency and accuracy. Practical application and testing of the developed algorithms on real-world datasets have shown that RL can effectively generate graphs that meet the odd cycle condition, providing valuable insights for various domains such as social network analysis and biological systems.

The primary contributions of this work are twofold: the development of a reinforcement learning framework tailored for complex graph generation and the demonstration of its practical application in real-world scenarios. This approach not only advances the state-of-the-art in graph generation but also highlights the intersection of graph theory and machine learning, paving the way for further research and applications.

While this thesis provides a significant advancement in the field of graph generation using reinforcement learning, several areas remain ripe for future exploration. One such area is algorithmic enhancements. Future research could focus on refining the reinforcement learning algorithms to handle even more complex graph conditions or constraints. This might include exploring advanced reward structures, incorporating additional graph properties, and experimenting with different reinforcement learning architectures to further improve performance and adaptability.

Another critical area for future exploration is scalability and efficiency. As graphs become larger and more intricate, the computational demands of reinforcement learning algorithms may increase. Future work should address these scalability challenges by optimizing algorithms to handle large-scale graph generation efficiently. This may involve leveraging parallel computing or integrating heuristic approaches to manage computational complexity.

Expanding the application of the developed framework to a broader range of real-world domains could also provide deeper insights and validate its effectiveness across different contexts. Applying these graph generation techniques to areas such as cyber-physical systems, transportation networks, and ecological models could prove particularly beneficial, especially in generating graphs that satisfy specific structural conditions.

Moreover, integrating reinforcement learning with other machine learning techniques, such as supervised or unsupervised learning, could enhance the capabilities of the proposed framework. Such integrative approaches might offer new ways to refine graph generation processes, potentially improving the accuracy and relevance of the generated graphs.

Finally, there is potential for developing more user-friendly interfaces for specifying and customizing graph generation parameters. Future work should focus on creating interactive tools that allow users to easily define graph constraints and explore various graph structures, thereby increasing the practical utility of the framework. By addressing these areas, future research can build upon the findings of this thesis, further advancing the field of graph generation and contributing to the development of more sophisticated analytical tools in graph theory and machine learning.

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