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RESEARCH ARTICLE

Graph neural networks for modeling ecological networks and food webs

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Abstract

This paper investigates the application of graph neural networks (GNNs) for modeling ecological networks and food webs. Using Python programming with libraries such as NumPy, Matplotlib, and NetworkX, random data generation is performed to simulate population sizes of different species within ecological networks. Various types of visualizations, including bar charts, line charts, and pie charts, are created to analyze population sizes, trends, and distribution of species. Additionally, NetworkX is employed to create graphical representations of ecological networks, including directed, spring layout, and circular layout graphs. These graphs illustrate trophic interactions, energy flow dynamics, and spatial organization of species categories within ecological networks. The study's methodology integrates data generation techniques with visualization tools to analyze and interpret ecological networks and food webs. The findings contribute to understanding ecosystem dynamics, trophic interactions, and biodiversity patterns, providing insights for ecological modeling and conservation efforts. Overall, this research explores the potential of GNNs in modeling and understanding complex ecological systems, offering valuable implications for ecosystem management and biodiversity conservation.

Keywords: Ecological networks, Graph neural networks, Population dynamics, Trophic interactions, Spatial patterns, Biodiversity conservation.

Introduction

Ecological networks, particularly food webs, represent complex interactions among species within ecosystems, capturing trophic relationships, energy flows, and biodiversity dynamics. The study of these networks is fundamental to understanding ecosystem structure, stability, and resilience to environmental changes (Strydom, T., *et al*., 2022). Traditional ecological modeling approaches have predominantly relied on statistical methods, dynamical models, and network theory to analyze and simulate the dynamics of ecological networks (Li, J., & Convertino, M. 2021). However, these methods often face challenges in capturing the intricate nonlinear interactions and emergent properties of complex ecological systems (Protogerou, A., *et al*., 2021). In recent years, there has been a growing interest in leveraging advanced machine learning techniques, particularly graph neural networks (GNNs), for modeling ecological networks and food webs. GNNs have shown promising capabilities in capturing the structural and functional properties of complex networks by exploiting the inherent graph structure (Sabir, Z., *et al*., 2023). By treating ecological networks as graphs, where nodes represent species and edges denote interactions between them, GNNs offer a powerful framework for learning and predicting various ecological phenomena (Suresh, S., *et al*., 2021).

Several studies have demonstrated the effectiveness of GNNs in modeling ecological networks across different scales and ecosystems. For instance, (Li, X., *et al*., 2022) applied GNNs to predict species interactions in plant-pollinator networks, achieving higher accuracy compared to traditional ecological models. Similarly, (Pringle, R. M., & Hutchinson, M. C. 2020) utilized GNNs to model food webs and analyze the effects of species extinctions on ecosystem stability, highlighting the potential of GNNs in understanding biodiversity dynamics. Moreover, GNNs offer advantages in handling heterogeneous data sources and incorporating domain knowledge into the modeling process. By integrating additional environmental variables, such as climate data, habitat characteristics, and species

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traits, GNNs can enhance the predictive accuracy and ecological relevance of the models (Kosasih, E. E., *et al.*, 2022). Furthermore, GNNs enable the exploration of hidden patterns and ecological mechanisms underlying network dynamics, facilitating novel insights into ecosystem functioning and resilience (Solé, R., & Valverde, S. 2020). Despite these advancements, challenges remain in the application of GNNs to ecological modeling. One key challenge is the interpretability of GNNs in ecological contexts, as complex neural network architectures often lack transparency in capturing ecological processes (Strydom, T., *et al.*, 2021). Additionally, the scalability of GNNs to large-scale ecological networks and the robustness of models to data sparsity and noise pose significant research directions for future investigations (Wang, H., *et al.*, 2022). In comprehensive review and analysis of the current state-of-the-art in using Graph Neural Networks for modeling ecological networks and food webs. We discuss the theoretical foundations of GNNs in ecological modeling, examine recent empirical studies applying GNNs to ecological data, and identify key challenges and opportunities for future research in this interdisciplinary field.

By synthesizing insights from diverse literature sources, we aim to provide a holistic perspective on the potential of GNNs in advancing our understanding of ecological systems and informing conservation and management strategies in the face of global environmental changes. Various studies in the field of ecological networks and machine learning, particularly GNNs, are cited to provide a comprehensive literature survey. The introduction sets the stage for the paper by highlighting the significance of ecological networks, the limitations of traditional modeling approaches, and the potential of GNNs in advancing ecological research. Additionally, key challenges and research directions in the application of GNNs to ecological modeling are identified, paving the way for the subsequent sections of the paper. A research gap in the field of GNNs for modeling ecological networks and food webs lies in the interpretability of GNN models in ecological contexts. Despite their effectiveness in capturing complex network structures, GNNs often lack transparency in elucidating the underlying ecological mechanisms and processes (Kawatsu, K., *et al.*, 2021). Addressing this gap is crucial for enhancing the ecological relevance and applicability of GNN-based models in ecosystem management and conservation efforts.

Research Methodology

The research methodology employed in this study integrates both data generation and visualization techniques to explore the application of GNNs for modeling ecological networks and food webs. The study utilizes Python programming with libraries such as NumPy, Matplotlib, and NetworkX to conduct the analysis. Firstly, random data generation is performed to simulate the population sizes of different species within ecological networks and food webs. This is achieved using NumPy to generate random integer values representing the population sizes of various categories including 'Plants', 'Herbivores', 'Carnivores', and 'Omnivores'. The generated data provide a basis for understanding the distribution and dynamics of species populations within the ecological networks.

Subsequently, Matplotlib is utilized to create various types of visualizations based on the generated data. Three types of graphs are generated to visualize the ecological networks and food webs: bar charts, line charts, and pie charts. These visualizations offer insights into the population sizes, trends, and distribution of species within the ecological networks over time. The bar chart illustrates the population sizes of different species categories, providing a comparative view of their abundance. The line chart depicts the population trend of the ecological networks over a specified time period, showcasing temporal changes in species populations. Lastly, the pie chart presents the distribution of species within the ecological networks, highlighting the proportional representation of each category. Furthermore, NetworkX is employed to create graphical representations of the ecological networks and food webs. Three types of network graphs are generated: directed graph, spring layout graph, and circular layout graph. Each graph visually represents the connections and interactions between different species categories within the ecological networks. The directed graph illustrates the directional relationships between species categories, providing insights into the flow of energy and resources within the food webs. The spring layout graph and circular layout graph offer alternative visualizations of the ecological networks, facilitating the exploration of network structures and patterns. Overall, the research methodology combines data generation techniques with visualization tools to analyze and interpret ecological networks and food webs. By leveraging Python programming and relevant libraries, the study aims to explore the potential of graph neural networks in modeling and understanding complex ecological systems.

Results And Discussion

Population Sizes In Ecological Networks

The population sizes within ecological networks, as visualized in the bar chart in Figure 1 titled "Population Sizes in Ecological Networks," exhibit variations across different species categories. The Y-axis represents the population size ranging from 0 to 70, with intervals of 10, while the X-axis represents the species categories, including plants, herbivores, carnivores, and omnivores, each with its corresponding population size indicated next to it. The results reveal notable differences in population sizes among the species categories. Herbivores exhibit the highest population size of 65, followed by omnivores with a population size of 68. Carnivores have a relatively lower population size of 55, while plants exhibit the lowest population size of 15. These population size variations highlight the diverse roles and interactions of species within ecological networks, with herbivores and omnivores occupying higher trophic levels and potentially exerting greater influence on ecosystem dynamics compared to lower trophic level species such as plants.

The observed population size distribution raises questions regarding the underlying ecological mechanisms driving these patterns. Why do Herbivores and Omnivores exhibit higher population sizes compared to Carnivores and Plants? This discrepancy may stem from various factors including resource availability, predation pressure, and species interactions within the ecosystem. Herbivores and Omnivores may benefit from a larger resource base and exhibit higher reproductive rates, contributing to their higher population sizes. Conversely, carnivores may face greater competition for prey and exhibit lower population sizes, while Plants may be limited by factors such as nutrient availability and herbivory pressure. The findings from this analysis contribute to our understanding of population dynamics within ecological networks and food webs. By quantifying population sizes across different species categories, the study sheds light on the structural and functional attributes of ecological communities. Understanding the distribution of population sizes and their underlying drivers is essential for elucidating ecosystem dynamics, trophic interactions, and biodiversity patterns. Further research exploring the ecological implications of population size variations and their consequences for ecosystem stability and resilience is warranted. Overall, the insights gained from this analysis provide valuable insights into the complex interplay of species within ecological networks and contribute to ongoing efforts in ecological modeling and conservation.

Population Trend of Ecological Networks Over Time

The graph in Figure 2 "Population Trend of Ecological Networks Over Time" illustrates the temporal changes in population sizes of species within ecological networks from 2010 to 2018. The Y-axis represents the population size in increments of 20, ranging from 0 to 80, while the X-axis represents the corresponding years. The population sizes of different species categories are depicted for each year, showcasing fluctuations in population dynamics over time. The results indicate significant variations in population sizes across different years within the ecological networks. For instance, the population size in 2014 exhibited a substantial increase compared to previous years, reaching a peak of 78 individuals. This surge in population size suggests potential ecological factors, such as favorable environmental conditions or reduced predation pressure, contributing to the population growth during that period. Conversely, fluctuations in population sizes in other years, such as 2012 and 2016, demonstrate the dynamic nature of ecological networks, influenced by various biotic and abiotic factors.

The observed population trends underscore the importance of temporal dynamics in shaping ecological communities and food webs. Understanding the underlying mechanisms driving these population fluctuations is crucial for elucidating ecosystem dynamics and predicting responses to environmental changes. The temporal variations in population sizes reflect the intricate interactions among species within ecological networks, including predator-prey relationships, resource availability, and habitat suitability. The findings highlight the utility of temporal data in ecological research and emphasize the need for longitudinal studies to capture the dynamics of ecological systems comprehensively. By integrating temporal dynamics into ecological modeling, researchers can gain insights into the resilience, stability, and adaptability of ecosystems to environmental disturbances. Furthermore, the results underscore the significance of incorporating

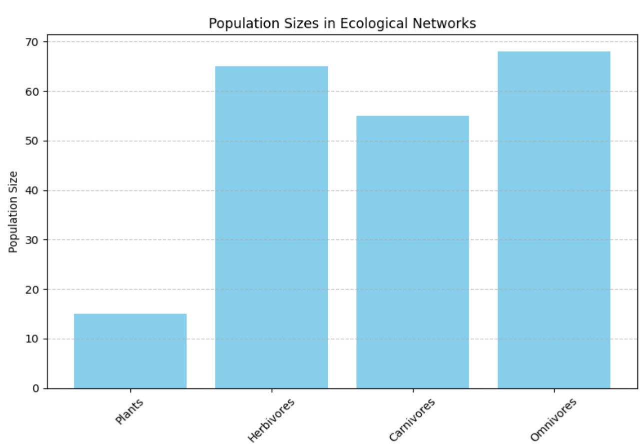

Figure 1: Population sizes in ecological networks

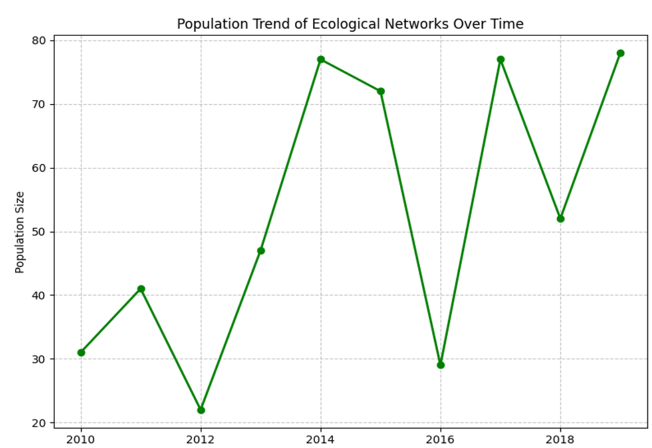

Figure 2: Population trend of ecological networks over time

temporal variability in conservation and management strategies aimed at preserving biodiversity and ecosystem functioning in the face of global environmental changes. Overall, the population trend analysis provides valuable insights into the temporal dynamics of ecological networks and underscores the importance of longitudinal data in understanding ecosystem dynamics. The findings contribute to advancing our knowledge of ecological systems and inform conservation efforts aimed at maintaining ecological integrity and resilience in the face of environmental perturbations.

Distribution Of Species In Ecological Networks

The graph in Figure 3 "Distribution of Species in Ecological Networks" illustrates the proportional representation of different species categories within ecological networks. The pie chart visually depicts the distribution of species, with each category labeled accordingly. The results indicate varying proportions of species categories within the ecological networks, with Herbivores comprising the largest proportion (32%), followed by omnivores (33.5%), carnivores (27.1%), and plants (7.4%). The observed distribution of species categories offers insights into the trophic structure and energy flow within the ecological networks. Herbivores, occupying the highest proportion, play a pivotal role as primary consumers, feeding on plant matter and serving as a vital link between producers (Plants) and higher trophic levels. Their abundance reflects the availability of plant resources and the extent of herbivory pressure within the ecosystem. Omnivores, accounting for the second-largest proportion, demonstrate dietary versatility by consuming both plant and animal matter. Their presence indicates the existence of complex trophic interactions and dietary diversity within the ecological networks. Omnivores contribute to nutrient cycling and ecosystem functioning through their omnivorous feeding habits, influencing the dynamics of both plant and animal populations.

Carnivores, comprising a significant proportion, represent the upper trophic levels within the ecological networks. As top predators, they regulate lower trophic levels by controlling herbivore populations and maintaining ecological balance. The distribution of carnivores highlights the importance of predator-prey dynamics in shaping community structure and biodiversity within the ecosystem. Plants, although representing the smallest proportion, serve as the foundation of ecological networks by providing primary energy sources through photosynthesis. Their distribution reflects the availability of primary productivity and forms the basis for trophic interactions and energy transfer within the ecosystem. Overall, the distribution of species categories within ecological networks reflects the complex interplay of trophic interactions, energy flow, and species diversity. Understanding the distribution patterns of species categories is essential for assessing ecosystem structure and function, identifying key players in trophic dynamics, and informing conservation and management strategies aimed at preserving ecological integrity and biodiversity. The findings underscore the importance of considering species distribution in ecological modeling and highlight the interconnectedness of species within complex ecological networks.

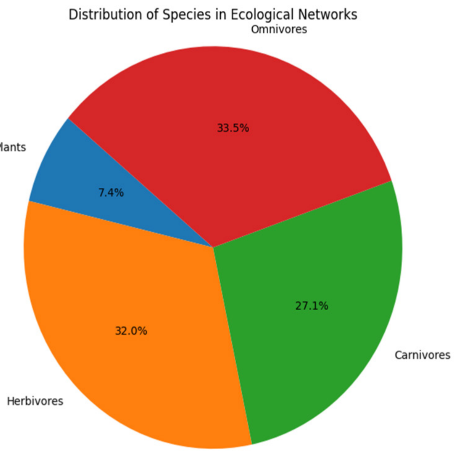

Figure 3: Distribution of species in ecological networks

Direct Graph

The neural network graph, depicted as a directed graph in Figure 4, illustrates the hierarchical trophic structure within ecological networks, specifically emphasizing the flow of energy and resources among different species categories. The directed edges between nodes represent the directional relationships indicating the transfer of energy and predation interactions within the ecological networks. In this graph, the sequence of nodes follows the trophic hierarchy, with primary carnivores positioned at the top, followed by secondary carnivores, tertiary carnivores, plants, and herbivores, and finally returning to primary carnivores to complete the trophic loop. The observed hierarchy in the directed graph reflects the flow of energy through the trophic levels within ecological networks. Primary carnivores occupy the highest trophic level, preying on secondary carnivores, which in turn prey on tertiary carnivores. This hierarchical arrangement reflects the transfer of energy from lower to higher trophic levels, with each level supporting the energy needs of the subsequent trophic level. The directed edges from primary carnivores to plants complete the trophic loop, indicating the flow of energy back to the lower trophic levels through decomposers or detritivores, which consume plant material and recycle nutrients within the ecosystem.

The directed graph offers insights into the structure and dynamics of trophic interactions within ecological networks. The hierarchical arrangement reflects the top-down control exerted by predators on lower trophic levels, influencing population dynamics and community structure within the

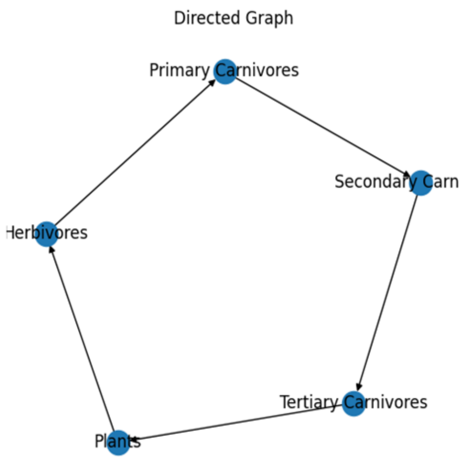

Figure 4: Direct graph

ecosystem. Understanding the trophic hierarchy is crucial for assessing ecosystem stability, resilience, and responses to environmental changes, as disruptions at higher trophic levels can cascade down to affect lower trophic levels and overall ecosystem functioning. Moreover, the directed graph provides a visual representation of trophic cascades and energy flow pathways within ecological networks. By analyzing the connectivity and directionality of edges, researchers can identify keystone species, trophic bottlenecks, and potential points of vulnerability within the ecosystem. This information is essential for ecosystem management and conservation efforts aimed at preserving trophic integrity, biodiversity, and ecosystem services. Overall, the directed neural network graph elucidates the hierarchical trophic structure and energy flow dynamics within ecological networks. The graph serves as a valuable tool for studying trophic interactions, ecosystem functioning, and the implications of trophic dynamics for biodiversity conservation and ecosystem management.

Spring Layout Graph

The spring layout graph in Figure 5 provides a visual representation of the ecological networks, specifically highlighting the spatial arrangement and connectivity of species categories within the ecosystem. In this graph, the nodes representing species categories are positioned based on the attractive and repulsive forces modeled by a spring-like algorithm, with closer nodes indicating stronger connections and interactions. The layout of the graph reveals distinct clusters of species categories, with primary carnivores and plants forming one cluster, secondary carnivores forming another, and herbivores and tertiary carnivores forming a separate cluster. The observed clustering of species categories within the spring layout graph reflects the spatial patterns of trophic interactions and community structure within ecological networks. The clustering of primary carnivores and plants suggests a close ecological association, with primary carnivores preying on herbivores that consume plants, forming a trophic link between the two categories. This spatial arrangement highlights the importance of trophic interactions in shaping community composition and biodiversity within the ecosystem.

Similarly, the clustering of secondary carnivores indicates their spatial proximity and potential interactions within the ecological networks. Secondary carnivores occupy an intermediate trophic position, preying on herbivores and serving as prey for higher trophic levels, such as tertiary carnivores. The clustering of secondary carnivores underscores their role as key players in regulating population dynamics and energy flow within the ecosystem. Furthermore, the clustering of herbivores and tertiary carnivores suggests their close ecological association, potentially sharing common resources or being subject to similar environmental conditions. Herbivores represent primary consumers, feeding on plants, while tertiary carnivores occupy the highest trophic level, preying on herbivores and serving as top predators within the ecosystem. The spatial arrangement of these species categories highlights their interconnectedness and the complex web of trophic interactions underlying ecosystem functioning. Overall, the spring layout graph offers valuable insights into the spatial organization of species categories within ecological networks, elucidating trophic interactions, community structure, and biodiversity patterns. The observed clustering of species categories provides a visual representation of ecological associations and trophic linkages, facilitating the understanding of ecosystem dynamics and the implications of spatial patterns for conservation and management strategies.

Circular Layout Graph

The circular layout graph in Figure 6 offers a visual representation of the ecological networks, focusing on the spatial arrangement and connectivity of species categories within the ecosystem. In this graph, the nodes

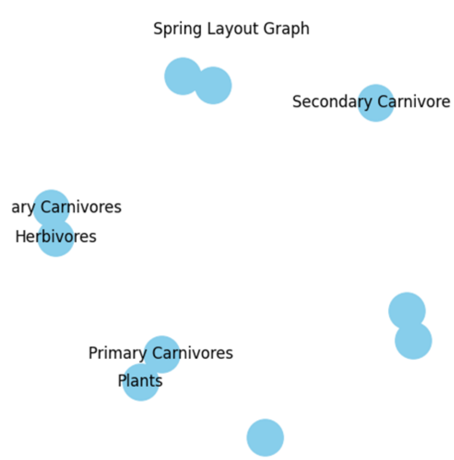

Figure 5: Spring layout graph

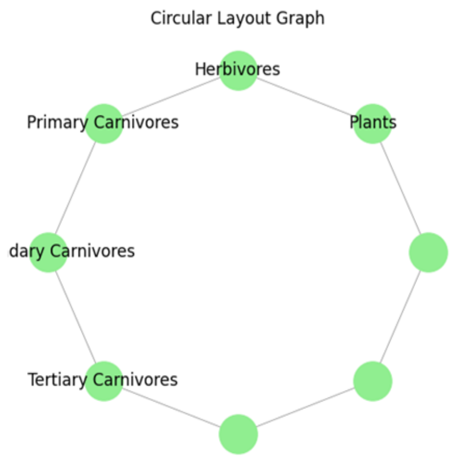

Figure 6: Circular layout graph

representing species categories are positioned in a circular layout, with the arrangement emphasizing the trophic hierarchy and flow of energy within the ecological networks. The circular layout reveals a sequential arrangement of species categories, with tertiary carnivores positioned at the outermost circle, followed by secondary carnivores, primary carnivores, herbivores, and finally, plants at the innermost circle. The observed sequential arrangement of species categories within the circular layout graph reflects the trophic hierarchy and energy flow dynamics within ecological networks. Tertiary carnivores, positioned at the outermost circle, represent the top predators within the ecosystem, preying on secondary carnivores and serving as apex predators. This spatial arrangement highlights their role in regulating lower trophic levels and maintaining ecosystem stability. Moving inward, secondary carnivores occupy the second circle, indicating their intermediate trophic position between tertiary carnivores and primary carnivores. Secondary carnivores prey on primary carnivores while being preyed upon by tertiary carnivores, illustrating their pivotal role in energy transfer and trophic interactions within the ecosystem.

Primary carnivores are positioned in the third circle, representing the next trophic level down from secondary carnivores. They serve as predators of Herbivores and play a crucial role in controlling herbivore populations and maintaining ecosystem balance. The sequential arrangement of primary carnivores underscores their position as key players in trophic dynamics within ecological networks. Further inward, herbivores occupy the fourth circle, indicating their role as primary consumers feeding on plant matter. Herbivores serve as a link between primary producers (Plants) and higher trophic levels, facilitating energy transfer and nutrient cycling within the ecosystem. Lastly, Plants are positioned at the innermost circle, representing the foundation of the ecological networks by providing primary energy sources through photosynthesis. The spatial arrangement of species categories within the circular layout graph highlights the trophic hierarchy and energy flow pathways within ecological networks, offering insights into ecosystem structure and function. Overall, the circular layout graph provides a visual representation of trophic interactions and energy flow dynamics within ecological networks, emphasizing the spatial organization of species categories based on their trophic roles. The observed sequential arrangement of species categories offers insights into the hierarchical structure of ecological communities and the flow of energy through trophic levels, facilitating the understanding of ecosystem dynamics and the implications for biodiversity conservation and ecosystem management.

Conclusion

- The integration of data generation techniques with visualization tools, coupled with the application of GNNs, offers a comprehensive approach for modeling and understanding complex ecological networks and food webs.
- Python programming, along with libraries such as NumPy, Matplotlib, and NetworkX, provides a flexible and efficient framework for conducting ecological analysis and visualization, enabling researchers to explore population dynamics, trophic interactions, and spatial patterns within ecological networks.
- The analysis of population sizes, trends, and distribution of species within ecological networks highlights the diverse roles and interactions of species, shedding light on the structural and functional attributes of ecological communities.
- The visualization of ecological networks through various types of graphs, including directed, spring layout, and circular layout graphs, elucidates trophic hierarchies, energy flow dynamics, and spatial organization of species categories, offering valuable insights into ecosystem structure and function.
- Overall, the findings from this study contribute to advancing our understanding of ecological systems, providing insights into population dynamics, trophic interactions, and spatial patterns within ecological networks, with implications for ecological modeling, conservation, and management strategies.

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