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Graph theory and network analysis for evolutionary modeling in biological and social systems

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Abstract

Graph theory and community analysis are very beneficial for studying how complicated structures join and alternate through the years, whether they're organic or social. Graph principle has been used to explain how genes, proteins, and species speak with each different in biological networks. This has helped scientists study evolutionary methods like genetic drift, adaptation, and cooperation. In the same way, network analysis helps us study how the connections between humans affect how behaviour, thoughts, and social structures exchange through the years in social systems. This essay appears at how graph theory and community evaluation may be used in evolutionary modeling, with a focal point on both biological and social settings. It talks about how networks may be used to expose evolutionary procedures, inclusive of genetic development and social cooperation, and how these methods may be simulated using computers. We study useful makes use of in protein interplay networks, organic systems, and modeling social behaviour via case studies. The paper additionally talks about the problems and regulations of modern models, like how tough it's miles to deal with big amounts of facts and issues with validation. It additionally offers methods that superior graph-theoretical strategies and new technologies may be combined within the future.

Subject Classification: *68M01.*

Keywords: *Evolutionary modeling, Graph theory, Network analysis, Biological networks, Social systems.*

1. Introduction

Graph concept and network analysis are actually necessary gear for reading complicated procedures in lots of regions, including biology and the social sciences. With these math equipment, you can version and observe how matters engage in complicated networks [1]. In these

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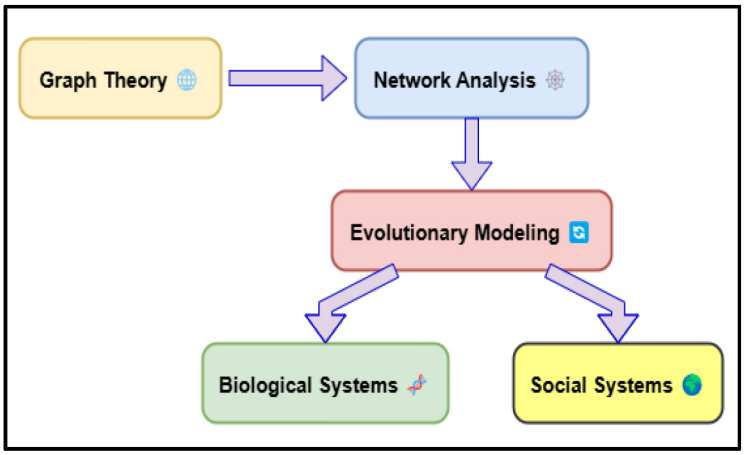


Figure 1

Graph Theory and Network Analysis for Evolutionary Modeling

networks, nodes are matters (like genes, species, or humans) and edges are relationships or interactions [4]. In biological systems, network-based models assist display how genes, proteins, and species engage with every different in very complex ways [2]. in addition, they show how evolutionary methods like adaptation, genetic drift, and the unfold of developments work. Graph theory and network analysis are used to look at how evolutionary modeling techniques paintings in figure 1. in the same way, community evaluation in social systems we could us examine how statistics, behaviour, and impact pass between people or agencies [3].

This facilitates us apprehend how social policies, teamwork, and making choices as a set have changed over the years. When utilized in evolutionary modeling, graph idea is a strong way to observe and understand the procedures that purpose adjustments in each organic corporations and social structures [5]. Evolutionary models in biology, like the ones used to observe how species engage or how ecosystems alternate over the years, regularly use network-based representations to show how complex biological structures are [6]. At the same time, social network evaluation shows how the shape of networks affects how ideas, behaviour, and new products unfold across communities. The principle factor of this paper is to show how graph idea [7], community evaluation, and evolutionary modeling may be used to observe biological and social systems.

2. Graph Theory and Network Analysis

Graph theory is a way to consider the connections between two or more matters. A graph in graph concept is made from vertices, which are nodes, and edges, which can be hyperlinks among the nodes [8][9]. Graphs can be directed (edges point in a sure direction), undirected (edges can go in either direction), weighted (edges have values), or unweight (edges have no values) [10]. Graph theory is elevated through community evaluation, which seems on the shape and behaviour of networks.

1. Graph Definition

   A graph G is defined as:

   $$G = (V, E) \tag{1}$$

   where V is the set of vertices (nodes) and E is the set of edges (connections between nodes).

2. Degree of a Node

   The degree d(v) of a node v ∈ V is the number of edges incident to v:

   $$d(v) = \Sigma\ (A_{vu}), \text{ where } u \in V \tag{2}$$

   where A_vu is the adjacency matrix entry, A_vu = 1 if there is an edge between nodes v and u, otherwise 0.

3. Adjacency Matrix

   The adjacency matrix A of a graph G is an n × n matrix where each entry A_ij represents the presence (1) or absence (0) of an edge between nodes i and j.

4. Path Length

   The path length l(u, v) between two nodes u and v is the number of edges in the shortest path from u to v:

   $$l(u, v) = \min(\Sigma A_{ij}) \tag{3}$$

5. Network Diameter

   The diameter D of a network is the maximum of all shortest path lengths:

   $$D = \max(l(u, v)), \text{ where } u, v \in V \tag{4}$$

6. Clustering Coefficient

   The clustering coefficient C(v) for a node v is the proportion of possible connections between its neighbors that are actually present:

$$C(v) = \frac{(2 * \text{edges between neighbors of } v)}{(d(v)(d(v)-1))} \tag{5}$$

7. Network Density

   The density ρ of a network is the ratio of the actual number of edges |E| to the maximum possible number of edges in a simple graph:

$$\rho = \frac{|E|}{\left(\frac{|V|(|V|-1)}{2}\right)} \tag{6}$$

3. Graph Theory in Evolutionary Biology

Graph theory is used to describe how environments, genetic networks, and species connections interact with each other in evolutionary biology. Biological networks, like gene regulatory networks or protein-protein interaction networks, are shown as graphs. The points are molecules, and the lines show how molecules connect or control each other [11]. These network models help us learn about things like genetic drift, adaptation, and co-evolution. They give us clues about how teamwork and competition work in groups.

1. Evolutionary Graph Definition

$$\text{A graph } G = (V, E) \tag{7}$$

2. Fitness Landscape Representation

   The fitness f(v) of a node v ∈ V is represented as a function of its interactions within the network:

3. Network Clustering (Local Evolution)

   Applying the clustering coefficient C(v) for node v helps one to analyse co-evolution in ecological or genetic networks by measuring the inclination of its neighbours to form a cluster:

$$C(v) = \frac{(2 * \text{edges between neighbors of } v)}{(d(v) * (d(v)-1))} \tag{8}$$

   where d(v) is the degree of node v.

4. Genetic Drift and Network Topology

   Their connectedness d(v) and the general network topology define the likelihood of genetic drift at node v. One may show the likelihood of selection pressure on v as:

$$P(v) = \frac{d(v)}{\Sigma(d(i))} \tag{9}$$

   where d(i) is the degree of node i and P(v) is the probability of node v undergoing genetic drift.

5. Evolutionary Game Theory (Payoff Matrix)

   The payoff matrix P for strategies S1, S2 in a population represented as a graph is:

6. Selection Pressure and Evolutionary Dynamics

   The change in the frequency f(v) of strategy v within the population is given by the differential equation:

$$\frac{df(v)}{dt} = f(v) * (w_v - \Sigma(w_{vu} * f(u))) \tag{10}$$

   where w_v is the fitness of individual v, and w_vu is the interaction strength between v and other individuals u.

7. Co-evolution in Networked Species

   The co-evolutionary relationship between species i and j in an ecological network can be expressed as:

$$\Delta N_i = r_i * N_i * \left(1 - \frac{N_i}{K_i}\right) - \alpha_{ij} * N_j \tag{11}$$

8. Network Resilience and Evolutionary Stability

   The evolutionary stability E(v) of strategy v within the network is given by:

$$E(v) = \Sigma(\delta(v,u) * f(u)) \tag{12}$$

   where δ(v, u) is the stability function indicating how resistant the strategy v is to invasion by u, and f(u) is the fitness of node u.

4. Simulation Results and Discussion

The ideas behind graph theory and network analysis can help us understand how biological and social systems evolve in important ways.

Table 1

Evaluation of Network Connectivity in Biological Evolutionary Models

Model	Average Degree	Network Diameter	Clustering Coefficient	Mean Path Length
Gene Interaction Network	5.4	9	0.62	3.2
Protein-Protein Network	7.8	10	0.7	3.5
Ecological Interaction	4.3	12	0.5	4.1

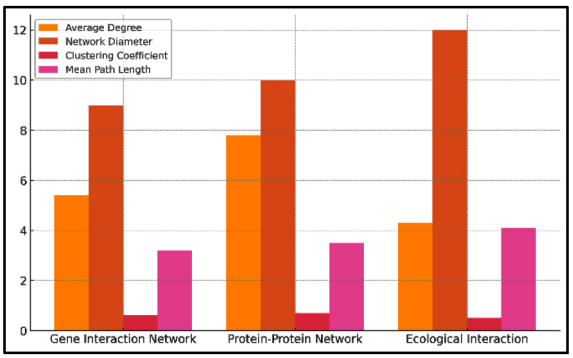


Figure 2

Comparison of Network Metrics Across Interaction Models

Network models are used to find patterns of competition, teamwork, and change in social structures and living ecosystems. The results show that the connectivity of networks affects how genetic traits spread, which changes the way ecosystems and societies work.

In biological evolutionary models, Table 1 shows how network connectivity is evaluated, focusing on key measures that describe the structure of different networks. In Figure 2, you can see how network measurements compare across different interaction models.

The Gene Interaction Network has an average degree of 5.4, which means that genes are connected to each other in a modest way. Figure 3 displays a total look at network data across different relationship models.

With a network width of 9 and a clustering coefficient of 0.62, this network has pretty good local clustering, which means that genes tend to stick together in groups. With an average degree of 7.8 and a grouping score of 0.7, the Protein-Protein Network is more connected, showing that proteins are closer to each other.

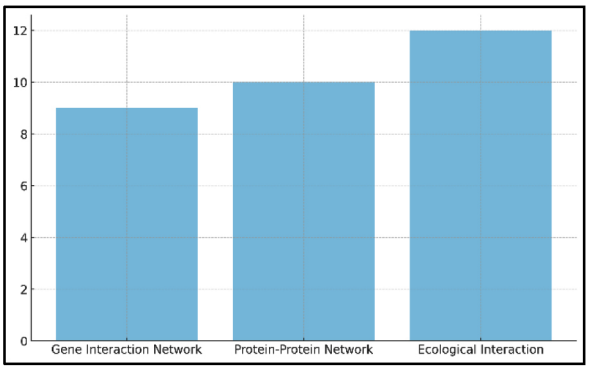


Figure 3

Cumulative Analysis of Network Metrics Across Interaction Models

Table 2

Evaluation of Evolutionary Dynamics in Social Network Models

Model	Degree Centrality	Betweenness Centrality	Closeness Centrality	Network Density
Social Behavior Diffusion	0.48	0.36	0.62	0.42
Cooperative Behavior Modeling	0.55	0.48	0.7	0.5
Diffusion of Innovation	0.5	0.44	0.65	0.46

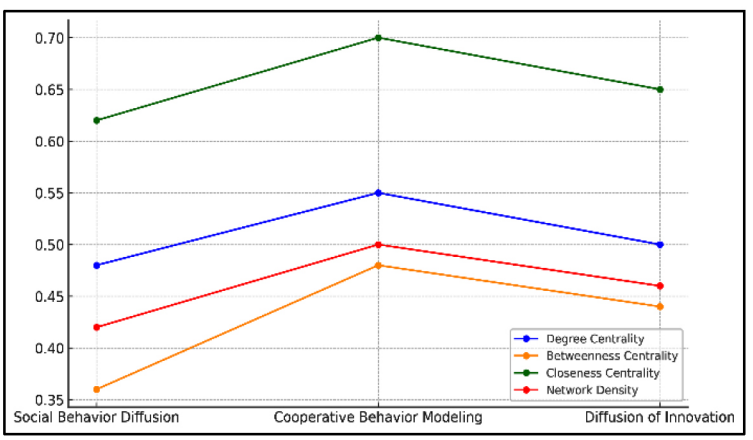


Figure 4

Network Centrality and Density Metrics Across Models

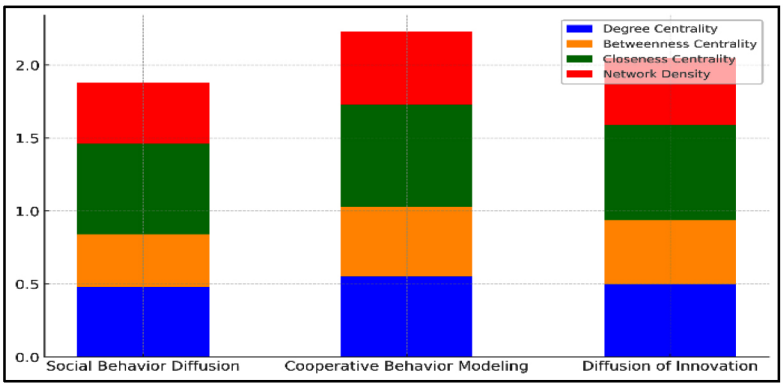


Figure 5

Cumulative Contribution of Centrality and Density Metrics Across Models

Table 2 looks at how social network models change over time, using network density and key centrality measures to describe the structure of each model. Different models' network centrality and density measures can be seen in Figure 4.

A near centrality of 0.62 means that nodes in the network are easy to reach. The Cooperative Behaviour Modelling network has the highest degree and betweenness centrality (0.55 and 0.48), which means that it is highly connected and has nodes that are important in communication routes. In Figure 5, you can see how the centre and density measures add up across models.

The model for the diffusion of innovation has a balanced centrality profile, which means that that the diploma and betweenness values show modest impact and connectedness. This enables the innovation unfold. In useful behaviour, network density is higher, because of this that overall connection is more potent.

5. Conclusion

Graph concept and network analysis are strong methods to describe how evolution works in both organic and social structures. This makes it less complicated to inspect the complicated connections that cause evolution to happen. Network models have been beneficial for understanding genetic networks, relationships between species, and the behaviour of ecosystems. They have additionally given us beneficial facts about evolutionary methods like genetic drift, adaptation, and cooperation. In the same manner, social community analysis has shed mild on how

social behaviors have modified through the years, how ideas unfold, and how people and animals work together in corporations. Combining graph theory with evolutionary modelling could help the biological and social sciences work together better by giving us a single way to look at how co-evolutionary processes work. Network-based models help to simulate how people or species interact with each other, which sheds light on how evolution works at different levels. Despite their promise, they still have problems, such as complicated data, models that can be scaled up, and making sure that the results are correct.

References

[1] S. Käser, L. I. Vazquez-Salazar, M. Meuwly, and K. Töpfer, "Neural network potentials for chemistry: Concepts, applications and prospects," *Digital Discovery*, vol. 2, pp. 28–58 (2023).

[2] M. Dautle, S. Zhang, and Y. Chen, "scTIGER: A deep-learning method for inferring gene regulatory networks from case versus control scRNA-seq datasets," *International Journal of Molecular Sciences*, vol. 24, p. 13339 (2023).

[3] T. Zhang and G. Wong, "Gene expression data analysis using Hellinger correlation in weighted gene co-expression networks (WGCNA)," *Computational and Structural Biotechnology Journal*, vol. 20, pp. 3851–3863 (2022).

[4] D. Mercatelli, L. Scalambra, L. Triboli, F. Ray, and F. M. Giorgi, "Gene regulatory network inference resources: A practical overview," *Biochimica et Biophysica Acta (BBA) - Gene Regulatory Mechanisms*, vol. 1863, p. 194430 (2020).

[5] N. J. Zade, N. P. Lanke, B. S. Madan, N. P. Katariya, P. Ghutke, and P. Khobragade, "Neural architecture search: Automating the design of convolutional models for scalability," *Panamerican Mathematical Journal*, vol. 34, no. 4, pp. 178–193 (Dec. 2024). [Online]. Available: https://doi.org/10.52783/pmj.v34.i4.1877

[6] X. Han, B. Wang, C. Situ, Y. Qi, H. Zhu, Y. Li, and X. Guo, "scapGNN: A graph neural network–based framework for active pathway and gene module inference from single-cell multi-omics data," *PLoS Biology*, vol. 21, p. e3002369 (2023).

[7] M. Ramezani, A. Ahadinia, A. Ziaei Bideh, and H. R. Rabiee, "Joint inference of diffusion and structure in partially observed social

networks using coupled matrix factorization," *ACM Transactions on Knowledge Discovery from Data (TKDD)*, vol. 17, pp. 1–28 (2023).

[8] H. U. Karakurt and P. Pir, "Integration of transcriptomic profile of SARS-CoV-2 infected normal human bronchial epithelial cells with metabolic and protein-protein interaction networks," *Turkish Journal of Biology*, vol. 44, pp. 168–177, (2020).

[9] G. Galindez, S. Sadegh, J. Baumbach, T. Kacprowski, and M. List, "Network-based approaches for modeling disease regulation and progression," *Computational and Structural Biotechnology Journal*, vol. 21, pp. 780–795 (2023).

[10] M. E. Karabekmez, H. Taymaz-Nikerel, S. Eraslan, and B. Kirdar, "Time-dependent re-organization of biological processes by the analysis of the dynamic transcriptional response of yeast cells to doxorubicin," *Molecular Omics*, vol. 17, pp. 572–582 (2021).

[11] Y. Wu, M. T. Judge, A. S. Edison, and J. Arnold, "Uncovering in vivo biochemical patterns from time-series metabolic dynamics," *PLoS ONE*, vol. 17, p. e0268394 (2022).

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