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RESEARCH PROJECT

BACHELOR'S THESIS

Simulation and Source Detection of Infectious Processes on Networks

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"At least I tried"

— Ann Brashares

Dedicated to the curious side of me that drives me crazy.

And to my idolized grandfather, who showered me with his fountain of knowledge.

Acknowledgements

I am grateful to Paula for her guidance throughout the entire semester. Her expertise has significantly shaped this project.

I am also thankful to my parents, who have provided emotional support throughout my bachelor studies. Their encouragement has been my foundation, and I owe them my heartfelt recognition.

Lastly, a hat tip to all the professors of the IC faculty who transmitted their knowledge and their passion for this domain.

Ahmed Abdelmalek

ABSTRACT

This project investigates the spread of infectious diseases on multiple network structures, with a dual focus on grid-based and graph-based models. At first, we implement and analyze various grid-based algorithms, then assess their performance based on specified criteria. Afterwards, we extend our analysis to more complex network models. We also analyze the differential equations for grid-based and network-based infections and access the reproduction number and the growth rate that determine if the infection dies out. We then explore some Stochastic and Probabilistic Approach using stochastic differential equations (SDEs). And we use Gillespie Algorithm to simulate our theoretical work.

Our results reveal that while homogeneous grid-based models simplify the identification of infection sources, certain complex network structures significantly enhance the traceability of these origins which offers promising strategies for more effective disease monitoring and control. Through this study, we contribute to the understanding of disease spread dynamics and the impact of network models on the detectability of infection sources.

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Chapter 1

Introduction

1.1 Background Information about the Problem

Infectious diseases have long posed significant threats to public health, necessitating the development of robust models to understand and predict their spread. Network analysis is an invaluable tool in this domain, allowing researchers to visualize and simulate how diseases propagate through different population structures. Traditional models such as Susceptible-Infected-Recovered (SIR) and Susceptible-Infected-Susceptible (SIS) have been fundamental in epidemiological studies. However, these models often fall short in capturing the complexities of real-world disease transmission, particularly when it comes to phenomena like waning immunity and recurrent infections, which are critical for understanding certain diseases such as COVID-19. As human interactions become increasingly complex, there is a pressing need to explore more sophisticated network models that can accurately represent the intricacies of disease spread in various contexts.

1.2 Main Challenges

One of the foremost challenges in this research is accurately identifying the source of an infection within a network. The diverse and intricate nature of network structures can significantly influence the propagation paths of infectious agents, making this task particularly complex. Grid-based models, while straightforward and easy to implement, often do not capture the heterogeneity of real-world interactions. Conversely, complex network models, although more realistic, pose significant computational challenges and require sophisticated algorithms for effective simulation. Balancing these two approaches and ensuring that the models accurately reflect real-world conditions are significant hurdles that this research seeks to overcome.

1.3 Thesis Statement

This project aims to investigate the spread of infectious diseases across various network structures, with a specific focus on both grid-based and graph-based models. The primary aim is to understand how these models can be used to simulate and analyze disease dynamics.

1.3.1 Introduction to the SIRS Model

The Susceptible-Infected-Recovered-Susceptible (SIRS) model, which accounts for waning immunity, is particularly applicable to diseases where immunity is not lifelong. This model rectifies the limitations of conventional epidemiological models by integrating waning immunity. This model forms the cornerstone of our study, enabling a more accurate representation of diseases where individuals can become susceptible again after a period of being recovered.

1.3.2 Approach Description

Our approach integrates simulating the spread of infectious diseases on both grid-based and graph-based models, followed by the application of our source recovery detection algorithms. We employ various centrality measures to enhance the accuracy of source identification. The goal is to achieve a clear success rate of infection source recovery over time and to understand the underlying reasons for these results. This comprehensive analysis accommodates the distinct features of each network type. The integration of multiple network models and centrality measures is essential for developing a nuanced understanding of disease spread.

The main idea of this project lies in its development of a simulation framework that adapts to various network structures, enhancing the accuracy of infection source detection. This project not only improves our theoretical understanding of network-based disease spread but also proves to be useful for assimilating all kind of source detection algorithms.

1.4 Limitations

While this study advances the understanding and implementation of network-based modeling for infectious disease spread, several limitations must be acknowledged. The algorithms employed, especially those involving centrality measures, can be computationally intensive, posing challenges when scaling up to larger networks or running extensive simulations over multiple iterations. The grid-based and network models used in this study rely on certain assumptions, such as homogeneous mixing within subpopulations and static network structures. These assumptions may not fully capture the complexities of real-world scenarios, where networks can be dynamic and heterogeneous. Additionally, the accuracy of the models heavily depends on the parameters chosen, such as infection rates (β), recovery rates (γ), and re-susceptibility rates (δ). Inaccurate estimation of these parameters can lead to significant deviations from real-world outcomes.

Boundary effects in grid-based models can significantly influence the accuracy of source detection algorithms. While wrap-around boundary conditions help mitigate some of these effects, they do not entirely eliminate the potential inaccuracies near the edges of the grid. The performance of the models, especially those employing machine learning techniques, depends on the availability and quality of historical data. In many real-world scenarios, such data may be incomplete or noisy, affecting the robustness and generalizability of the models. Although the simulation framework developed in this study shows promise, its scalability to large real-world networks and diverse epidemiological contexts remains an area for further exploration and refinement. The transition from theoretical models to practical applications involves challenges such as handling incomplete data and integrating with real-time surveillance systems. Addressing these limitations in future work will be crucial for enhancing the accuracy, and applicability of network-based models in epidemiological research.

Chapter 2

Literature Review

2.1 Evolution of Propagation Sources Identifying studies

For decades, researchers have been captivated by the challenge of identifying propagation sources within networks, a quest that extends across diverse domains, from managing disease outbreaks in biological networks to tracking the genesis of rumors across social media platforms. This introduction sets out to explore the evolutionary trajectory of methodologies used to address this pivotal challenge.

Early approaches focused on leveraging **centrality measures** within network structures, as explored by Granovetter [1]. These pioneering works investigated concepts like Degree Centrality, Closeness Centrality, Betweenness Centrality, and Eigenvector Centrality to identify influential nodes within a network. Nodes with high centrality scores were considered potential sources of propagation.

However, as network research matured, limitations of centrality measures became apparent. Researchers turned to more sophisticated approaches that incorporated information about the underlying propagation processes. Statistical methods emerged, capitalizing on the **temporal dynamics** of propagation [2, 3]. These methods exploited the fact that information typically spreads outward from the source, allowing for inferences based on the timing and directionality of propagation events.

The rise of **complex network theory** further diversified source identification methodologies. Researchers recognized the intricate structures of real-world networks, such as community structures and varying node degrees. Works by Zhou et al. [4] and Gomez-Rodriguez et al. [5] explored leveraging these features for improved source identification accuracy. Their approaches incorporated information about community memberships and node connectivity patterns to refine the search for potential sources.

The landscape continues to evolve. Recently, researchers have begun integrating **machine learning** and **data-driven techniques**. Studies by Zhao et al. [6] and Gao et al. [7] explored the use of supervised learning algorithms to predict the source of propagation events based on historical data. These methods offer promising results in specific scenarios but often require access to large datasets for effective training.

This literature review builds upon this rich history, exploring the strengths and limitations of existing methodologies for source identification in networks. By examining various approaches across different studies [8, 9, 10, 11], we aim to identify areas for improvement and pave the way for the development of more robust and adaptable source identification techniques. Ultimately, this pursuit holds significant implications for understanding and potentially controlling various processes unfolding within complex networks.

2.2 Key Findings and Insights

An extensive review by Wang et al. [8] explores a broad spectrum of centrality measures, including Degree Centrality, Closeness Centrality, Betweenness Centrality, and Eigenvector Centrality, evaluating their applicability and effectiveness for source detection within various network structures. This comprehensive analysis highlights how different centrality

measures perform in identifying the origin of propagation across diverse network types. Shelke & Attar [9] offer a structured taxonomy categorizing source detection techniques into structural, diffusion-based, and probabilistic approaches. Their methodology emphasizes the role of network features, such as topology (network structure) and dynamics (how information or disease spreads over time), in determining the accuracy of source detection, helping us understand how different techniques leverage network properties to pinpoint the source of propagation. Doe et al. [10] investigate the use of classical graph centrality measures specifically for identifying infection sources, employing a range of measures including Degree, Betweenness, Closeness, and Eigenvector Centrality to assess their performance across different network structures. This work sheds light on the variability in performance of these centrality measures depending on network characteristics, informing the selection of appropriate centrality measures for source identification within chosen network models (grid-based and graph-based). While previous studies focused on network analysis techniques, Liu et al. [11] introduce a novel approach using stochastic modeling. They propose a stochastic SIRS epidemic model incorporating logistic growth and stochastic perturbations, developing stochastic differential equations (SDEs) to model disease dynamics. By evaluating the impact of stochastic perturbations (random variations) on epidemic spread, this work highlights the inherent randomness present in real-world outbreaks.

These methodologies showcase the multifaceted approach needed for identifying propagation sources in networks, enriching the field with diverse perspectives. Several key findings emerge from these studies. Wang et al. [8] demonstrated that integrating multiple centrality measures improves source detection accuracy in networks, finding that specific combinations like Closeness Centrality and Eigenvector Centrality are particularly effective in pinpointing the origin of spread. Shelke & Attar [9] emphasized the effectiveness of structural methods for static networks, while diffusion-based methods perform better in dynamic environments. Doe et al. [10] highlighted the variability in centrality measure performance across different network structures, underscoring the need for careful selection based on network characteristics. Finally, Liu et al. [11] illustrated the significant impact of stochastic perturbations on epidemic dynamics, highlighting the role of stochasticity in shaping the long-term behavior of epidemics, affecting their persistence and stability. These findings contribute to a deeper understanding of infection source detection in networks and emphasize the complex interplay between network structure, dynamics, and stochasticity.

2.3   Limitations and Areas for Improvement

While these studies offer valuable insights, there are areas for improvement and limitations to consider. Wang et al. [8] acknowledge the need for more robust algorithms capable of handling dynamic and real-time data streams. Additionally, they highlight the importance of integrating probabilistic models to account for uncertainties inherent in network propagation. Shelke & Attar [9] provide a comprehensive framework for hybrid detection approaches, but their study lacks practical implementation details. Doe et al. [10] offer valuable insights into centrality measure performance but acknowledge limitations in real-time detection capabilities. Finally, Liu et al. [11] call for more empirical validation of their stochastic SIRS model and suggest exploring different types of stochastic perturbations.

2.4   Thesis Contributions and Impact on the Field

The methodologies and findings from the reviewed studies provide crucial guidance for this thesis, particularly in the selection of centrality measures for infection source detection. These contributions are instrumental in developing robust simulation frameworks that enhance the accuracy of infection spread models. Insights from these papers enrich the understanding of disease dynamics in networked environments.

By examining the strengths and limitations of these methods [8, 9, 10, 11], this thesis lays the groundwork for a comprehensive framework for source identification within the context of our research project. The core of this project focuses on investigating disease spread across different network structures. By integrating established centrality measures with potentially more nuanced approaches, the aim is to develop a robust framework for source identification within both grid-based and graph-based network models.

This project contributes to the field by understanding the interplay between network structure and source identification. Leveraging a combination of established and tailored methods aims to achieve a higher success rate in pinpointing infection sources compared to existing approaches that rely on singular techniques. The comparative study across grid-based and graph-based models will illuminate how network characteristics influence the effectiveness of different source identification algorithms. This knowledge will contribute to developing more adaptable frameworks that can be tailored to specific network types.

Chapter 3

Mathematical Modeling

Understanding the spread of infectious diseases in complex networks is critical for effective epidemic control [14, 26]. Network theory provides valuable insights into how diseases propagate through populations [17], and centrality measures play a crucial role in identifying influential spreaders and potential epidemic sources [5].

This chapter provides the foundational knowledge necessary for modeling infectious diseases, focusing on one key model: **SIRS**. We will discuss the differential equations governing this model and methods to quantify the speed of infection.

3.1 Mathematical Modeling of an SIRS process

Infectious diseases can be modeled using differential equations that describe the changes in the number of susceptible (S), infected (I), and recovered (R) individuals over time.

The SIRS model includes a return to susceptibility after recovery, accounting for waning immunity. The compartments are:

- **Susceptible (S):** Individuals who can contract the disease.

- **Infected (I):** Individuals who have contracted the disease and can transmit it.

- **Recovered (R):** Individuals who have recovered from the disease but can become susceptible again.

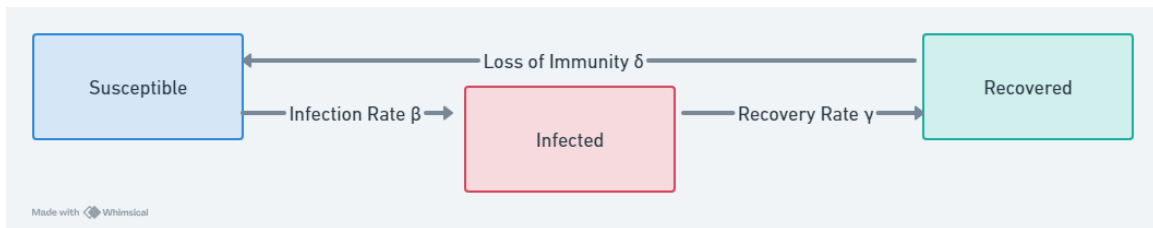Figure 3.1: SIRS model dynamics

The differential equations for the SIRS model are [27, 28]:

$$\frac{dS}{dt} = \delta R - \beta S I, \tag{3.1}$$

$$\frac{dI}{dt} = \beta S I - \gamma I, \tag{3.2}$$

$$\frac{dR}{dt} = \gamma I - \delta R, \tag{3.3}$$

where β is the infection rate, γ is the recovery rate, and δ is the rate at which recovered individuals become susceptible again.

To capture the inherent randomness in disease spread, the stochastic version of the model can be represented using stochastic differential equations (SDEs) [11, 12]:

$$dS = (\delta R - \beta SI)\, dt + \sigma_S S\, dW_S, \tag{3.4}$$

$$dI = (\beta SI - \gamma I)\, dt + \sigma_I I\, dW_I, \tag{3.5}$$

$$dR = (\gamma I - \delta R)\, dt + \sigma_R R\, dW_R, \tag{3.6}$$

Here, dW_S, dW_I, and dW_R are increments of independent Wiener processes representing random fluctuations in the susceptible, infected, and recovered populations, respectively. The terms σ_S, σ_I, and σ_R denote the intensities of these fluctuations.

Explanation of Terms:

- **Wiener Processes:** dW_S, dW_I, and dW_R are continuous-time stochastic processes with the following properties:
    - $E[dW_t] = 0$
    - $E[dW_t^2] = dt$

- **Noise Intensities:** The parameters σ_S, σ_I, and σ_R control the amplitude of the stochastic perturbations. Larger values indicate stronger random effects.

3.1.1 Speed of Infection

Quantifying the speed of infection involves understanding how quickly the disease spreads through a population. This can be achieved using the basic reproduction number (R_0) and growth rate (λ), as well as a probabilistic approach using the binomial distribution.

Basic Reproduction Number (R_0): R_0 is defined as the average number of secondary infections produced by a single infected individual in a fully susceptible population. It is given by:

$$R_0 = \frac{\beta}{\gamma} \tag{3.7}$$

R_0 indicates whether the infection will spread ($R_0 > 1$) or die out ($R_0 \leq 1$).

Growth Rate (λ): The growth rate λ quantifies the rate of change of the infected population: The deterministic growth rate is given by:

$$\lambda_{\text{det}} = \beta S_0 - \gamma$$

The stochastic growth rate incorporates noise intensities:

$$\lambda_{\text{stoch}} = \beta S_0 - \left(\gamma + \frac{\sigma^2}{2}\right)$$

where σ^2 is the combined variance of the noise terms affecting the susceptible, infected, and recovered compartments. Specifically, $\sigma^2 = \sigma_S^2 + \sigma_I^2 + \sigma_R^2$ and S_0 is the initial number of susceptible individuals.

Infection Models on Grids

Grid-based models are fundamental in studying the spread of infectious diseases due to their simplicity and structured layout. In these models, the population is represented as nodes in a grid, where each node can be in one of several states: susceptible, infected, or recovered. The disease spreads to neighboring nodes based on defined rules, which makes the grid model particularly suitable for capturing local interactions and spatial dynamics of infection.

In grid-based models, the infection spreads according to specific rules:

- A susceptible node becomes infected with probability β if it has one or more infected neighbors.

- An infected node recovers with probability γ.

- A recovered node can become susceptible again with probability δ.

This structured interaction makes grid-based models ideal for exploring the dynamics of infection spread, especially in scenarios where spatial factors play a significant role.

Probability and Binomial Distribution Approach

In a grid-based network, the speed of infection can be estimated using probability. The infection probability β and the number of nodes n along the shortest path are crucial factors. **Binomial Distribution Approach:** Consider a grid where the probability of infection transmission between neighbors is β. The expected number of infected nodes at distance k can be modeled with a binomial distribution:

$$P(X = k) = \binom{n}{k} \beta^k (1-\beta)^{n-k} \tag{3.8}$$

Conclusions from the Probability and Binomial Distribution Approach: The binomial distribution approach provides an upper bound on the speed of infection spread in a grid-based model. By calculating the expected number of infected nodes at each distance, we can estimate the maximum potential spread of the infection over time. This approach highlights the importance of the infection probability β. Higher values of β significantly increase the likelihood of infection spread, which underscores the critical role of infection control measures in reducing β. Lastly, this approach provides a foundation for comparing different grid configurations or network structures. By analyzing how changes in network topology affect the binomial distribution of infection spread, we can gain insights into the resilience and vulnerability of different network designs.

3.2 Conclusion

This chapter has provided a comprehensive overview of the mathematical models used to study infectious disease spread, with a focus on the SIRS model. We discussed the differential equations governing these models and methods to quantify the speed of infection using both reproduction number and probabilistic approaches. These foundational concepts are crucial for understanding the dynamics of disease transmission and will inform the subsequent research and analyses in this thesis.

Chapter 4

Proposed Work

The study aims to explore both grid-based algorithms and more complex network models, focusing on understanding disease spread dynamics and improving the traceability of infection sources.

4.1 Grid-Based Models

Grid-based models are fundamental in epidemiological studies due to their simplicity and structured nature. These models represent the population as nodes in a grid, where each node can be in one of several states: susceptible, infected, or recovered. The spread of disease is simulated by allowing the infection to propagate from one node to its neighboring nodes.

The infection probabilities on neighbors in a grid-based model were discussed in detail in the Mathematical Modeling chapter along with the interaction rules (Section 3.1.1).

Moreover, boundary conditions are crucial in grid-based models as they influence the spread of infection, especially at the edges of the grid. There are two primary types of boundary conditions:

- **Fixed Boundary:** In a fixed boundary grid, nodes at the edges have fewer neighbors compared to nodes in the interior. This can create edge effects where the infection dynamics at the boundaries differ significantly from those in the central region.

- **Wrap-Around Boundary (Toroidal Grid):** In a wrap-around grid, the edges are connected in such a way that the grid forms a torus. This means that nodes at the edges are connected to nodes on the opposite edge, eliminating boundary effects and creating a uniform infection spread throughout the grid.

The structure and configuration of the grid, along with the interaction rules, determine how the infection spreads. In our project, the grid is configured as a square lattice where each node has up to four neighbors (north, south, east, west).

Note that grid-based models provide a foundational approach to studying the spread of infectious diseases. By carefully considering infection probabilities, boundary conditions, and interaction rules, these models can offer valuable insights into the dynamics of disease transmission and the effectiveness of various intervention strategies.

4.1.1 Algorithm Selection

Three primary algorithms were selected for their distinct approaches and potential effectiveness in source identification within grid-based models:

1. Jordan Center Identification using BFS

2. Euclidean Distance Minimization

3. Center of Mass Identification

4.1.2 Performance Metrics

The performance of the selected algorithms is evaluated based on the following criteria:

1. Accuracy

2. Complexity

3. Handling Boundaries

4.2 Complex Network Models

The exploration of complex network models is essential for a comprehensive understanding of disease spread dynamics in real-world scenarios. Unlike grid-based models, complex networks exhibit diverse structures and connectivity patterns, which can significantly influence the spread of infections.

4.2.1 Network Types

Erdős–Rényi Graphs

Erdős–Rényi graphs are characterized by having a fixed number of nodes where each pair of nodes is connected with a fixed probability. They are useful for modeling random connections in a network, providing a basis for understanding the impact of randomness on disease spread.

Random Regular Graphs

Random Regular graphs consist of nodes each with the same number of connections (degree), ensuring uniformity in node connectivity. They help in examining disease spread in networks with uniform connectivity, highlighting the effect of equal distribution of contacts.

Random Geometric Graphs

Random Geometric graphs are constructed by placing nodes randomly in a geometric space and connecting nodes that are within a certain distance from each other. They simulate spatial networks, making them suitable for studying geographic constraints on the spread of infections.

4.2.2 Algorithm Selection

For the analysis of infection spread on complex networks, several algorithms were selected based on their effectiveness in identifying the source of infection:

1. Jordan Center Identification

2. Eccentricity and Closeness Centrality

3. Betweenness Centrality

4. Eigenvector Centrality

5. Closeness Centrality

4.2.3 Performance Metrics

The performance of the algorithms on complex networks is measured based on the following criteria:

1. Accuracy: The precision of the algorithm in correctly identifying the source of infection.

2. Scalability: The ability of the algorithm to handle increasing network sizes effectively.

4.3   Stochastic Approach: Stochastic Differential Equations (SDEs)

We employed stochastic differential equations to introduce randomness into the infection spread models. They allow for the incorporation of stochastic variations and uncertainties in the transmission process. The Gillespie Algorithm will be employed to simulate the stochastic models. This algorithm is particularly suitable for simulating the time evolution of systems with random events, such as the spread of infectious diseases. We'll then compare the stochastic approach to the deterministic approach.

4.4   Conclusion

This chapter has outlined the proposed work, detailing the objectives and expected outcomes of the research. The focus is on comparing grid-based algorithms and complex network models to enhance the understanding of disease spread dynamics.

In the next chapter, we will detail the design and implementation of the models and algorithms used in this study.

Chapter 5

Project Design

This chapter details the design and implementation of the models and algorithms used in this study. The goal is to simulate the spread of infectious diseases on different network structures and apply source detection algorithms to identify the origins of the infection. The design choices, methodologies, and tools used in this study are discussed comprehensively.

5.1 Model Structures and Algorithm Implementation

5.1.1 Grid-based models

The spread of disease in grid-based models is simulated by allowing the infection to propagate from one node to its neighboring nodes. The infection probabilities on neighbors in a grid-based model were discussed in detail in the Mathematical Modeling chapter along with the interaction rules in Section 3.1.1.

The structure of the grid-based model and the importance of boundary conditions were previously outlined in Section 4.1. To summarize, the boundaries of the grid significantly affect the spread dynamics. Fixed boundaries can limit the spread, while periodic boundaries simulate an infinite plane by wrapping around edges, allowing the infection to propagate without edge effects.

Equilibrium State in Grid-Based Models

An equilibrium state in a grid-based model is reached when the number of individuals in each state (susceptible, infected, recovered) stabilizes and no longer changes significantly over time. This state indicates a balance between the rates of infection, recovery, and return to susceptibility. Understanding the equilibrium state helps in predicting the long-term behavior of the disease spread and in designing effective intervention strategies.
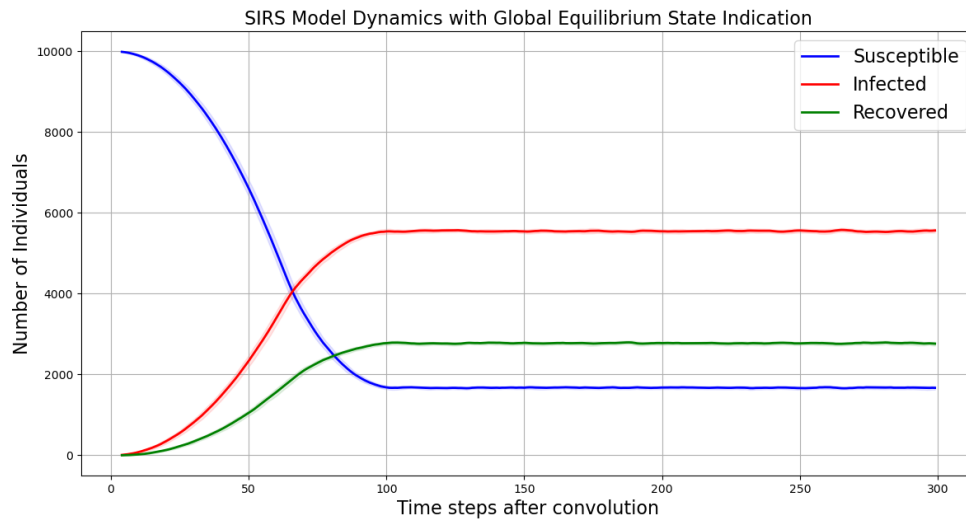
Figure 5.1: SIRS Model Dynamics and Equilibrium State

Figure 5.1 shows the dynamics of the SIRS model reaching an equilibrium state. Initially, the number of susceptible individuals (blue) decreases as the infection spreads, while the number of infected (red) and recovered (green) individuals increase. Over time, the system stabilizes, and the number of individuals in each state remains constant, indicating that the model has reached an equilibrium.

Impact of Initial Infection Sources

The initial number and location of infected nodes significantly impact the disease spread dynamics. Multiple initial infection sources can lead to a rapid spread and a higher initial peak of infected individuals, as the infection can propagate from several points simultaneously. Conversely, a single initial infection source typically results in a slower spread and a delayed peak.
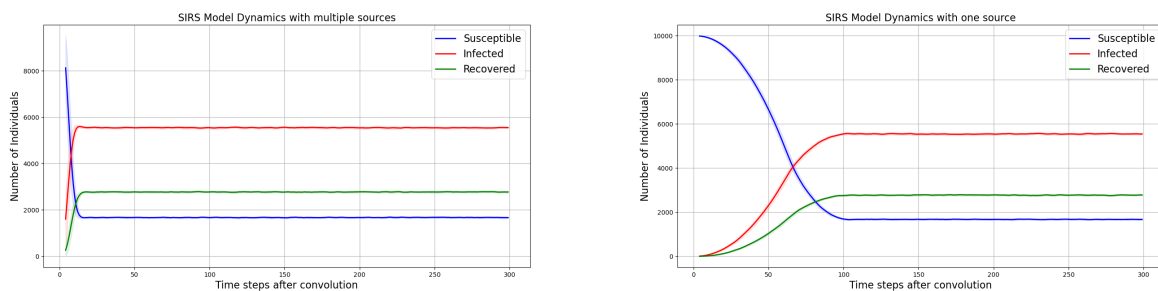
Figure 5.2: Impact of Initial Infection Sources on Disease Spread

Figure 5.2 illustrates the difference in disease spread dynamics between multiple and single initial infection sources. In the left panel, with multiple sources, the number of infected nodes rises sharply and then stabilizes as the disease quickly reaches an equilibrium. In the right panel, with a single source, the infection spreads more slowly, taking longer to reach the peak and stabilize.

By analyzing these dynamics, we can better understand how initial conditions affect the spread and control of infectious diseases in grid-based models. This understanding is essential for designing effective intervention strategies and predicting the outcomes of different epidemic scenarios.

Comprehensive Insight into Grid-Based Models

Grid-based models offer a controlled environment to study the spread of infectious diseases. By manipulating parameters such as infection probability, recovery rate, and initial infection sources, researchers can gain insights into the disease dynamics and the effectiveness of various intervention strategies. These models also provide a basis for comparing different algorithms for infection source detection, as discussed in the subsequent sections of this chapter.

Source Detection Algorithms

For source detection within the grid-based model, we implemented three primary algorithms: Jordan Center Identification using Breadth-First Search (BFS), Euclidean Distance Minimization, and Center of Mass Identification. These algorithms were evaluated based on their accuracy, complexity, and ability to handle boundary conditions.

Accuracy: The accuracy of each algorithm was measured by its ability to correctly identify the infection source within the grid. This was quantified by running multiple simulations (400 different grids each step) and recording the percentage of times the algorithm correctly identified the actual source. Higher accuracy indicates a more reliable algorithm for source detection.

Complexity: Complexity was evaluated based on the computational resources required by each algorithm, particularly focusing on time complexity. The Jordan Center Identification algorithm, using BFS, typically has a higher time complexity due to the exhaustive search required to compute the centrality scores for all candidate nodes. In contrast, the Center of Mass algorithm is computationally simpler as it only involves calculating the mean position of the external boundary nodes.

Boundary Handling: Boundary handling refers to the algorithm's ability to effectively manage the edges of the grid, where interactions may be limited or different from the interior. Algorithms that consider wrap-around boundaries or effectively account for fixed boundaries were rated higher in this metric. The performance in boundary handling was assessed by comparing the accuracy of each algorithm in grids with different boundary conditions (fixed and wrap-around).

The **Jordan Center algorithm** employs a Breadth-First Search (BFS) approach to identify the central node that minimizes the maximum distance to all other nodes. This method calculates the centrality score for each candidate node, selecting the node with the highest score as the source. The detailed implementation of this algorithm is presented in the Implementation chapter.

The next figures illustrate the performance of the Jordan Center algorithm in different grid configurations. The titles of the figures, such as "source_recovery_30_70_fixed_grid," indicate that the true source node used in the algorithm is located at (30, 70) and that the grid has fixed boundaries. These images represent the results of running the source location algorithm on 400 different grids at each time step, with each grid being a 100x100 grid.
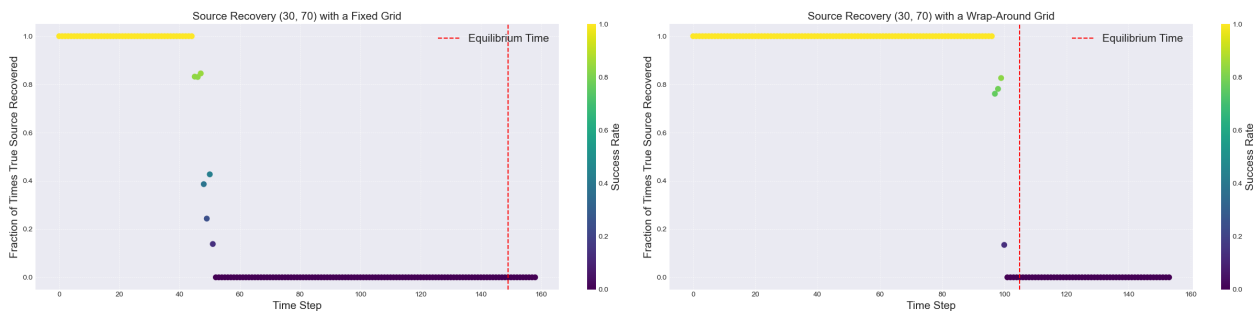

Figure 5.3: Source Recovery at (30, 70) with Jordan Center Algorithm on Fixed Grid (Left) and Wrap-Around Grid (Right)

Figure 5.3 shows the performance of the Jordan Center algorithm in both fixed boundary and wrap-around grid configurations. In the fixed boundary grid (left), the accuracy of source recovery decreases significantly as the infection reaches the boundaries. This is because edge nodes have fewer neighbors, which skews the centrality calculations, leading to less accurate source detection. In contrast, the wrap-around grid configuration (right) maintains high accuracy due to consistent node behavior across the grid. The wrap-around boundaries eliminate the edge effects seen in fixed boundary grids, allowing for more accurate centrality measurements and, consequently, more precise source detection.
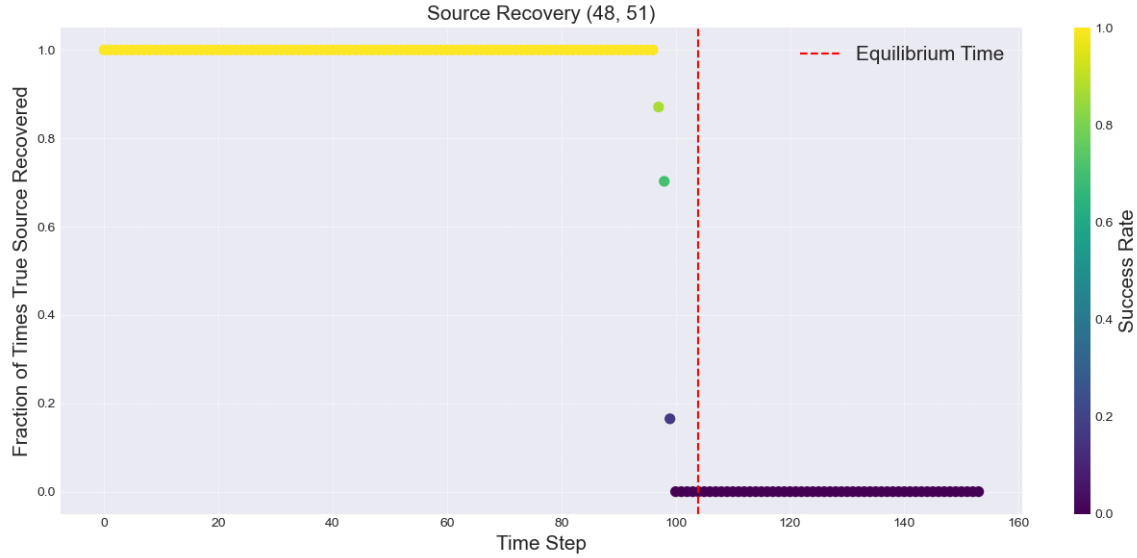

Figure 5.4: Source Recovery (48, 51) with Jordan Center Algorithm

Figure 5.4 demonstrates the high effectiveness of the Jordan Center algorithm when detecting the source at central nodes. The symmetric conditions in the center of the grid favor accurate source detection due to the uniform connectivity of nodes.

The **Jordan Center algorithm** performs exceptionally well in wrap-around grid configurations due to the consistent node behavior across the grid. This consistency allows for accurate centrality measurements, resulting in high source recovery accuracy. However, in fixed boundary grids, the algorithm's performance deteriorates as the infection reaches the boundaries. This analysis provides critical insights into selecting and adapting source detection algorithms based on the grid configuration and boundary conditions in epidemiological models.

We then explored the **Center of Mass Algorithm** for source detection. The Center of Mass algorithm calculates the mean position of all infected nodes and designates this point as the source of the infection. While this method is computationally efficient, it has limitations in terms of accuracy, particularly near the boundaries of the grid.

Initially, we applied the Center of Mass algorithm to detect the source node using the regular method. The results are depicted in Figure 5.5, which shows a poor recovery of the source node.
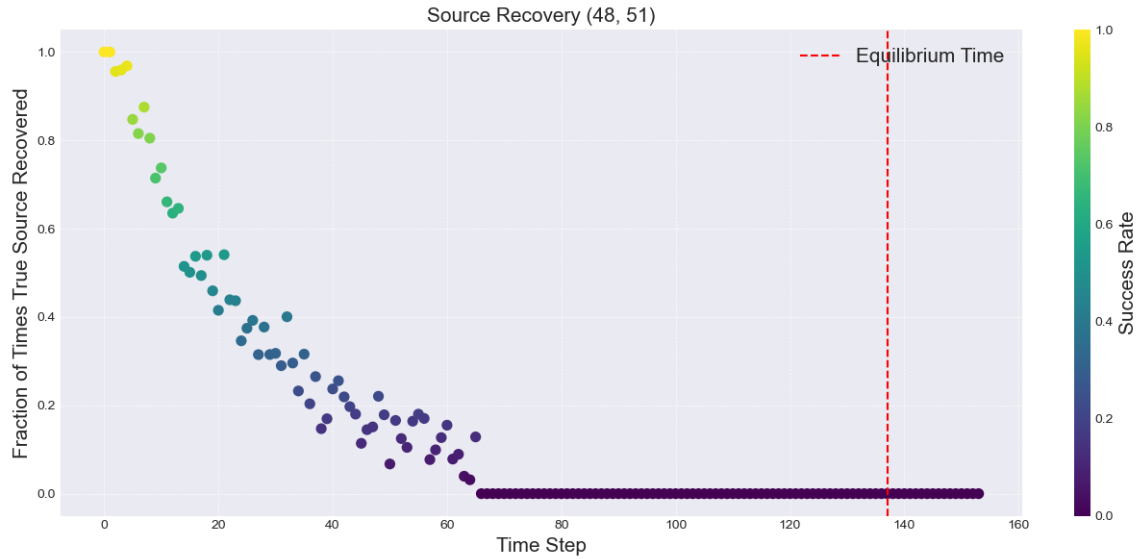
Figure 5.5: Source Recovery (48, 51) with Center of Mass Algorithm

Upon analyzing the distance error between the true source node and the recovered one, we observed that the error distance was usually small, especially in the initial stages of the infection spread. To better understand this, we plotted the distance error between the predicted source and the true source over time, as depicted in Figure 5.6. This analysis shows that the distance error remains relatively small in the initial stages of infection spread, justifying the one-node error margin approximation.
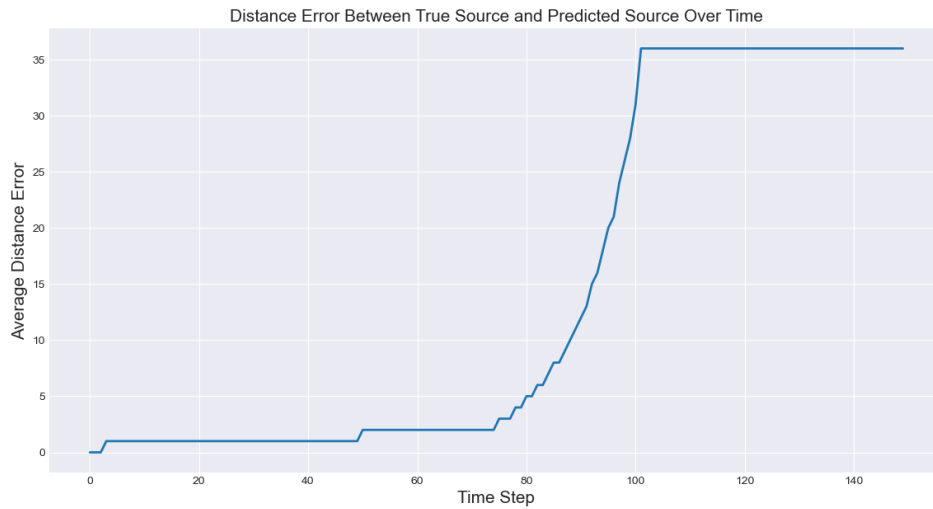
Figure 5.6: Distance Error Between True Source and Predicted Source Over Time with Center of Mass Algorithm

Given the proximity of the recovered nodes to the true source, we considered an approximation approach, allowing for a *one-node error margin*. This means that if the true source node is a neighbor of the recovered source node, it is considered a successful recovery. When we applied this approximation, the source recovery improved significantly, as shown in Figure 5.7.

Figure 5.7: Approximate Source Recovery (48, 51) with Center of Mass Algorithm allowing one-node error

However, the Center of Mass algorithm's performance near the boundaries remained poor, regardless of whether the grid had wrap-around or fixed boundaries. This is illustrated in Figure 5.8, where the handling of boundary conditions showed poor performance.
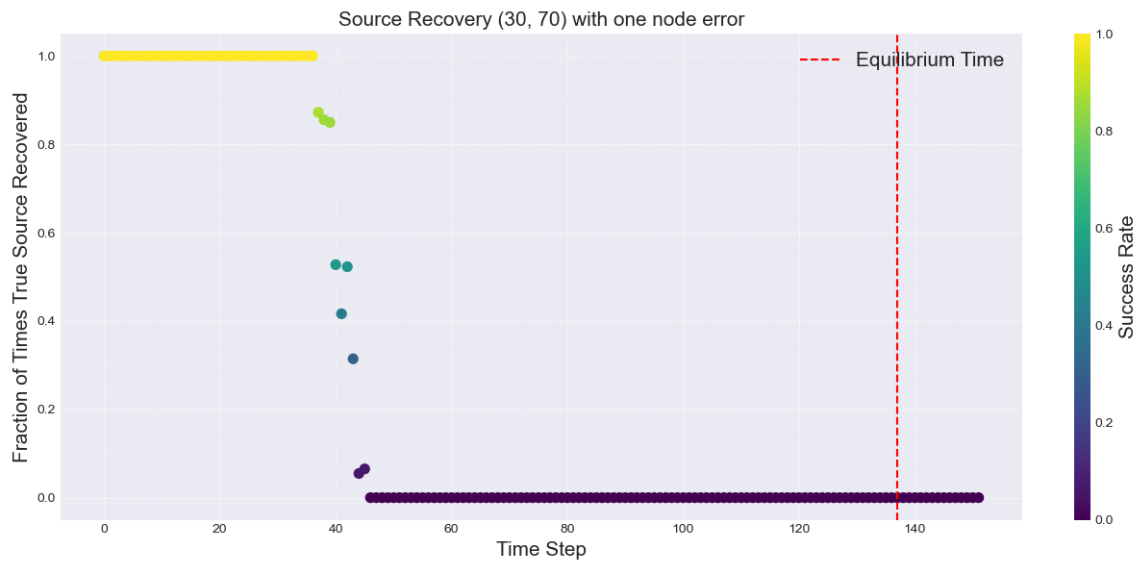
Figure 5.8: Approximate Source Recovery (30, 70) with Center of Mass Algorithm allowing one-node error

While the Center of Mass algorithm is computationally efficient, its accuracy is limited, particularly near grid boundaries. By considering a one-node error margin, we can improve the recovery accuracy, but the method still faces challenges in boundary conditions. These findings highlight the importance of adapting source detection algorithms to the specific characteristics and constraints of the grid configuration.

Next, we examined the **Distance Analysis Algorithm**, utilizing Manhattan or Euclidean Distance to identify the source of infection. The algorithm determines the node whose cumulative distance to all infected nodes is minimized. This method, while computationally efficient, suffers from inaccuracies near boundaries.

Initially, the Distance Analysis algorithm demonstrated significant errors in identifying the exact source node. However, when we considered the approximate approach, allowing for a *one-node error margin*, the performance improved markedly. Figure 5.9 show the results for the central node scenario, indicating better recovery rates with the one-node

error margin.

Figure 5.9: (Left) Source Recovery (30, 70) with Distance Analysis Algorithm without one-node error margin. (Right) Approximate Source Recovery (48, 51) with Distance Analysis Algorithm allowing one-node error

In boundary conditions, the Distance Analysis algorithm performed poorly, as illustrated in Figure 5.10. The accuracy significantly drops when the infection reaches the boundaries, indicating a loss of critical information for source detection.
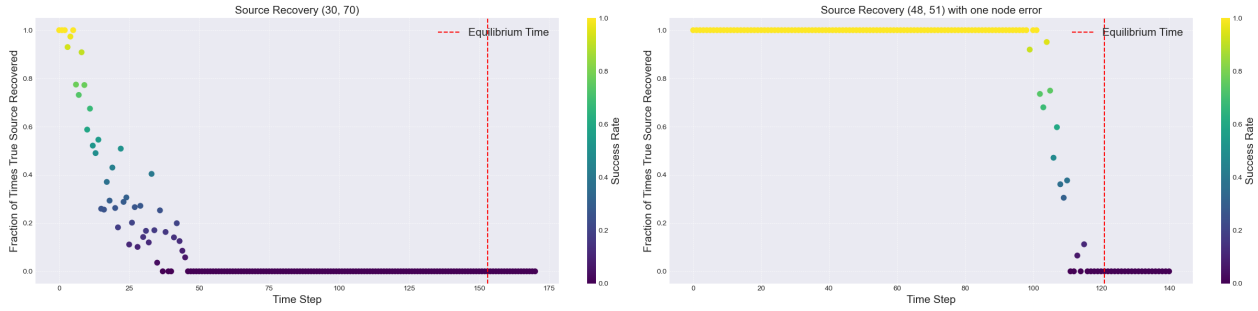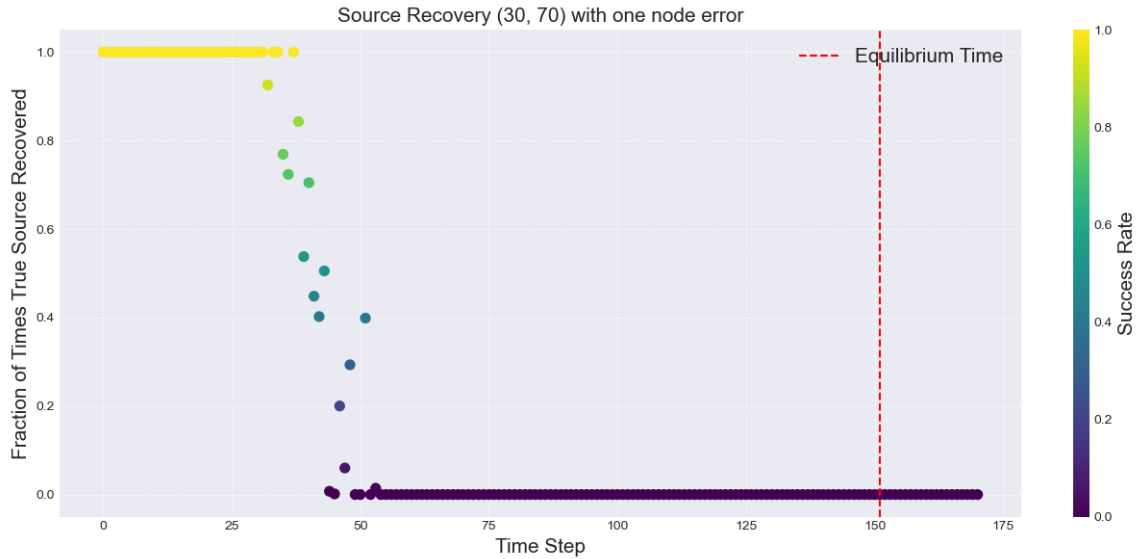

Figure 5.10: Approximate Source Recovery (30, 70) with Distance Analysis Algorithm allowing one-node error

Upon comparing the three algorithms, the Jordan Center algorithm consistently demonstrated the highest accuracy in source detection, particularly in wrap-around grid configurations. This can be attributed to its ability to handle uniform connectivity across the grid, which is not affected by boundary conditions. The Center of Mass and the Distance Analysis algorithms, while computationally efficient, showed limitations in accuracy, especially near grid boundaries. The one-node error margin approach significantly improved their performances, making them a viable option for quick approximations.

In summary, the grid-based algorithms implemented in this study provided valuable insights into the effectiveness of different approaches for source detection in epidemiological models. The Jordan Center algorithm emerged as the most accurate, especially in wrap-around grid configurations, making it suitable for both grid-based and complex network models. The Center of Mass and Distance Analysis algorithms, while less accurate, offered computational efficiency and improved performance with the one-node error margin approach.

Moving forward, we will explore the application of these algorithms to complex network models to further enhance our understanding of disease spread dynamics and improve the traceability of infection sources.

5.1.2 Centrality Measures in Complex Network Models

We move on now to complex network models, which are crucial for a comprehensive understanding of disease spread dynamics in real-world scenarios. Unlike grid-based models, complex networks exhibit diverse structures and connectivity patterns that significantly influence the spread of infections. We used several types of complex networks, including Erdős–Rényi graphs, Random Regular graphs, and Random Geometric graphs. These network types are illustrated in Figure 5.11.

(a) Erdős–Rényi Graph   (b) Random Regular Graph   (c) Random Geometric Graph
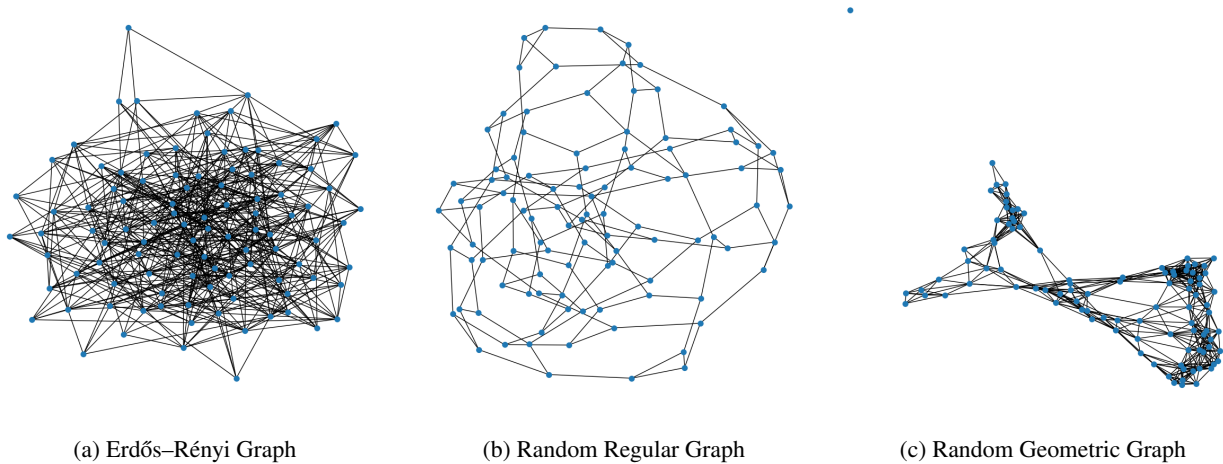
Figure 5.11: Examples of Complex Network Structures

We chose these networks due to their varying structural properties. Erdős–Rényi graphs are simple random graphs where each edge is included with a fixed probability. Random Regular graphs have a fixed degree for each node, ensuring uniform connectivity. Random Geometric graphs represent spatial networks where nodes are connected if they are within a certain distance, introducing heterogeneity in node degrees.

To enhance source detection in these complex networks, we employed various centrality measures [12]:

1. **Eccentricity + Closeness Centrality:** This combined measure uses both eccentricity and closeness scores to identify central nodes.

2. **Eccentricity:** Defined as the greatest distance between a node and any other node in the network, used to find the "central" node [17].

3. **Betweenness Centrality:** Measures the extent to which a node lies on the shortest paths between other nodes, highlighting nodes critical for the flow of infection [15].

4. **Eigenvector Centrality:** Assigns relative scores to all nodes based on the principle that connections to high-scoring nodes contribute more to a node's score.

5. **Closeness Centrality:** Measures the average length of the shortest path from a node to all other nodes in the network, indicating how quickly information spreads from a given node to others.

The implementation of these centrality measures was integrated into the network simulation, and their performance was tested on various network structures. The evaluation criteria included accuracy and time complexity under varying network conditions and infection parameters.

Figure 5.12 from Jiang et al. [12] provides a comprehensive illustration of these centrality measures.
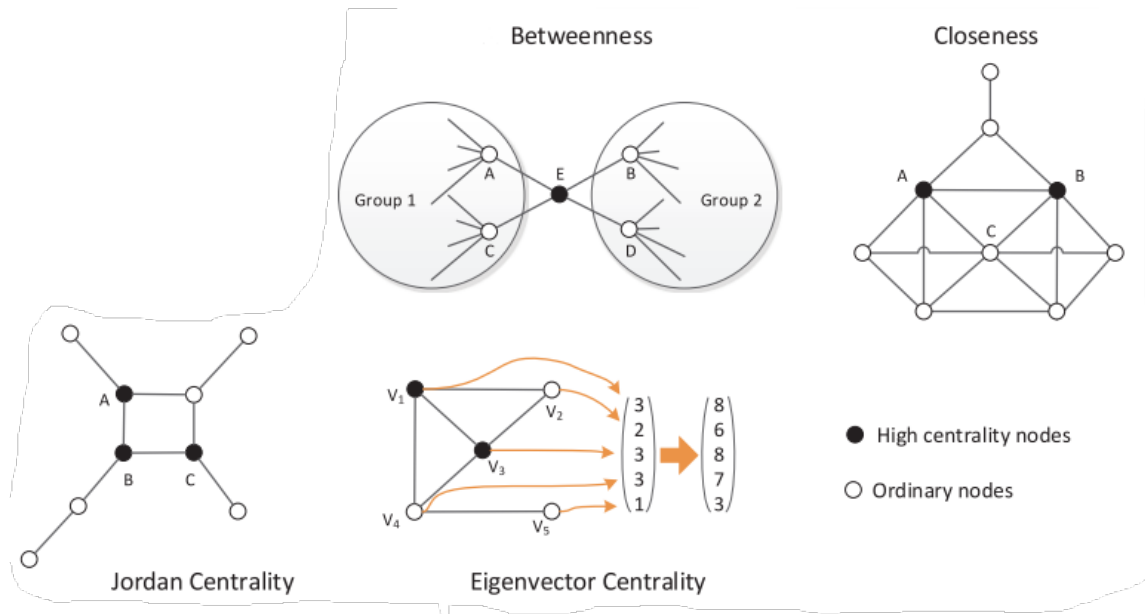
Figure 5.12: Centrality Measures Explained (Jiang et al., 2017)

In this figure, different centrality measures are visually explained:

- **Betweenness:** Nodes that frequently appear on shortest paths between other nodes.

- **Closeness:** Nodes that can reach other nodes most quickly.

- **Jordan:** Nodes that minimize the maximum distance to other nodes.

- **Eigenvector:** Nodes that are connected to other well-connected nodes.

These centrality measures offer different insights into network structure and dynamics, aiding in the accurate identification of infection sources. The implementation of these centrality measures was integrated into the network simulation, and their performance was tested on various network structures. The evaluation criteria included accuracy and computational efficiency under varying network conditions and infection parameters [2]. Their performance is further analyzed in the subsequent sections.

First, let us delve into the accuracy of these centrality measures. Figure 5.13 shows the accuracy of various centrality measures on different network types. We executed each of the source detection algorithms 400 times across various stages of the infection and different graph configurations to generate this plot.

Figure 5.13: Accuracy of Centrality Measures on Different Graphs

From the accuracy plot, we observe that the combination of Eccentricity and Closeness Centrality (EC_CC) consistently demonstrates the hi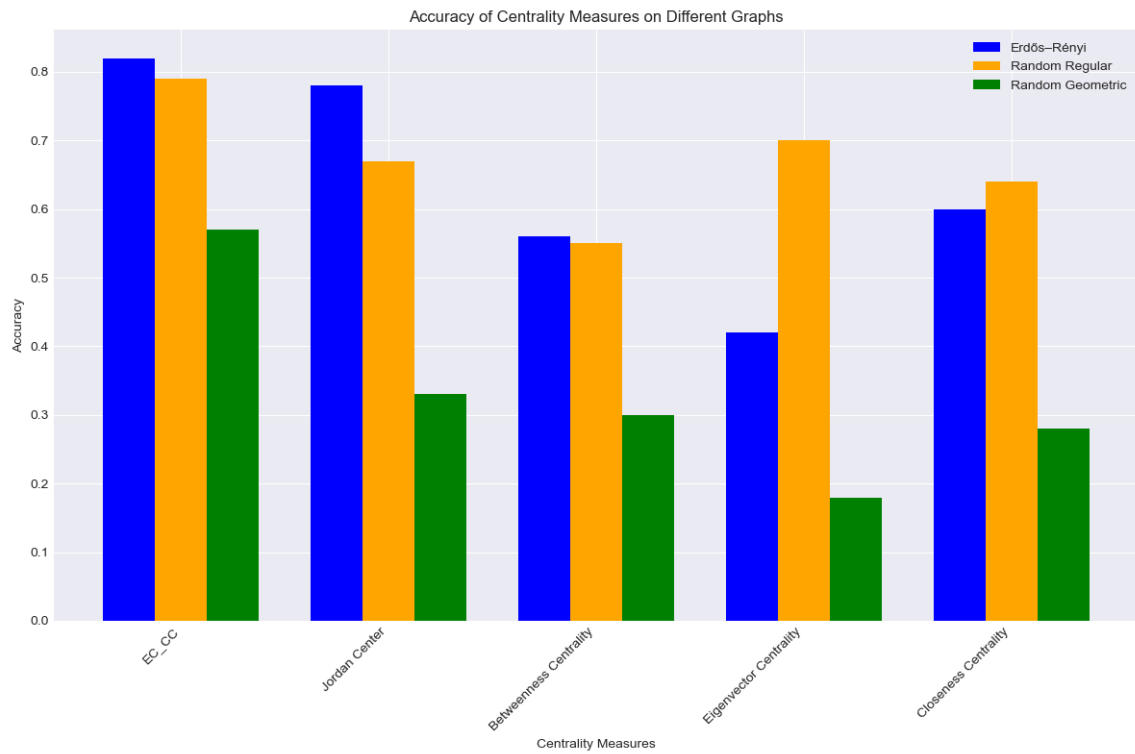ghest accuracy across all network types. This is likely because Eccentricity identifies the node that minimizes the maximum distance to all other nodes, while Closeness Centrality ensures that the node is centrally located in terms of average shortest path distances. Together, they provide a robust indication of the central node, which is often the source of the infection.

For Erdős–Rényi and Random Regular graphs, the accuracy is relatively high. This can be attributed to the regularity and homogeneity of these graphs, where nodes tend to have similar numbers of neighbors, allowing centrality measures to perform effectively. The consistent connectivity patterns in these graphs make it easier for the algorithms to identify the central nodes accurately.

In contrast, the accuracy is lower for Random Geometric graphs. These graphs have irregular structures, with varying node degrees and connectivity patterns, especially near the boundaries. The irregularities and the presence of boundary nodes, which have fewer neighbors, make it challenging for centrality measures to accurately identify the infection source. The varying density and proximity-based connections disrupt the uniformity, leading to lower accuracy in source detection.

However, accuracy is not the only criterion to consider. The computational efficiency of these algorithms is equally important, especially for large-scale networks. Figure 5.14 illustrates the average time taken by various centrality measures on different network types.
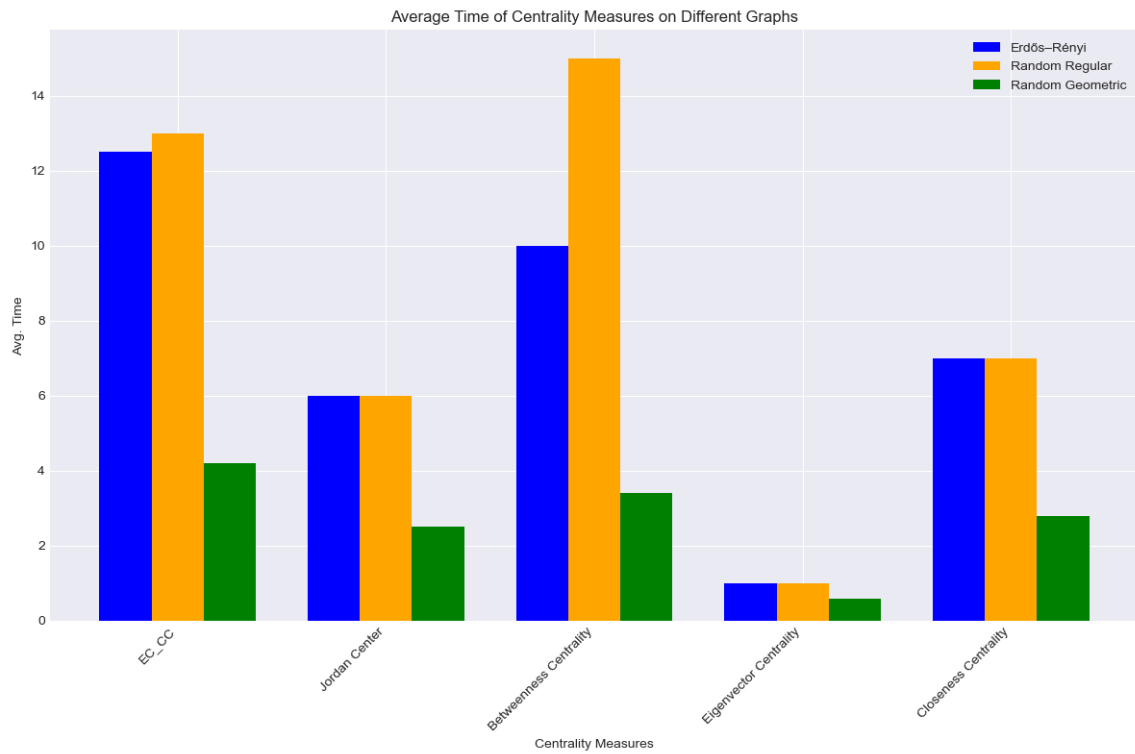
Figure 5.14: Average Time of Centrality Measures on Different Graphs

The combination of Eccentricity and Closeness Centrality (EC_CC), while accurate, is the most time-consuming. This is because these measures involve complex calculations that consider the distances between all pairs of nodes. The high time complexity can be a significant drawback in large networks where quick decision-making is crucial.

Betweenness Centrality also takes a considerable amount of time due to its dependency on the shortest paths between all node pairs. It provides valuable insights into the network's flow structure but at the cost of computational efficiency.

Eigenvector Centrality is relatively fast but sacrifices accuracy, particularly in irregular networks. It assigns scores based on the principle that connections to high-scoring nodes contribute more to a node's score. While this is useful in some contexts, it may not always accurately identify the infection source, especially in heterogeneous networks.

Closeness Centrality strikes a balance between time and accuracy, performing well across different network types. It measures the average length of the shortest path from a node to all other nodes, providing a good indication of centrality without the computational overhead of Betweenness or EC_CC.

Jordan Centrality provides a favorable balance between accuracy and time complexity, making it an excellent choice for source detection algorithms. It performs effectively on both grid-based and network-based models.

In summary, the choice of centrality measure depends on the specific requirements of the analysis. For high accuracy, especially in regular networks, EC_CC is preferred despite its higher computational cost. For faster computations, Eigenvector or Closeness Centrality might be more suitable, particularly in large or irregular networks.

The results from our study highlight the strengths and weaknesses of various centrality measures for source detection in complex networks. By understanding these trade-offs, we can select the most appropriate algorithm based on the network structure and the specific requirements of the task at hand.

5.2 Stochastic Approach

Given that our models already incorporate stochasticity through probabilistic spreading, we explored an additional route to simulate infection spread: the stochastic approach model. This approach differs from our current models, which

advance one step at a time using timestamps. Instead, the stochastic approach uses continuous-time Markov processes to simulate the timing of infection events, providing a more nuanced understanding of disease dynamics and allowing for real-time simulations.

We implemented this new stochastic model using the Gillespie Algorithm, which is suitable for simulating systems with random events such as disease spread. The Gillespie Algorithm allows us to model the discrete nature of infection events and the inherent randomness in the timing of these events. The infection times follow an exponential distribution, capturing the stochastic nature of real-world scenarios. The mathematical foundation of the stochastic approach involves Stochastic Differential Equations (SDEs) for the SIRS model, which incorporate Wiener processes to account for random perturbations in the state of susceptible, infected, and recovered individuals. This allows for the incorporation of random fluctuations and noise into the infection dynamics [11, 13, 30].

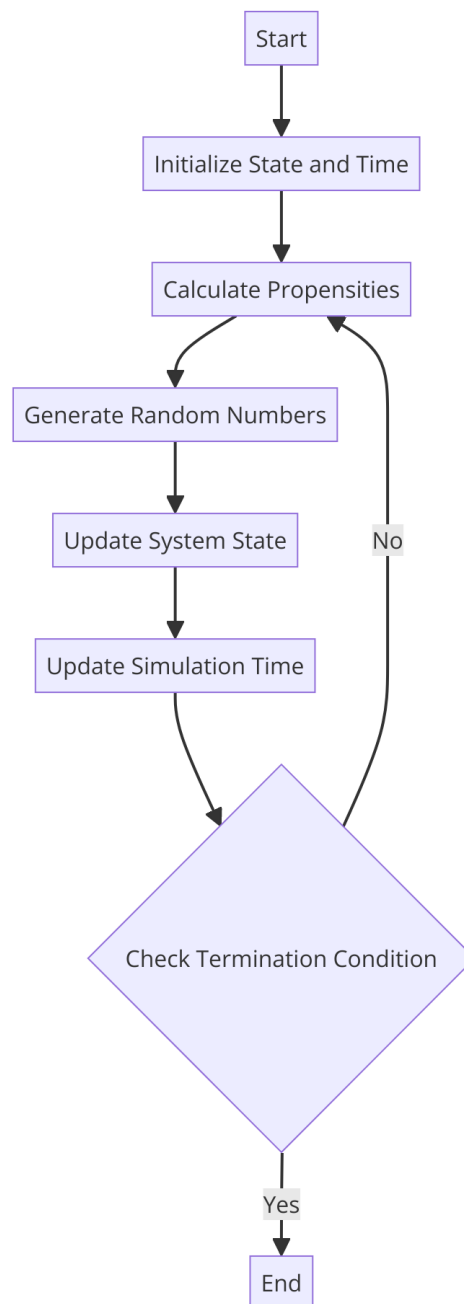The flowchart of the Gillespie Algorithm is shown in Figure 5.15.

Figure 5.15: Flowchart of the Gillespie Algorithm

By incorporating stochastic elements, we can capture the unpredictable fluctuations that occur in real-world disease spread scenarios. This randomness affects the performance of source detection algorithms, as the spread patterns are less

predictable and more diverse [33, 32].

We performed a comparative analysis between our probabilistic spreading models and the new stochastic approach to highlight the differences and advantages. The stochastic models provide a more realistic simulation of infection dynamics, accounting for the inherent uncertainties in real-world scenarios [29, 31].

The comparison of the probabilistic and stochastic models is illustrated in Figure 5.16.
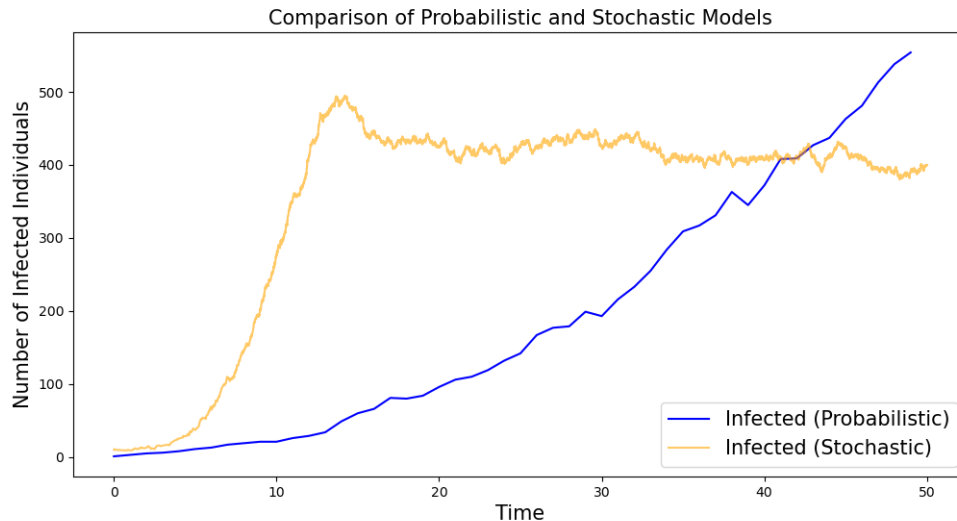

Figure 5.16: Comparison of Probabilistic and Stochastic Models

From Figure 5.16, several key differences and observations can be made:

- **Variability and Noise:** The stochastic model (orange line) shows significant variability and noise, capturing the random fluctuations in the number of infected individuals. This is consistent with real-world scenarios where infection dynamics are influenced by numerous unpredictable factors. The probabilistic model (blue line) shows a smoother trajectory, representing the average behavior of the infection spread over discrete time steps.

- **Peak Infection:** The stochastic model reaches a higher peak of infection more quickly, reflecting the potential for rapid outbreaks due to random events. The probabilistic model shows a more gradual increase in infections, highlighting the average spread without accounting for sudden changes.

- **Equilibrium State:** Both models eventually reach an equilibrium state, but the stochastic model's equilibrium fluctuates more due to ongoing random events. The probabilistic model's equilibrium is more stable, reflecting the average steady-state behavior.

Advantages of the Stochastic Approach:

- Captures the randomness and variability observed in real-world infection spread, which deterministic models may overlook.

- Provides a more nuanced understanding of disease dynamics by accounting for random fluctuations and noise.

- Leads to more robust and reliable predictions of disease spread and source detection, better reflecting the inherent uncertainties in real-world scenarios [27].

- Allows for real-time simulations, making it suitable for dynamic and rapidly changing epidemic scenarios.

In summary, incorporating stochastic elements into infection spread models significantly enhances their realism and reliability. The stochastic models account for the inherent randomness and noise present in real-world disease spread,

leading to more accurate and robust predictions. This comparative analysis underscores the importance of stochastic modeling in epidemiological research and the need for further development of these models to better understand and control disease spread [34].

5.3 Conclusion

This chapter has detailed the design and implementation of grid-based and complex network models for simulating infectious disease spread. By employing various source detection algorithms and centrality measures, we aimed to improve the traceability of infection sources. The integration of stochastic elements further enhanced the realism of our simulations, providing a comprehensive framework for understanding disease dynamics.

The Jordan Center algorithm demonstrated high accuracy in wrap-around grid configurations but showed limitations in fixed boundary scenarios. Centrality measures like EC_CC proved to be the most effective for source detection in complex networks, although at the cost of higher computational time.

In summary, our findings highlight the importance of selecting appropriate algorithms and centrality measures based on the network structure and the specific requirements of the analysis. The choice of algorithm significantly impacts the accuracy and computational efficiency of source detection in epidemiological models.

Chapter 6

Implementation

6.1 Introduction

This chapter details the implementation of the models, algorithms, and simulations discussed in this study. The focus is on providing the necessary code snippets and explaining the logic behind the implementations. Additionally, we discuss the computational complexity of each algorithm.

6.2 Model Structures and Algorithms

6.2.1 Grid-Based Model Implementation

We chose to use NumPy for grid-based algorithms due to its efficiency in handling large arrays and performing mathematical operations. NumPy's operations are optimized for performance, making it faster than using a network library like NetworkX for grid-based structures. Additionally, we used the JIT (Just-In-Time) compilation feature from the Numba library to further optimize our distance calculations, ensuring that our algorithms run efficiently even on large grids.

Jordan Centrality

The Jordan Center Identification algorithm utilizes the Breadth-First Search (BFS) to determine the central node that minimizes the maximum distance to all other nodes. This method calculates the centrality score for each candidate node, selecting the node with the highest score as the source.

Algorithm 1 Jordan Centrality using BFS

1: Initialize centrality scores for each node.
2: **for** each candidate node **do**
3:     Perform BFS to calculate distances.
4:     Compute centrality score based on distances.
5: **end for**
6: Select the node with the highest centrality score as the source.

Time Complexity: The BFS algorithm has a time complexity of $O(V + E)$, where V is the number of vertices (nodes) and E is the number of edges (connections). Since this algorithm is applied to each candidate node, the overall complexity can be considered $O(N(V + E))$ where N is the number of candidate nodes.

Center of Mass

The Center of Mass algorithm calculates the mean position of all infected nodes and designates this point as the source of the infection. This method is computationally efficient but can be less accurate, especially near grid boundaries.

Algorithm 2 Center of Mass Algorithm

1: Identify all boundary nodes.

2: Perform flood fill to isolate internal and external boundaries.

3: Calculate the centroid of the boundary nodes.

4: Designate the centroid as the source.

Time Complexity: The flood fill algorithm has a time complexity of $O(N)$, where N is the number of nodes in the grid. The overall complexity for finding the centroid is also $O(N)$ since it requires visiting each node.

Distance Analysis

The Distance Analysis algorithm calculates the maximum Euclidean distance from each candidate node to any point on the boundary and identifies the node that minimizes this maximum distance.

Algorithm 3 Distance Analysis Algorithm

1: Identify all boundary nodes.

2: **for** each candidate node **do**

3:     Calculate the maximum Euclidean distance to the boundary nodes.

4:     Track the node that minimizes this maximum distance.

5: **end for**

6: Designate the node with the minimum maximum distance as the source.

Time Complexity: The main operations in this algorithm involve iterating over the grid nodes and computing Euclidean distances. The time complexity is $O(N \cdot M)$, where N is the number of nodes and M is the number of boundary nodes.

6.2.2 Complex Network Models Implementation

In this section, we focus on the implementation of centrality measures for source detection in complex network models. We use various centrality measures to identify the infection source within networks such as Erdős-Rényi graphs, Random Regular graphs, and Random Geometric graphs.

The centrality measures we implemented include those mentioned and explained in 5.1.2, which are:

- Eccentricity + Closeness Centrality

- Jordan Center

- Betweenness Centrality

- Eigenvector Centrality

- Closeness Centrality

We used the NetworkX library to implement these centrality measures. The library provides efficient functions to compute the various centrality metrics, allowing us to focus on integrating these measures into our source detection framework.

Each centrality measure has its own strengths and weaknesses, and the choice of measure depends on the specific characteristics of the network and the requirements of the analysis.

This concludes the implementation section for the complex network models. Next, we will discuss the stochastic approach.

6.2.3 Stochastic Approach Implementation

In this section, we detail the implementation of the stochastic approach to model infection spread using the Gillespie Algorithm.

Gillespie Algorithm

The Gillespie Algorithm is used to simulate the time evolution of systems with random events, such as the spread of infectious diseases. Its flowchart is shown in Figure 5.15.

It involves calculating propensities for each possible event, generating random numbers to determine the next event and its timing, and updating the system state accordingly. The following code snippet demonstrates the implementation of the Gillespie Algorithm for the SIRS model:

Algorithm 4 Gillespie Algorithm for SIRS Model

1: Initialize S, I, R, and time.
2: **while** time $<$ T **do**
3:     Calculate rates: infection, recovery, loss of immunity.
4:     Calculate total rate.
5:     **if** total rate == 0 **then**
6:         break.
7:     **end if**
8:     Draw time step from exponential distribution.
9:     Update time.
10:     Draw event type.
11:     **if** infection event **then**
12:         Update S, I, R.
13:     **else if** recovery event **then**
14:         Update S, I, R.
15:     **else if** loss of immunity event **then**
16:         Update S, I, R.
17:     **end if**
18: **end while**

6.3 Conclusion

In this chapter, we have detailed the implementation of the models, algorithms, and simulations used in this study to analyze the spread of infectious diseases. We provided code snippets for key components, including the grid-based models and stochastic approaches.

For the grid-based models, we implemented three main algorithms: Jordan Centrality, Center of Mass, and Distance Analysis. Each algorithm was discussed in terms of its implementation details, time complexity, and space complexity. We used NumPy for efficient computation and the JIT compiler from Numba to optimize performance.

For the complex network models, we implemented various centrality measures such as Eccentricity + Closeness Centrality, Jordan Centrality, Betweenness Centrality, Eigenvector Centrality, and Closeness Centrality.

In the stochastic approach, we incorporated randomness into the models using the Gillespie Algorithm. The implementation of this method was described along with its computational complexity.

By implementing these models and algorithms, we were able to simulate the spread of infectious diseases in different network structures and compare the effectiveness of various source detection methods. The detailed implementation provided in this chapter serves as a foundation for further analysis and experimentation in the field of epidemiological modeling.

Chapter 7

Conclusion and Future Scope

In conclusion, this thesis has provided a detailed examination of infectious disease spread across various network structures. The study explored both grid-based algorithms, which are fundamental in epidemiological studies due to their simplicity and structured nature, and more complex network models focusing on understanding disease spread dynamics. The aim is to improve the traceability of infection sources, which are crucial for a comprehensive understanding of disease spread dynamics in real-world scenarios.

The research highlights the importance of selecting appropriate modeling approaches to accurately simulate and trace infection dynamics. By integrating grid-based, network-based, and stochastic models, this work offers valuable insights into the complexities of disease transmission and the potential for improved disease monitoring and control.

The proposed future research directions aim to build on these findings, enhancing the robustness and applicability of simulation models in real-world contexts. Continued investigation in these areas will contribute to the ongoing efforts to understand and combat infectious diseases, ultimately supporting public health initiatives and improving outcomes for populations worldwide.

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Appendix A

Algorithm Implementations

A.1 Jordan Center

```python
import numpy as np
import time
from collections import deque

def bfs(grid, start_pos):
    # Implement BFS to calculate distances
    pass  # Omitted for brevity

def infection_nodes(grid):
    # Identify all infected or previously infected nodes
    pass

def find_infection_source_bfs(grid):
    height, width = grid.shape

    # For SIRS, we take nodes that are infected or were infected
    candidate_nodes = infection_nodes(grid)

    centrality_scores = np.zeros_like(grid, dtype=np.float32)

    global_start_time = time.time()
    for i, start_pos in enumerate(candidate_nodes):
        start_time = time.time()
        start_pos_tuple = tuple(start_pos)

        # Pass the precomputed infected nodes if applicable
        distances = bfs(grid, start_pos_tuple)

        # Compute centrality score considering distances to other nodes
        reachable_nodes = distances[distances != -1]  # Exclude unreachable nodes
        num_reachable_nodes = len(reachable_nodes) - 1  # Exclude the start node itself
        total_distance = np.sum(reachable_nodes)

        if num_reachable_nodes > 0:
            average_distance = total_distance / num_reachable_nodes
            centrality_scores[start_pos_tuple] = 1 / average_distance
        else:
            centrality_scores[start_pos_tuple] = 0

    # Find the node with the highest centrality score
    source_node = np.unravel_index(np.argmax(centrality_scores), grid.shape)
```

```
42
43        return source_node
```

Listing A.1: Jordan Centrality using BFS

A.2 Center of Mass

```python
1  import numpy as np
2
3  def flood_fill(grid, mask, start_i, start_j, target_val, fill_value):
4      stack = {(start_i, start_j)}  # Using a set to avoid duplicate positions
5      while stack:
6          x, y = stack.pop()
7          if mask[x, y] != fill_value and grid[x, y] == target_val:
8              mask[x, y] = fill_value
9              base_idx = (x * width + y) * 4
10             for k in range(4):  # Changed loop variable to k to avoid confusion with i, j
11                 neighbor_idx = neighbors_map[base_idx + k]
12                 if neighbor_idx != -1:  # Valid neighbor index
13                     nx, ny = divmod(neighbor_idx, width)  # Convert flat index to 2D indices
14                     if mask[nx, ny] != fill_value:
15                         stack.add((nx, ny))
16
17 def find_external_boundary_grid(grid):
18     height, width = grid.shape
19     infected_val = 0  # Infected nodes
20     susceptible_val = -1  # Susceptible nodes
21
22     # Step 1: Identify All Potential Boundary Nodes
23     potential_boundary = np.zeros_like(grid, dtype=bool)
24     for i in range(height):
25         for j in range(width):
26             if grid[i, j] == infected_val:
27                 base_idx = (i * width + j) * 4
28                 for k in range(4):
29                     neighbor_idx = neighbors_map[base_idx + k]
30                     if neighbor_idx != -1:
31                         nx, ny = divmod(neighbor_idx, width)
32                         if grid[nx, ny] == susceptible_val:
33                             potential_boundary[i, j] = True
34                             break
35
36     # Step 2: Flood Fill from Grid Edges
37     mask = np.zeros_like(grid, dtype=bool)
38     edge_indices = np.hstack((np.arange(0, width), np.arange(grid.size - width, grid.size)))
39     for edge_idx in edge_indices:
40         i, j = divmod(edge_idx, width)
41         if grid[i, j] == susceptible_val and not mask[i, j]:
42             flood_fill(grid, mask, i, j, susceptible_val, True)
43
44     # Step 3: Identify Internal Potential Boundary Nodes
45     internal_potential_boundary = np.zeros_like(grid, dtype=bool)
46     for i in range(height):
47         for j in range(width):
48             if potential_boundary[i, j]:
49                 base_idx = (i * width + j) * 4
50                 for k in range(4):
51                     neighbor_idx = neighbors_map[base_idx + k]
```

```
52                    if neighbor_idx != -1:
53                        nx, ny = divmod(neighbor_idx, width) # Convert flat index to 2D indices
54                        if mask[nx, ny]:
55                            internal_potential_boundary[i, j] = True
56                            break
57
58      # Step 4: Isolate Actual Boundary Nodes
59      actual_boundary = potential_boundary & internal_potential_boundary
60
61      return actual_boundary
62
63  def find_centroid_mean(external_boundary_grid):
64      boundary_indices = np.argwhere(external_boundary_grid)
65
66      # Calculate the centroid (mean position) of the boundary points.
67      centroid_x, centroid_y = np.mean(boundary_indices, axis=0)
68
69      # The centroid coordinates are given as (centroid_x, centroid_y).
70      # If you need to round them to the nearest integer (since grid indices are integers), you can
              do:
71      centroid_x = int(round(centroid_x))
72      centroid_y = int(round(centroid_y))
73
74      centroid = (centroid_x, centroid_y)
75      return centroid
76
77  centroid = find_centroid_mean(find_external_boundary_grid(grid))
78  print(centroid)
```

Listing A.2: Center of Mass Algorithm

A.3 Distance Analysis

```
1  import numpy as np
2  from numba import jit
3  from collections import deque
4
5  @jit(nopython=True)
6  def max_euc_distance_to_boundary(x0, y0, boundary_indices):
7      """Calculate the maximum Euclidean distance from (x0, y0) to any boundary point."""
8      max_distance = 0.0
9      for index in range(boundary_indices.shape[0]):
10         x, y = boundary_indices[index]
11         euc_distance = np.sqrt((x - x0) ** 2 + (y - y0) ** 2)
12         if euc_distance > max_distance:
13             max_distance = euc_distance
14     return max_distance
15
16  def find_infection_source_euc_distance(grid):
17      """Find the source of infection by minimizing the maximum distance to the external boundary."""
18      height, width = grid.shape
19      start_pos = (height // 2, width // 2)
20
21      # Convert the external boundary to a NumPy array of indices for efficient processing
22      external_boundary_grid = find_external_boundary_grid(grid)
23      external_boundary_indices = np.argwhere(external_boundary_grid)
24
25      # Initialize queue and visited set
```

```
26    queue = deque([start_pos])
27    visited = set([start_pos])
28    current_best_node = start_pos
29    current_min_max_distance = max_euc_distance_to_boundary(start_pos[0], start_pos[1],
          external_boundary_indices)
30
31    while queue:
32        x0, y0 = queue.popleft()
33
34        # Check all neighbors to find the one with the smallest maximum distance to the boundary
35        min_neighbor_distance = float('inf')
36        next_node = None
37
38        base_index = (x0 * width + y0) * 4
39        for i in range(4):
40            neighbor_idx = neighbors_map[base_index + i]
41            if neighbor_idx == -1:
42                continue
43
44            nx0, ny0 = divmod(neighbor_idx, width)
45            if (nx0, ny0) not in visited:
46                visited.add((nx0, ny0))
47                n_max_distance = max_euc_distance_to_boundary(nx0, ny0, external_boundary_indices)
48                if n_max_distance < min_neighbor_distance:
49                    min_neighbor_distance = n_max_distance
50                    next_node = (nx0, ny0)
51
52        if next_node and min_neighbor_distance < current_min_max_distance:
53            # Only proceed if the next node improves the maximum distance
54            queue.append(next_node)
55            current_min_max_distance = min_neighbor_distance
56            current_best_node = next_node
57
58    return current_best_node
```

Listing A.3: Distance Analysis Algorithm

A.4   Gillespie Algorithm

```
1  import numpy as np
2
3  def gillespie_sirs(S0, I0, R0, beta, gamma, delta, T):
4      S, I, R = [S0], [I0], [R0]
5      t = 0
6
7      while t < T:
8          N = S[-1] + I[-1] + R[-1]
9          rates = [
10             beta * S[-1] * I[-1] / N,   # Infection rate
11             gamma * I[-1],              # Recovery rate
12             delta * R[-1]               # Loss of immunity rate
13         ]
14         rate_sum = sum(rates)
15
16         if rate_sum == 0:
17             break
18
19         tau = np.random.exponential(1 / rate_sum)
```

```
20          t += tau
21          rand = np.random.random() * rate_sum
22
23          if rand < rates[0]:
24              S.append(S[-1] - 1)
25              I.append(I[-1] + 1)
26              R.append(R[-1])
27          elif rand < rates[0] + rates[1]:
28              S.append(S[-1])
29              I.append(I[-1] - 1)
30              R.append(R[-1] + 1)
31          else:
32              S.append(S[-1] + 1)
33              I.append(I[-1])
34              R.append(R[-1] - 1)
35
36      return np.array(S), np.array(I), np.array(R)
```

Listing A.4: Gillespie Algorithm for SIRS Model