Study of Assortativity in Configuration Networks via Newman Rewiring

A dissertation submitted to the Jawaharlal Nehru University

in partial fulfilment of the requirements

for the award of the degree of

MASTER OF TECHNOLOGY

IN

COMPUTER SCIENCE AND ENGINEERING

By

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2024

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Declaration

I declare that the project work entitled "**Study of Assortativity in Configuration Networks via Newman Rewiring**" which is submitted by me in partial fulfilment of the requirement for the award of degree Master of Technology (a part of a Five-Year Dual Degree Course) to School of Engineering, Jawaharlal Nehru University comprises only my original work and due acknowledgement has been made in the text to all other material used.

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CERTIFICATE

May 10, 2024

This is to certify that this dissertation entitled "**Study of Assortativity in Configuration Networks via Newman Rewiring**" submitted by Nitish Kumar Sharma to the School of Engineering, Jawaharlal Nehru University, New Delhi for the award of the degree of Master of Technology in Computer Science and Engineering, as part of the dual degree programme in the School of Engineering, is a research work carried out by him under the supervision of Dr. Krishnan Rajkumar.

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Dedicated to my Friends and family

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Acknowledgements

I would like to express my deepest gratitude and appreciation to all those who have contributed to the successful completion of my M. Tech program and the preparation of this thesis. First and foremost, I am sincerely thankful to my supervisor, Dr. Krishnan Rajkumar, for their invaluable guidance, constant support, and encouragement throughout this research journey. Their expertise, insightful feedback, and patience have been instrumental in shaping the direction of this work. I am also grateful to all the faculty members for their extensive knowledge and engaging lectures.

I extend my heartfelt appreciation to my parents and family for their unwavering love, support, and belief in my abilities. Their encouragement and sacrifices have been the foundation of my educational journey, and I am truly grateful for their presence in my life. Furthermore, I would like to express my gratitude to my fellow classmates and colleagues for their collaboration and stimulating discussions. Thank you all for being an integral part of this M. Tech endeavour and for your support.

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Abstract

This thesis studies assortativity in networks through the development of an Python framework, utilizing the NetworkX library. The focus is on implementing Newman's rewiring technique within the configuration model to precisely control the assortative mixing in networks, with a special emphasis on scale-free networks. The "random hubs" method is employed to generate degree sequences that ensure minimal fluctuations, optimizing the structural stability of the networks.

Thesis studies the effectiveness of various rewiring matrices in different works adoption of more sophisticated matrices that manage off-diagonal elements effectively. This adjustment is critical for realizing statistically plausible correlations within practical network constructs.

The application of these methodologies is exemplified through modifications to Barabasi-Albert (BA) networks, leveraging recent analytical insights into their natural correlations. This allows for a direct comparison between networks formed through preferential attachment and those configured through the enhanced rewiring techniques developed in this study. For scale-free distributions with a β parameter of 2 or greater, the networks achieved complete connectivity, demonstrating the effectiveness of the configuration model in producing robust network structures.

This thesis not only deepens theoretical understanding of network assortativity but also provides a comprehensive toolkit for researchers and practitioners to explore and manipulate network dynamics effectively in real-world scenarios.

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Chapter 1

Introduction

1.1 Introduction

In the realm of network science, understanding assortativity—specifically, nodes' preference to attach to similar others in terms of degree—is vital for predicting network behavior under various operational scenarios. This thesis undertakes a comprehensive analysis of existing research on assortativity modeled through Newman's rewiring technique within configuration networks. The study aims to elucidate the implications of these network characteristics on the stability and performance of both social and technological systems.

Configuration networks,are a type of random network model where each node is assigned a degree from a given degree distribution before the network is constructed. The degrees are paired randomly to form edges, subject to the constraint that the total degree is even. This model is particularly useful for studying theoretical properties of networks because it allows for precise control over the degree distribution while maintaining a random structure elsewhere.[18]

Assortativity in networks refers to the tendency of nodes to connect with other nodes that are similar in certain attributes, such as degree, which is the number of connections a node has. This characteristic is crucial in understanding how networks behave under various conditions because it affects the network's resilience to attacks and its overall connectivity. Assortative mixing in networks leads to a robust structure where high-degree nodes are more likely to be connected to other high-degree nodes, potentially enhancing the network's resistance to random failures.

The interaction between assortativity and the structure of configuration networks, especially under Newman's rewiring technique, offers a fascinating avenue for exploring

how assortative mixing can be artificially introduced or adjusted in network models. Newman's rewiring is a process that selectively reorganizes the links in a network to increase or decrease assortative mixing without altering the underlying degree distribution. This technique has profound implications for the study of network dynamics and is central to the investigations carried out in this thesis.

1.2 Structure of the Thesis

Following the introductory chapter that sets the stage by introducing the key concepts of assortativity and configuration networks, this thesis delves deeper into the realm of random graphs, scale-free properties, and the Barabási-Albert (BA) model in Chapter (2). This chapter lays the foundational knowledge of network science necessary to build a comprehensive understanding of the field.

Chapter 3 details the analytical methodologies employed for synthesizing and evaluating the collected literature, articulating the criteria used to assess the effectiveness of assortative mixing models . This methodological framework is crucial for the rigorous analysis that follows.

In Chapter 4, an in-depth analysis of the literature underscores the theoretical and practical implications of Newman's rewiring technique across different network models (4). This analysis explores the effects of assortative and disassortative mixing on network functionality, providing critical insights into the dynamics of network behavior.Chapter 4 broadens the discussion to explore the wider implications of these findings, particularly their applications in enhancing the resilience of infrastructural and social networks (5).

The thesis concludes with Chapter 5, which summarizes the findings and reflects on the contributions of this study to the field of network science (**??**). It emphasizes the significance of assortativity in understanding and managing complex network behaviors, highlighting how this characteristic influences network resilience and stability.

1.3 Concluding Note

This thesis provides a critical examination of the role of assortativity in networks, enhancing our understanding of how assortative properties can be manipulated to optimize network behavior. By connecting theoretical research with practical implications, this

work explores foundational knowledge necessary for advancing network design and strategy in complex technological and social landscapes.

Chapter 2

Related Work

2.1 The Random Network Model: $G(N, p)$

A random network simplifies the complex real-world structure to two basic components: nodes and links. The challenge lies not just in the creation of these components but in their interconnection, which must accurately reflect the complexity of the actual systems they model. The $G(N, p)$ model, introduced by Gilbert, posits a straightforward yet profound approach: it constructs networks where each pair of N nodes is connected with a probability p, independent of other pairs. This model captures the essence of randomness in network formation and is favored for its clarity and mathematical tractability in exploring network properties.[12]

Constructing a Random Network

To construct a random network using the $G(N, p)$ model, the procedure involves:

1. **Initialization:** Start with N isolated nodes.
2. **Connection:** For every distinct pair of nodes, generate a random number between 0 and 1. If the number is less than or equal to p, establish a link between the pair; otherwise, leave them disconnected.
3. **Iteration:** Repeat the connection step for each of the $\frac{N(N-1)}{2}$ possible pairs, ensuring that all potential connections are evaluated.[2]

The resulting structure, often referred to as the Erdős-Rényi network or random graph, symbolizes the inherent randomness and unpredictability of complex networks. This

model allows researchers to simulate and study the basic properties of network connectivity and resilience.

Mathematical Description

In the $G(N, p)$ model, the number of links L in any given realization is subject to stochastic variations. The probability of observing exactly L links follows a binomial distribution:

$$P(L) = \binom{N(N-1)/2}{L} p^L (1-p)^{N(N-1)/2-L}$$

This equation combines the probability p^L of L connections occurring, the probability $(1-p)^{N(N-1)/2-L}$ of the remaining potential connections not occurring, and the combinatorial factor $\binom{N(N-1)/2}{L}$, which counts the number of ways to choose L links from $\frac{N(N-1)}{2}$ possible pairs.

From this distribution, the expected number of links $\langle L \rangle$ in the network is:

$$\langle L \rangle = p\frac{N(N-1)}{2}$$

Moreover, the expected average degree $\langle k \rangle$ of each node, which is the average number of connections per node, is given by:

$$\langle k \rangle = p(N-1)$$

2.1.1 The Watts-Strogatz Model

The Watts-Strogatz model, [20], extends the random network model by incorporating the real-world observations of network structures. This model is a cornerstone in understanding the phenomena of 'small-world' networks, characterized by two distinct features:

Small World Property

Real-world networks demonstrate that the average path length between two nodes grows logarithmically with the number of nodes N, as opposed to the polynomial growth observed in regular lattices. This observation suggests a more efficient connectivity in natural networks than what would be expected in uniformly structured designs.

High Clustering

Contrary to the predictions for random networks, real networks exhibit a significantly higher clustering coefficient for the same number of nodes N and links L. This indicates a

tendency for nodes to create tightly knit groups, enhancing the network's overall robustness to disruptions.

Model Description

The Watts-Strogatz model bridges the gap between a regular lattice, which has high clustering but does not exhibit the small-world property, and a random network, which shows low clustering but demonstrates the small-world phenomenon. The model initiates with a ring of nodes where each node connects not only to its immediate neighbors but also to the next ones, thus ensuring a high initial clustering coefficient $\langle C \rangle = 0.75$ when the rewiring probability $p = 0$[2].

With a small probability p, each link in the network is rewired to a random node. This minor adjustment significantly decreases the average path length while maintaining a high clustering coefficient, effectively capturing the small-world phenomenon. As p approaches 1, all links are likely to be rewired, transitioning the network towards a random network structure.

Model Dynamics

The impact of the rewiring probability p on the network's average path length $d(p)$ and clustering coefficient $\langle C(p) \rangle$ is profound. Both metrics are normalized by their values in a regular network (i.e., $d(0)$ and $\langle C(0) \rangle$) for comparison. As p varies from 0 to 1, average path length experiences a decline, indicating the onset of the small-world phenomenon, while $\langle C(p) \rangle$ remains compa high in the range of $0.001 \leq p \leq 0.1$. This range is crucial as it supports the coexistence of short path lengths and high clustering, which are characteristic of many real-world networks. The parameters for these observations typically include node $N = 1000$ and $\langle k \rangle = 10$.

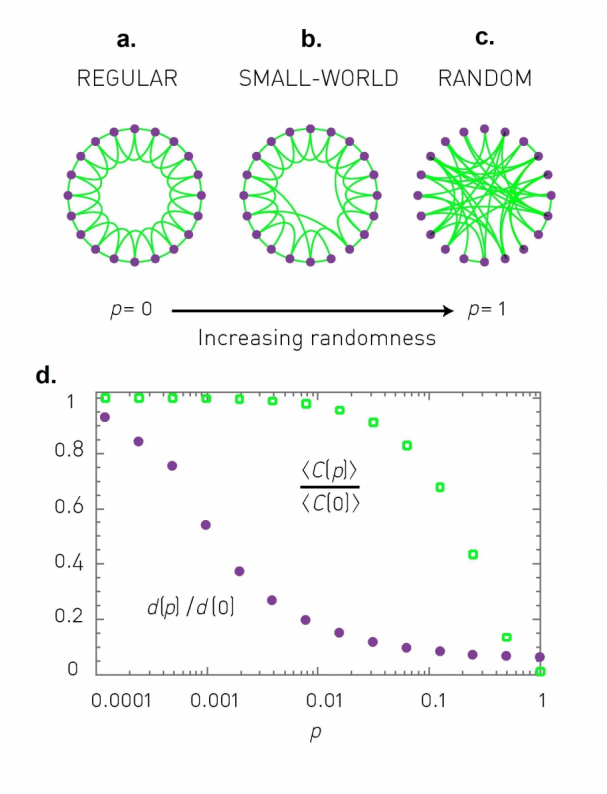

Figure 2.1: The Watts-Strogatz Model showing the transition from a normal network to a small-world network as a function of p.

2.2 Scale-Free Networks

Scale-free networks are distinguished by a degree distribution that follows a power law, which contrasts sharply with the Poisson distribution expected in random networks. This distinct characteristic is fundamental in understanding many complex network behaviors[2].

Characteristics of Scale-Free Networks

The term ”scale-free” refers to the network’s degree distribution following a power law, typically observable across several orders of magnitude in real-world networks. Mathematically, the power law distribution for a network’s degree k is expressed as:

$$p(k) \sim k^{-\gamma}$$

where γ is the degree exponent. This relationship suggests that the probability $p(k)$ that a node in the network connects to k other nodes decreases polynomially with k.

In logarithmic terms, this distribution implies a linear relationship on a log-log scale:

$$\log p(k) \approx -\gamma \log k$$

which signifies a straight line with a slope of $-\gamma$.

Mathematical Formalism

To analyze scale-free networks, two formalisms are generally employed:

- **Discrete Formalism:** Suitable for situations where node degrees are integers, the probability p_k that a node has exactly k links is given by:

  $$p_k = \frac{k^{-\gamma}}{\zeta(\gamma)}$$

  where $\zeta(\gamma)$ is the Riemann-zeta function, ensuring normalization.

- **Continuum Formalism:** Useful for analytical calculations assuming degrees can take any positive real value, the form of $p(k)$ becomes:

  $$p(k) = (\gamma - 1)k_{\text{min}}^{\gamma-1}k^{-\gamma}$$

  where k_{min} is the minimum degree for which the power law holds.[2]

Implications for Network Dynamics

Scale-free networks are particularly notable for their robustness against random failures but vulnerability to targeted attacks. The presence of hubs(nodes with high degrees) — influences both the structural properties and the dynamics of the network, such as spreading processes and community formation.

In summary, the scale-free nature of a network significantly impacts its topology and dynamics. Understanding these networks involves not just identifying the presence of power-law degree distributions but also examining how these properties influence network behavior across various domains, from technological to biological systems.

2.3 The Barabási-Albert Model

2.3.1 Introduction

The Barabási-Albert (BA) model marks a significant shift from traditional random network models by integrating growth and preferential attachment into its framework. These principles elucidate the ubiquitous presence of hubs in complex networks, ranging from the Internet to biological systems, nodes exhibit a power-law like distribution.

2.3.2 Mathematical Description

The model begins with an initial set of m_0 interconnected nodes. Each subsequent node is added with $m \leq m_0$ edges that link to existing nodes with a probability proportional to their degree. The probability, $\Pi(k_i)$, that a new node will connect to node i with degree k_i is defined a[2]s:

$$\Pi(k_i) = \frac{k_i}{\sum_j k_j} \tag{2.1}$$

[**H.**]

where $\sum_j k_j$ is the sum of the degrees of all existing nodes in the network. This preferential attachment rule encapsulates the "rich get richer" phenomenon, a fundamental characteristic of scale-free networks.[2]

2.3.3 Role in Assortativity and Network Dynamics

While the BA model inherently generates disassortative mixing due to its preferential attachment mechanism, it serves as an insightful platform for studying how deviations from this model can affect network dynamics. Introducing additional mechanisms such as node fitness or aging could influence the assortative or disassortative mixing patterns, thus impacting the network's structural robustness and functionality.[5]

2.3.4 Analysis and Simulation

Simulations of the BA model, implemented using the NetworkX library in Python, demonstrate the scale-free nature of the BA network. The degree distribution of these BA network follows power-law, confirming the model's theoretical predictions:

$$p(k) \sim k^{-\gamma} \tag{2.2}$$

with γ typically close to 3, characteristic of scale-free networks. These empirical findings not only validate the model but also enhance our understanding of the dynamics of network growth and topology.

2.3.5 Visualization of Growth and Preferential Attachment

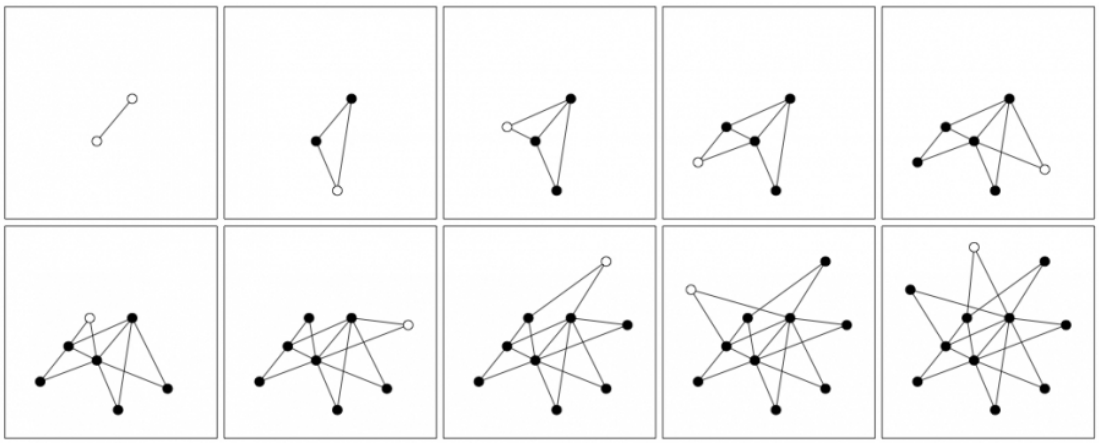

Figure 2.2: The set of images sequentially illustrates the development of the Barabási-Albert model across nine steps. Each image highlights the latest node, represented by empty circles, which determines the placement of its two links (m=2) according to the principle of preferential attachment.

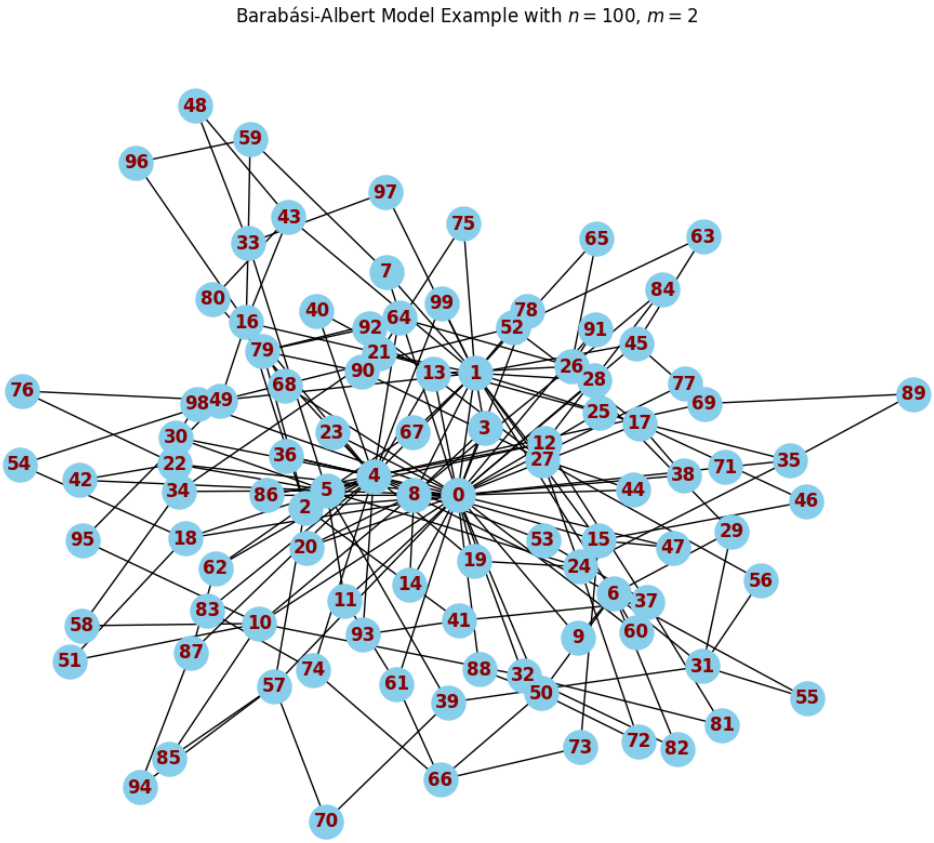

Figure 2.3: provides a visual representation of the network's evolution, illustrating how new nodes preferentially attach to existing nodes with higher degrees. This visual aid helps to conceptualize the dynamic process of network growth and the emergence of hubs within the network.

Chapter 3

Study of Assortatativity

3.1 Assortative Mixing in Network Models

Network structures, from social and computer networks to biological systems, are fundamentally graphs composed of nodes (vertices) interconnected by links (edges) [16, 18]. Although various network models have been explored within the realm of physics to mirror real-world network characteristics , a critical aspect often neglected is the phenomenon of assortative mixing. This phenomenon involves a preference among high-degree nodes to connect with other high-degree nodess, whereas disassortative mixing involves high-degree nodes connecting to low-degree ones.

3.1.1 Assortative Mixing and Its Impact on Network Dynamics

The concept of assortative mixing by degree is not just a structural curiosity but influences the dynamics and functionality of networks. To demonstrate this, we start by considering a network as a simple undirected graph with N vertices and M edges, characterized by a degree distribution p_k, where p_k is the likelihood a randomly selected vertex will have a degree k[17].

Upon following a randomly chosen edge to a vertex, the degree of this vertex tends to be higher than average due to the increased probability of connecting to vertices with a high degree. Consequently, the degree distribution of this vertex deviates from p_k to being proportional to kp_k. If we are interested in the degree minus the edge just traversed, termed the remaining degree, it follows a distribution proportional to $(k-1)p_{k-1}$.

3.1.2 Quantifying Assortative Mixing

The degree distribution q_k is given by:

$$q_k = \frac{(k-1)p_{k-1}}{\sum_j jp_j}.$$

Following the Newman [16], defined as e_{jk} as the joint probability distribution for the remaining degrees of two vertices at either end of a chosen edge. This matrix e_{jk} is symmetric ($e_{jk} = e_{kj}$) and satisfies:

$$\sum_{jk} e_{jk} = 1, \quad \sum_j e_{jk} = q_k.$$

In uncorrelated networks, e_{jk} simplifies to $q_j q_k$. In networks exhibiting assortative mixing, e_{jk} deviates from this product, reflecting a preference for connection between vertices of similar degree. The degree of assortative mixing can be given by a correlation function:

$$\langle jk \rangle - \langle j \rangle \langle k \rangle = \sum_{jk} jk(e_{jk} - q_j q_k),$$

which measures the deviation from the expected value under no assortative mixing. To compare networks, this measure is normalized by the maximal value obtainable on a perfectly assortative network, yielding:

$$r = \frac{1}{\sigma_q^2} \sum_{jk} jk(e_{jk} - q_j q_k),$$

where σ_q^2 is the variance of the distribution q and r serves as the Pearson correlation coefficient for the degrees at the ends of an edge, ranging from -1 to 1.

This metric is further refined for practical computation on actual networks as follows:

$$r = \frac{M^{-1} \sum_i j_i k_i - M^{-1} \sum_i \frac{1}{2}(j_i + k_i)^2}{M^{-1} \sum_i \frac{1}{2}(j_i^2 + k_i^2) - M^{-1} \sum_i \frac{1}{2}(j_i + k_i)^2},$$

[18] where j_i and k_i are the degrees of vertices at the ends of the i^{th} edge. This formulation provides a straightforward method for evaluating the assortative or disassortative nature of any given network.

3.2 The Configuration Model with Newman Rewiring

The configuration model is a fundamental framework used to create uncorrelated networks with specified degree distributions. This model is invaluable for creating network environments that are ideal for analyzing dynamic behaviors and diffusion processes. One of the primary types of networks studied using this model are scale-free networks, defined by a degree distribution $P(k) = c_\gamma k^{-\gamma}$. This function $P(k)$ represents the likelihood that any given node has k connections. Libraries such as Python's `networkX` and `igraph` provide essential tools for generating these networks and performing the necessary uncorrelated connections between node "stubs".[10]

3.2.1 Discretized Degree Distribution

In constructing networks with specific degree distributions, a precise methodological approach is essential. For a network comprising N total nodes, each node i (where i ranges from 1 to N) is assigned a degree D_i from a power-law distribution $P(k) = \frac{c_\gamma}{k^\gamma}$. The theoretical maximum degree n within the network is derived using the relationship:

$$\int_n^\infty P(k)\, dk = \frac{1}{N}$$

This integral suggests n as the threshold degree above which the network is unlikely to find more than one node, particularly when $\gamma = 3$, resulting in $n \approx \sqrt{N}$. For practical implementation in finite networks, $P(k)$ is set to zero for $k > n$ and the distribution is normalized accordingly:

$$\frac{1}{c_\gamma} = \sum_{k=1}^{n} P(k)$$

This normalization process allows for the calculation of N_k, the expected number of nodes with degree k, typically rounded to the nearest integer:

$$N_k = \text{Round}[P(k)N]$$

However, this method often results in N_k becoming zero for $k > n_1$, where $n_1 \approx (2Nc_\gamma)^{1/\gamma}$, significantly smaller than the calculated n. This issue arises from discarding fractional values during the rounding process, leading to inaccuracies for higher degrees[5].

To address this and better capture the presence of high-degree nodes, the **Random Hubs Method**[10] is utilized:

- **Random Hubs Method:** If the average number of nodes with a particular degree k is less than one, specifically $NP(k) = X < 1$, a node with that degree is introduced into the network with probability X. For each degree k, a random number ξ between 0 and 1 is generated. If ξ exceeds the decimal part of $NP(k)$, N_k is set to the integer part of $NP(k)$; otherwise, N_k is increased by one. This probabilistic approach ensures that the degree distribution adheres to the theoretical probabilities across multiple network realizations, accommodating the natural variability seen in real-world networks.[9]

This adaptation of the Random Hubs Method significantly refines the traditional configuration model, enabling more realistic simulations of network structures where high-degree hubs play critical roles in network dynamics and functionality.

The assignment of degree correlations in a network hinges on the properties of the statistical degree correlation matrix $P(h|k)$, which should uphold criteria of positivity, normalization, and pseudo-symmetry. The key question addressed is under what conditions can we assert the existence of scale-free networks exhibiting these correlations on an average level?

We define $\bar{k}_{nn}(k)$, the average neighbor degree of nodes[11] of degree k, as:

$$\bar{k}_{nn}(k) = \sum_{h=1}^{n} hP(h|k) \tag{3.1}$$

While various networks may share identical $\bar{k}_{nn}(k)$ profiles, they can differ in their underlying degree correlations $P(h|k)$, as discussed in [5]. Further details on the convergence behaviors of $\bar{k}_{nn}(k)$ in random and configuration model networks are documented in [5].

The assortativity coefficient r is explicitly incorporated into this definition, generally spanning from -1 to 1, with the focus here on $0 \leq r \leq 1$.

This sets the stage for subsequent sections that explore Newman's rewiring on Erdös-Rényi and Barabási-Albert networks, investigate the general case of scale-free networks with varying exponents, and present methods for inducing assortativity in these networks. Theoretical insights are supported by implementations in `networkX` and simulations aimed at comparing different network configurations and their impact on diffusion processes.

3.2.2 Rewiring process

Upon allocating a specific degree D_i to each node, or "stub," in the network, the classical configuration model traditionally attaches links randomly until each node achieves its designated degree. However, our approach modifies this procedure by introducing a partly deterministic wiring process. This method enhances efficiency, especially since it is followed by an extensive phase of random rewiring that maintains the node degrees while aligning their correlations closely with the predefined "target" correlations e_0^{jk}[16].

Initial Wiring Process

The wiring begins with the highest-degree node, Node 1, and proceeds to connect it with D_1 other distinct nodes selected randomly. As each connection is made, the number of available stubs for the connected nodes decreases by one. This step is iteratively applied to the subsequent nodes in descending order of their degree, ensuring that no node whose stubs are fully connected is selected again. The outcome of this phase is a set of links L, represented as pairs (a, b), where 'a' and 'b' are the connected nodes. For an even total node count N, the total number of links L is given by[2]:

$$L = \frac{1}{2}\sum_{j=1}^{N} D_j = \frac{1}{2}\sum_{k=1}^{n} kN_k = \frac{1}{2}\sum_{k=1}^{n} kP(k)N = \frac{1}{2}\langle k\rangle N$$

Rewiring Procedure

For the rewiring phase, based on the Newman method, two links, (a, b) and (c, d), are randomly chosen from the network. Their respective nodes possess excess degrees denoted by A, B, C, and D. The rewiring decision is driven by comparing the current link configuration's probability $E1 = e_0^{AB}e_0^{CD}$ against the alternate configuration $E2 = e_0^{AC}e_0^{BD}$. Rewiring actions are determined through a Metropolis-like decision rule[5]:

- If $E1 = 0$, the rewiring is immediately performed, replacing links (a, b) and (c, d) with (a, c) and (b, d).

- If $E1 > 0$, the rewiring probability is set by the ratio $E2/E1$, executing the rewiring if a randomly generated number ξ is less than P, where $P = E2/E1$.

Rewiring Efficacy

The algorithm's performance is quantified by tracking the successful rewirings per node, aiming for a predefined benchmark to ensure adequate reshuffling of connections to reflect the target correlations closely. Typically, this benchmark was set at approximately 1000 rewirings per node, although significant convergence is often observed with fewer cycles.

The r-coefficient and $\bar{k}_{nn}(k)$ functions are recalculated after each rewiring cycle to monitor the evolution of network properties towards the desired correlation structure. The procedure's effectiveness in managing network dynamics is thus continuously evaluated, ensuring that the final network structure robustly represents the predefined correlation patterns without significant deviations from expected behaviors.

3.2.3 Characteristics of BA Networks in the Configuration Model

In the Barabási-Albert model with parameter $\beta = 1$ (referred to as BA1), the correlation $P(1|1)$ is inherently zero, consistent with the theoretical frameworks presented by Fotohui and Rabbat. This is a direct consequence of the fully connected growth process of preferential attachment, where nodes of degree 1 are precluded from forming connections amongst themselves to avoid isolated pairs.

Applying the configuration model to scale-free networks along with random rewiring typically results in the formation of numerous isolated pairs, significantly reducing the size of the largest connected component. However, with BA1 networks designed to adhere to specific degree distributions and subjected to Newman rewiring aimed at achieving target correlations e_0^{jk} derived from $P(h|k)$, the emergence of isolated pairs is effectively prevented. This rigorous enforcement of $P(1|1) = 0$ ensures a coherent connectivity throughout the network,. Most of the smaller disconnected components tend to form as triples, which presents an interesting dynamic within the network structure.

Furthermore, the correlation $P(2|1)$ remains non-zero within BA1 networks, leading to the formation of extended tail structures where the terminal nodes enhance the $P(2|1)$ correlation, while intermediate nodes support the $P(2|2)$ correlation. When such networks are reconstructed under the configuration model, this leads to isolated triples due to the permissible connections between two nodes of degree 1 and a central node of degree 2, which remains disconnected from the main network body on the opposing side. This exemplifies the limitation of defining networks solely based on degree distributions and pairwise correlations, illustrating the need for a comprehensive network understanding.

For networks where $\beta > 1$, such as the BA2 configuration, Newman rewiring invariably leads to a fully connected network. This high level of connectivity is less influenced by the targeted correlations and more by the inherent high connectivity $h_k = 2\beta$ typical of these networks. This characteristic demonstrates that within the configuration model, the proportion of the giant component rapidly expands as the average connectivity increases. This phenomenon can be effectively observed through initial setups using the BA2 degree distribution and then Newman rewiring to achieve specific e_0^{jk} correlations.

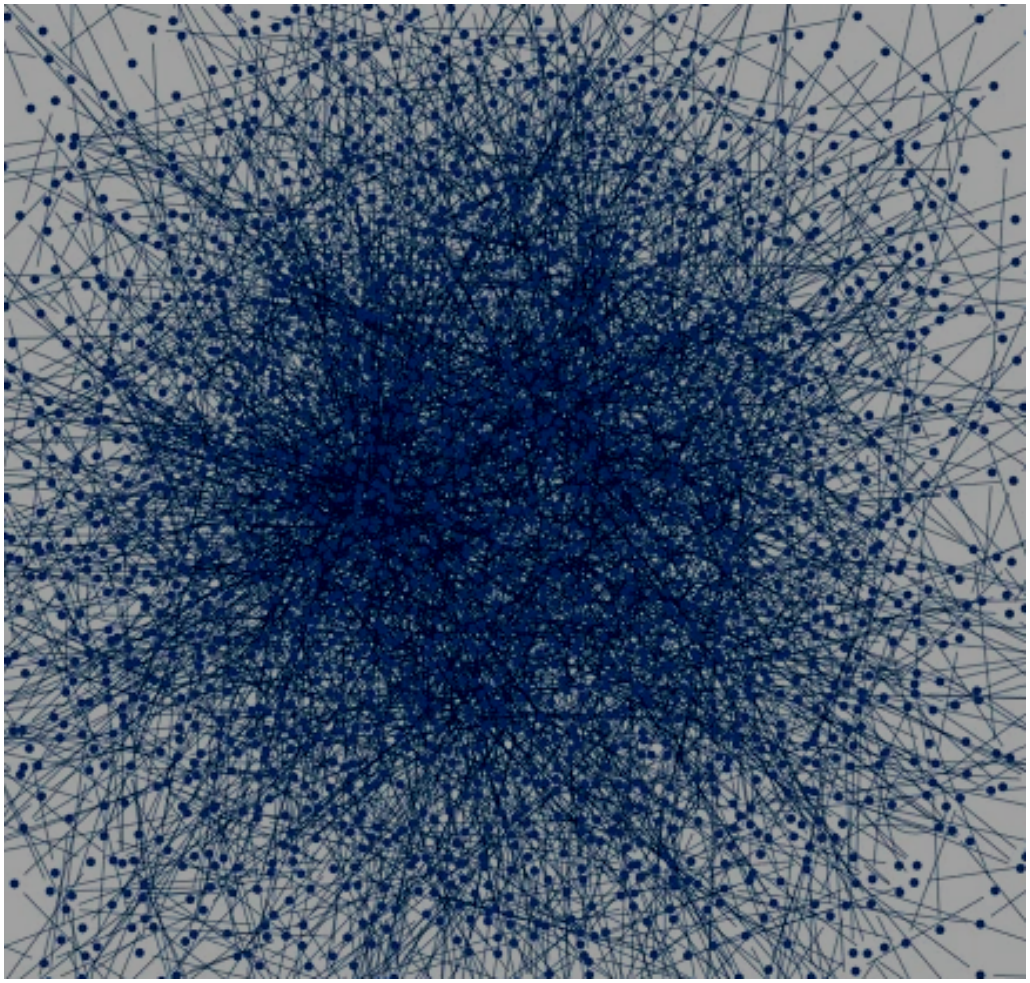

Figure 3.1: A network with N=2000 nodes obtained in Newman rewiring of BA network with =2 (“BA2”). The largest hubs have degree n80 with ⟨k⟩=3.5, compared to ⟨k⟩=2 of the BA1.

Chapter 4

Simulation

4.1 Simulation Analysis of Assortativity Coefficient

To further investigate the impact of assortative mixing parameters on network structure, we conducted a series of simulations. These simulations aimed to explore how varying the parameter p and κ influences the assortativity coefficient r within the framework of a network described by a symmetric binomial form. The binomial form is given by[16]:

$$e_{jk} = \mathcal{N} e^{-(j+k)/\kappa} \left[\binom{j+k}{j} p^j q^k + \binom{j+k}{k} p^k q^j \right], \tag{4.1}$$

where $\mathcal{N} = \frac{1}{2}(1 - e^{-1/\kappa})$ is a normalizing constant, p and q are probabilities such that $p + q = 1$, and $\kappa > 0$ is a parameter that scales the exponential decay[16].

4.1.1 Methodology for Varying p

For the simulation, we varied p from 0 to 1 in increments of 0.05. For each value of p, the assortativity coefficient r was computed based on the distribution:

$$r = \frac{1}{\sigma_q^2} \sum_{jk} jk(e_{jk} - q_j q_k), \tag{4.2}$$

where σ_q^2 is the variance of the distribution q_k, and q_k is given by:

$$q_k = \frac{(k+1)p_{k+1}}{\sum_j j p_j}, \tag{4.3}$$

with p_k following a power-law distribution $p_k \propto k^{-2.5}$.

4.1.2 Results for Varying p

The simulation revealed that the assortativity coefficient r varies significantly with p. The results, plotted in Figure 4.1, show how r changes with p, indicating the degree of assortative or disassortative mixing in the network.

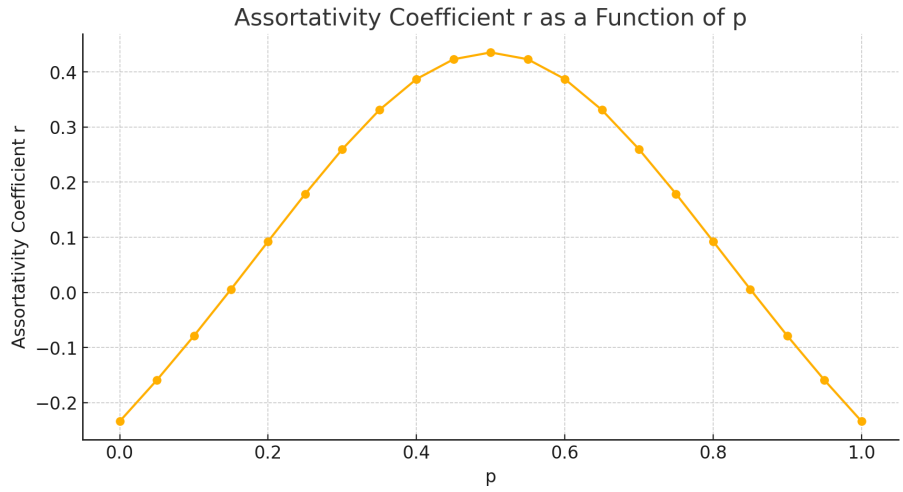

Figure 4.1: Assortativity Coefficient r as a function of p

A specific test was conducted to check if r is zero at $p = 0.1464$. The results showed that r is approximately -0.000366, indicating a nearly non-assortative mixing at this parameter setting to confirm the finding with the paper[16] as mentioned in paper at $p = 0.1464$ r is zero.

4.1.3 Methodology for Varying kappa

To understand the effect of the parameter κ on network assortativity, κ was varied from 0.1 to 5.0. For each κ, the assortativity coefficient r was computed to observe how it influences network behavior.

4.1.4 Results for Varying kappa

The graph below presents how the assortativity coefficient r changes as κ varies, reflecting its impact on network structure.

The fluctuating values of r suggest a complex interaction between κ and the network's assortative or disassortative properties, indicating that even subtle changes in κ can significantly affect network dynamics.

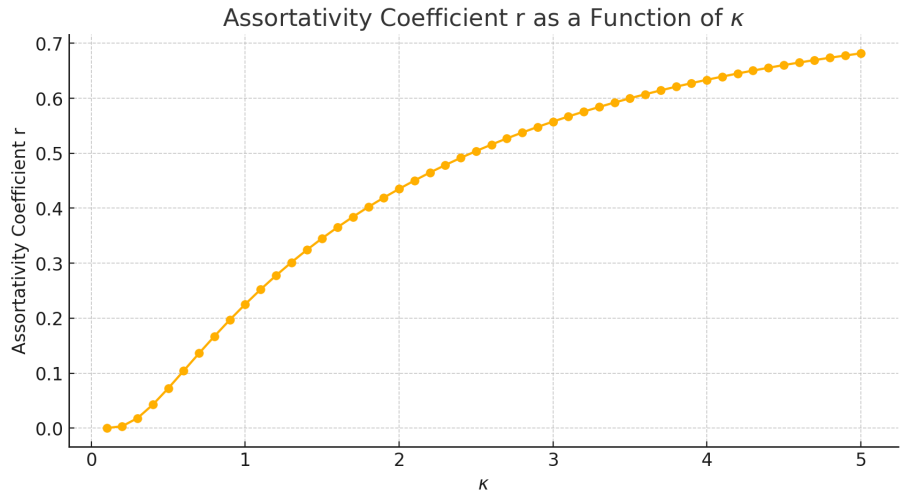

Figure 4.2: Assortativity Coefficient r as a Function of κ

4.1.5 Discussion

The analysis highlights the sensitivity of network structure to the parameters p and κ. Understanding these relationships is crucial for designing and interpreting the behavior of complex networks in various domains.

4.1.6 Detailed Findings and Discussion

These findings align with theoretical expectations about network dynamics. Assortative mixing, where high-degree vertices connect predominantly with other high-degree vertices, leads to the formation of a densely connected core group with a higher mean degree than the overall network. This structure can result in earlier percolation within these subnetworks.

Our simulations, which varied the parameters p and κ, demonstrated that the assortativity coefficient r is sensitive to these parameters. Specifically, changes in p, controlling the degree of assortative mixing, and κ, influencing the exponential decay in the degree distribution, significantly impact the network's structure and behavior. For instance, when p was set to 0.1464, the assortativity coefficient r approached zero, indicating nearly non-assortative mixing at this parameter setting.

The practical implications of these observations are substantial, particularly in scenarios such as the spread of diseases on social networks, which often exhibit assortative mixing. According to our model, such networks could maintain a 'reservoir' of disease within the core group of high-degree vertices, potentially sustaining an epidemic even

when overall network density is low. This scenario would likely confine the disease to a smaller segment of the population compared to diseases spreading on disassortative or neutral networks.

Moreover, our analysis suggests that assortative mixing increases network resilience, especially against strategies that aim to disrupt connectivity by removing high-degree vertices. This strategy is less effective in assortative networks due to the clustering of high-degree vertices within the core group, rendering such removals somewhat redundant. Conversely, in disassortative networks, where high-degree vertices are more dispersed, targeting these vertices disrupts connectivity more effectively.

In summary, our comprehensive analysis and simulation of networks reveal that assortative mixing by degree not only facilitates earlier percolation but also enhances network resilience, particularly in social networks. Conversely, disassortative networks, such as many technological and biological networks, percolate less easily and are more vulnerable to targeted disruptions. This distinction underscores the importance of understanding specific mixing patterns of networks when devising strategies for intervention and protection.

Chapter 5

Conclusion

5.1 Conclusion

In this thesis, we have conducted a thorough exploration of the structural characteristics of networks, particularly focusing on degree distribution, correlation functions, and assortativity. These features are crucial as they significantly influence the dynamics and functional behaviors observed in various network types. By leveraging advanced computational models and algorithms, this research has enabled the generation of networks with predetermined structural attributes, allowing for detailed studies of their dynamic processes and the simulation of these networks under various conditions.

The core of the methodology was the adaptation and enhancement of the traditional configuration model. This model typically facilitates the generation of uncorrelated networks by assigning a predefined degree distribution. However, one of the longstanding challenges in applying the configuration model to scale-free networks has been the accurate representation of high-degree stubs. This was addressed by refining the degree distribution definition to align with the integral criterion, which ensures a more accurate representation of scale-free networks.

Building upon this foundational model, incorporated a sophisticated rewiring algorithm initially proposed by Newman, which was designed to introduce and control assortative and disassortative mixing in the network structure. This algorithm has traditionally been applied to enhance our understanding of scale-free networks' assortative properties. In our work, we rigorously tested and validated this algorithm against networks directly generated through the preferential attachment scheme, known for naturally incorporating such assortative characteristics.

This simulations provided clear evidence supporting the effectiveness of the Newman rewiring algorithm. Notably, the analysis of the k_{nn} function across multiple network ensembles demonstrated that the rewiring algorithm could consistently reproduce expected assortative behaviors, thereby affirming the validity of our approach. These results not only corroborated the algorithm's robustness but also its applicability to exploring a broader spectrum of correlation functions, particularly in Barabási-Albert (BA) networks.

Furthermore, new rewiring criterion that minimizes fluctuations in the resulting network ensembles, allowing for the precise tuning of the assortativity coefficient. This approach enabled us to systematically investigate and manipulate specific components of network correlations. For example, in our adapted configuration model for BA1 networks, we observed the complete absence of isolated pairs, which was directly attributable to the effective nullification of the e_{00} correlation by our method. In contrast, in maximally disassortative networks with a BA2 degree distribution, we consistently found that all significant hubs were exclusively connected to nodes of degree 2.

The implications of these findings extend beyond theoretical advancements in network science. By enhancing the configurational model and developing a refined rewiring method, we have provided tools that can simplify the understanding and manipulation of complex networks. These tools are invaluable for researchers and practitioners who require precise control over network characteristics to simulate and predict network behavior under various theoretical and real-world scenarios.

In conclusion, this thesis has significantly deepened the theoretical understanding of assortative mixing patterns within different graphsical models. The knowledge and methods developed in previous works contributed profoundly to both the theory and practical applications of network dynamics, setting a robust foundation for future research in this vibrant field.

5.2 Future Scope

As observed during the course of this study, the simulations required extensive computational time and resources. This highlights a critical need for future research in the following areas:

Development of Faster Algorithms and Libraries

The development of more efficient algorithms and the optimization of existing libraries are essential to reduce the computational demands of network simulations. Future work should focus on creating and refining computational techniques that can handle large-scale networks more rapidly. This could involve leveraging parallel computing architectures or developing new algorithms that minimize computational complexity.

Analytical Approaches to Network Dynamics

While simulations provide valuable insights, there is a pressing need to complement these findings with analytical studies. Future research should aim to develop theoretical models that can predict network behaviors under various assortativity settings without relying solely on computational simulations. Analytical methods would provide a deeper understanding of the fundamental principles governing network dynamics and assist in verifying and refining simulation results.

Multi-Metric Assortativity Analysis

Assortativity analysis for complex networks has primarily been conducted using single metrics, such as degree centrality or other node-level metrics of interest, without considering the interactions between multiple metrics. Future studies should explore assortativity from a multi-dimensional perspective, incorporating various node attributes simultaneously. This approach could reveal more complex and nuanced patterns of connectivity and influence within networks, offering richer insights into their structural and functional properties.

Software and Tool Development

To make the advanced techniques developed in this thesis more accessible, there is a need for dedicated software tools that practitioners and researchers can use without extensive

programming knowledge. Developing user-friendly software that incorporates these new algorithms and analytical methods would significantly enhance the utility and applicability of network assortativity studies.

Machine Learning Models for Network Analysis

Integrating machine learning models to predict and analyze network behavior based on assortativity metrics offers a promising direction for future work. Machine learning could automate the optimization of network configurations and rewiring strategies based on desired outcomes, such as maximizing robustness or enhancing diffusion processes. Furthermore, machine learning techniques could be used to identify patterns in network changes over time, providing predictive insights into network evolution.

These areas of future work not only aim to enhance the computational efficiency and analytical depth of network assortativity studies but also seek to make these advanced methods more accessible and applicable to a broader range of real-world problems. This will facilitate a greater understanding and manipulation of complex networks across various disciplines.

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Appendix A

Appendix A

A.1 Introduction

This document provides the implementation of a scale-free network generation using the configuration model, improved discretized degree distribution methods, and the Newman rewiring algorithm. The provided code is structured into different functions for clarity and modularity.

A.2 Scale-Free Network Generation

```
import numpy as np
import networkx as nx
import random
from collections import Counter

# Constants
GAMMA = 3.0
N = 2500

# Step 1: Degree distribution and maximum degree n
def max_degree(N, gamma):
    return int(N**(1/(gamma-1)))

n = max_degree(N, GAMMA)

# Step 2: Normalized degree distribution P(k)
def degree_distribution(gamma, n):
```

```
    degrees = np.arange(1, n + 1)
    pk = degrees**(-gamma)
    c_gamma = 1 / np.sum(pk)  # Normalizing constant
    pk_normalized = c_gamma * pk
    return degrees, pk_normalized

degrees, pk_normalized = degree_distribution(GAMMA, n)

# Step 3: Cumulation Method
def cumulation_method(degrees, pk_normalized, N):
    Nk = pk_normalized * N
    degree_sequence = []
    cumulative_sum = 0
    for k, nk in zip(degrees, Nk):
        cumulative_sum += nk
        while cumulative_sum >= 1:
            degree_sequence.append(k)
            cumulative_sum -= 1
    # Fill to exactly N nodes
    while len(degree_sequence) < N:
        degree_sequence.append(random.choices(degrees, pk_normalized)
    [0])
    return degree_sequence[:N]

degree_sequence = cumulation_method(degrees, pk_normalized, N)

# Step 4: Configuration model network creation
G = nx.configuration_model(degree_sequence)
G = nx.Graph(G)  # Convert to simple graph
G.remove_edges_from(nx.selfloop_edges(G))  # Remove self-loops

# Step 5: Newman rewiring algorithm
def target_correlation(a, b):
    return 1  # Placeholder for the target correlation matrix function

def newman_rewiring(G, num_rewirings=10**6):
    edges = list(G.edges())
    for _ in range(num_rewirings):
        (a, b), (c, d) = random.sample(edges, 2)
        if len(set([a, b, c, d])) == 4:
```

```
            E1 = target_correlation(a, b) + target_correlation(c, d)
            E2 = target_correlation(a, c) + target_correlation(b, d)
            if E1 == 0 or (E2 / E1) >= 1 or random.random() < (E2 / E1)
    :
                G.remove_edges_from([(a, b), (c, d)])
                G.add_edges_from([(a, c), (b, d)])
                edges = list(G.edges())
    return G

G_rewired = newman_rewiring(G)

# Step 6: Validate network properties
def average_neighbor_degree(G):
    return nx.average_neighbor_degree(G)

def assortativity_coefficient(G):
    return nx.degree_assortativity_coefficient(G)

avg_neighbor_degree = average_neighbor_degree(G_rewired)
assortativity = assortativity_coefficient(G_rewired)

print("Average Neighbor Degree:", avg_neighbor_degree)
print("Assortativity Coefficient:", assortativity)

# Visualize the degree distribution
import matplotlib.pyplot as plt

degree_counts = Counter(dict(G_rewired.degree()).values())
degrees, counts = zip(*sorted(degree_counts.items()))

plt.figure(figsize=(10, 6))
plt.loglog(degrees, counts, 'bo-')
plt.xlabel('Degree')
plt.ylabel('Count')
plt.title('Degree Distribution')
plt.show()
```

Listing A.1: Scale-Free Network Generation

A.3 Explanation

- **Degree Distribution**: Computes the maximum degree n using the formula for a power-law distribution and generates the normalized degree distribution $P(k)$.
- **Cumulation Method**: Ensures the correct number of nodes for each degree, handling the tail of the distribution properly.
- **Configuration Model**: Creates the initial graph using the configuration model, converts it to a simple graph, and removes self-loops.
- **Newman Rewiring Algorithm**: Implements the Newman rewiring algorithm to adjust correlations using a placeholder function `target_correlation`, which should be replaced with the actual target correlation calculation.
- **Validation**: Calculates and prints the average neighbor degree and assortativity coefficient to validate the network properties.
- **Visualization**: Plots the degree distribution of the rewired network to verify the scale-free property.

The code in Appendix A provides a complete workflow for generating a scale-free network with specific degree distributions and performing the Newman rewiring process to achieve the desired network properties. Adjust the `target_correlation` function as needed to match your specific requirements.

Appendix B

Appendix B

B.1 Extended Simulation Code

The Python code below has been enhanced to simulate and analyze the effects of varying both κ and p on the assortativity coefficient r. This comprehensive simulation illustrates how r is influenced by these parameters, providing deeper insights into network behavior under different assortative mixing conditions.

```
import numpy as np
import matplotlib.pyplot as plt

# Define the function to calculate the assortativity r
def assortativity_coefficient(kappa, p, max_degree=50):
    degrees = np.arange(1, max_degree + 1)
    pk = degrees ** -2.5
    pk /= pk.sum()  # Normalize the degree distribution

    # Calculate qk based on pk and kappa
    qk = np.array([(k + 1) * pk[k] for k in range(len(pk))])
    qk /= (degrees * pk).sum()

    # Compute ejk using the normalized pk and qk
    ejk_matrix = np.zeros((max_degree, max_degree))
    for j in range(max_degree):
        for k in range(max_degree):
            ejk_matrix[j, k] = np.exp(-(j + k) / kappa) * (pk[j] * qk[k
    ] + pk[k] * qk[j])

```

```
    # Normalize ejk to ensure sum(ejk) = 1
    ejk_matrix /= ejk_matrix.sum()

    # Calculate r using the definition
    qj = pk.copy()
    mean_q = (degrees * qj).sum()
    var_q = ((degrees ** 2) * qj).sum() - mean_q ** 2
    r = (np.sum(degrees[:, None] * degrees[None, :] * ejk_matrix) -
    mean_q ** 2) / var_q

    return r

# Plot r for different values of kappa and p
kappa_values = np.linspace(0.1, 5, 50)
p_values = np.linspace(0.1, 0.9, 9)

plt.figure(figsize=(10, 8))

for p in p_values:
    r_values = [assortativity_coefficient(kappa, p) for kappa in
    kappa_values]
    plt.plot(kappa_values, r_values, label=f'p={p:.2f}')

plt.xlabel('Kappa')
plt.ylabel('Assortativity Coefficient r')
plt.title('Variation of Assortativity Coefficient r with Kappa and p')
plt.legend()
plt.show()
```

Listing B.1: Extended Python Simulation Code for Assortativity Coefficient

B.2 Explanation

The code in Appendix B extends our previous model by varying both κ and p, the key parameters in our assortativity model. The results from this comprehensive simulation are visualized in the plot, showing the variation of the assortativity coefficient r across a range of values for κ and p. This detailed analysis allows us to observe the direct effects of these parameters on network dynamics, particularly on how high-degree vertices tend to connect in different network configurations.