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# A Survey of the Analysis of Complex Systems based on Complex Network Theory and Deep Learning

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#### **Abstract**

From the perspective of complex network theory, complex systems can be characterized by the interaction of microscopic units through nonlinear effects, yielding macroscopic emergent behavior. In light of the powerful capability of deep learning in feature extraction and model fitting from large amount of datasets, we try to overview the benefits of combining the complex network analysis with deep learning techniques to investigate complex systems. We first explore the existence of complexity in complex systems. In what followed, we first give a brief description of complex network theory. Then, we present an overview of deep learning technology. Subsequently, we focus on the research advances and applications in the analysis of complex systems based on complex network theory and deep learning. The last section is further discussion and prospects for the combination of these two methods. In a nutshell, the development of deep learning combined with complex network theory allows for exploring the complexity in complex systems at a higher level.

Keywords: complexity; complex systems; complex networks; deep learning

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## 1. Introduction

Complexity in complex systems has always been a problem that scientists are committed to pursuing and deeply exploring. Truthfully, its development has been entirely driven by research methods. For example, before the advent of computers, people mainly employ the method of reductionism to study complex systems which are questionable due to the discovery of nonlinear interactions [1]. In the 1990s, the research groups from Santa Fe Institute gradually formed, giving rise to the birth of network science which is capable of characterizing the complex systems in various fields [2]. In the course of research, graph theory provides a highly effective mathematical tool used to model complex systems as a network. Afterwards, network analysis based on small-world model, scale-free model and various kinds of network models permeated all corners of complexity research [3,4]. Since 2010, in light of the advent of big data and computational social science, complexity research has gradually stepped into a new stage of development with deep learning techniques involved.

The complex network theory is mainly employed to characterize network structure and explore the function of complex systems. In the course of theory development, there have been a lot of fundamental quantities and relevant measurements developed [5]. However, it has been clearly noticed that with the rapid development of information technology, the increasing amounts of data are more readily available than before. Therefore, it is becoming increasingly imperative in complex network research to discover the desired nodes relationship from the vast amount of data, to find the patterns and "extra" features hidden in the data, and to use them rationally to build a close-to-reality network under study as the scale and type of data we are able to collect continues to grow [6]. To this end, the advances in machine learning (ML) techniques come into play.

Machine learning refers to a large set of algorithms for data mining, which include logistic regression, decision trees, collaborative filtering, etc [7]. The development of machine learning is divided into two parts, Shallow Learning and Deep Learning. Shallow learning originated in the 1920s with the invention of the back-propagation algorithm for artificial neural networks, which led to the popularity of statistical-based machine learning algorithms. Afterwards, in 2006, Hinton proposed the Deep Neural Network algorithm, which greatly improved the capability of neural networks [8]. The advantages of deep

learning mainly lie in automatically extracting hidden features and pattern recognition in massive datasets. The first conjunction point between complex network theory and deep learning technology is that deep learning algorithms as an advanced and intelligent tool for data analysis can be used to exploit the hidden information behind network structure. The characteristic features of network structure (e.g. average degree, node centrality, degree distribution, average short path) can be applied as the input variables for training the DL algorithms to predict those properties. Another point where complex network theory and deep learning can be combined lies in that data can be represented by means of networks to capture the relations among data space, topology, and functions of systems. Accordingly, in this work, we focus on the benefits and necessities of combining complex network theory with deep learning techniques to study complex systems from above mentioned two points of combination.

The contents of this work are organized as follows. In section 2, we review the complexity in the complex networks. Then, we present a brief introduction of complex network theory in section 3. Once a short overview of deep learning in section 4 is conducted, we place emphasis on the combination of complex network theory and deep learning in terms of their applications in section 5. Following that, we discuss the prospects for deployment of deep learning in complex systems concerning complex network theory in the last section.

## 2. Complexity in Complex Networks

The universe and everything in it can be regarded as Complex Systems composed of intricately connected segments. Since Newton established the three laws of mechanics, it is generally believed that as long as we can figure out the properties of the components of a system and their interactions between them, then the future behaviors of these systems can be accurately predicted, which makes the primary argument of early methodology *Reductionism* [1,9] for the analysis of the real-world systems. Thereafter, Laplace proposed the well-known *Laplacian determinism*. Accordant with the belief expressed in reductionism, the statement emphasizes that it is possible to give a precise prediction of future states at an arbitrary time according to the fundamental equations of the evolution of a system and the initial states [10].

However, there exists a plethora of systems that are not suited to be discussed with the reductive method. In addition, the great success of reductionism in physics does not mean that it can achieve the same success in different disciplinary fields, such as in social sciences, biological sciences, and so on [11]. In 1972, the famous paper `More is Different" written by Anderson criticized the argument of reductionism, pointing out that the fundamental laws obtained by reducing systems into the basic structural units do not imply that systems can be reconstructed [12].

Admittedly, the interaction of basic elements involves an immense amount of complicated factors which are intricately interlinked. Therefore, not only is it impossible to carry out an analytical discussion of dynamics, but it is also impossible to calculate from scratch with "ideal precise" values without considering approximations. Moreover, as the "organization" of the elementary units of such a system will present many *emergent* properties that will not be exhibited by a considerable number of discrete individuals, it is impossible to make predictions about the rich behavior of the entire system solely based on the characteristics of an independent unit, such as the typical *adaptive systems*. Broadly speaking, the above-mentioned circumstances have contributed to the *complexity* of complex systems simultaneously.

## 3. Introduction of Complex Network Theory

From the previous statements, it can be concluded that complex systems must be explored from a holistic perspective, taking into account the mechanisms of individual behaviors and their interactions. There is no denying that complex network theory has certainly become the most ubiquitous and powerful tool to characterize the complexity in complex systems. Broadly speaking, a large number of complex systems can be modeled as complex networks composed of a group of components and connections [5,13,14,15]. In this sense, exploring the relationship between network structure and function is closely related to understanding the nature of complex systems. In a special issue on complex systems published in Science [16], there is an enlightening quote from Barabási who pointed out that since the underlying structure has a crucial effect on the behavior of the system, there is no way to understand complex systems without exploring the network structure, which also promotes the use of complex network theory to study complex systems.

To conduct complex network research, the knowledge from different fields, such as statistical physics, game theory, probability and mathematical statistics is required. Among them, graph theory is recognized as the mathematical basis of complex network research. Currently, it is widely accepted that the first theorem in graph theory is specifically originated from the solution of the Königsberg bridge problem solved by great Swiss mathematician Leonhard Euler [17,18]\cite{Euler1741,Biggs1986}. As shown in Fig.1, Euler proposed that the bridge crossing problem can be abstractly reduced to the combination of points and lines on the plane, i.e., interpreting it to be a graph by considering the land portions as four points (*vertex*) and the seven bridges as connections (*edge*) between them.

From 1736 to 1950s, the field of graph theory was substantially expanded, but it was limited by the lack of tools for large-scale computation. With the invention of modern computers, the matrix description of graphs attracted a lot of attention. Afterwards, massive problems sprung up about using *graph* to describe the large real networks, e.g. power grids, traffic networks, communication networks and so on. In the decades that followed, a remarkable collection of scientists introduced ideas, methods, and analysis tools of statistical physics into graph theory, giving birth to *network science* [19,20].

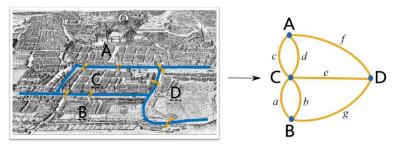


Figure 1. Illustration of the problem of the Seven Bridges of Königsberg.

According to the complex network theory, a system can be reduced to an abstract structure, only capturing the basic patterns of interactions which are crucial to comprehend the behavior of complex systems. Put in the simple terms, a network is a collection of discrete objects joined together, usually described as *nodes* connected by *links* in the jargon of the field [21]. When looking at a network, the research task of interest usually can be phrased in terms of its topological properties reflected by its unique connection patterns. Hence, the statistical summaries of network structure can support us in comprehending their topology and, consequently, understanding the mechanisms behind their dynamical processes. There are many fundamental quantities and corresponding measures developed to characterize networks, such as, degree, clustering, path and so on [5,22,23]. The commonly used statistical metrics in complex networks mainly include three categories as shown in Table 1:

Table 1. Summary of statistical descriptions of complex networks

	Classification	Metrics			
local information Node degree		gree			
	Global information	Network diame	eter, Average degree, Cl	lustering c	oefficient, Modularity, Network Radius, etc.
	Mixed local and global information	Betweenness	centrality, degree centra	ality, Eiger	nvector centrality, PageRsnk algorithm, etc.

Along with richer available data in recent decades, the scientific interest has shifted from the application of concepts developed based on graph theory to the investigation of the dynamical evolution of network topology, structural representation, pattern recognition, etc. [13]. It is thus clear that the most primitive driving force behind the development of complex networks is the acquisition and exploitation of the new data as Barabási's view [24] states:

"Fuelled by cheap sensors and high-throughput technologies, the data explosion that we witness today, from social media to cell biology, is offering unparalleled opportunities to document the inner workings of many complex systems."

--- Albert-László Barabási

Thanks to advances in high technology, it has become effortless and inexpensive to collect massive amounts of multirelational data [6]. Nevertheless, for many complex systems, it has not been possible to obtain a complete data of network structure [13, 25]. The challenges posed by the era of big data leads to the realization that deeper exploration of big data has far surpassed the ability of manual analysis. Moreover, despite the powerful calculation capability of computers, the algorithmic problems pertaining to complex network analysis, such as community structure mining and link prediction in giant social networks [26,27], need to be addressed in depth. Faced with huge amounts of data, to end the era when researchers dedicated to the study of complexity in complex systems by manually inventing characteristic metrics, we have to draw on the techniques of machine learning, especially deep learning technology.

## 4. Overview of Deep Learning

Recently, more and more researchers pay attention to the crossover study of complex systems by complex network theory and deep learning technology. Before introducing deep learning, we should first introduce *Artificial Intelligence* (AI) and *Machine Learning* (ML) in order to clarify the relationship between AI, Machine Learning, and Deep Learning. In 1956, the concept of "artificial intelligence" is formally introduced by several scientists at a conference in USA. Literally, the term of Artificial Intelligence can be simplified as "a man-made thinking capability"," including learning, reasoning, and self-correction.

Machine learning is both a core technology to implement artificial intelligence and a discipline used to study how to achieve a technology that allows machines to solve complicated problems like a human [28]. In simple terms, machine learning can be explained to learn patterns from historical data and apply them into future predictions to improve certain performance measurements. The learning paradigms are mainly divided into three ways, i.e., unsupervised learning, semi-supervised learning, and supervised learning [29,30]. Unsupervised learning mainly learns and discovers the internal connections among to explore the overall structure by taking advantage of samples similarity or topologies. In this process, the training samples exclusively use unlabeled data without the guidance of output variables and feedback functions. However, supervised learning uses a group of labeled samples to achieve the required performance. Semi-supervised training methods lies between the above two learning paradigms and primarily considers how to use a small number of labeled samples and a large number of unlabeled samples to conduct training and classification problems [31].

Deep learning is a sub-field of machine learning which uses more than three layers of neural networks, also known as deep neural networks [8]. It uses multi-level nonlinear information processing and abstraction for feature learning, representation, classification, regression, and pattern recognition in a way of supervised learning, unsupervised learning, and semi-supervised learning [32]. Each module in Deep learning transforms the low-layer representation into the high-layer one, composing enough transformations layer by layer to learn very complex functions. Currently according to different structures, commonly accepted models of DL are Deep belief network (DBN) based on Restricted Boltzmann machine (RBM) [8], Deep neural network (DNN), Stacked Autoencoder (SAE) based on Autoencoder (AE) [33], Deep Boltzmann machine (DBM) [34], Convolutional neural networks (CNN) [35] and Recurrent neural networks (RNN) [36]. Deep learning technology conducts data processing by combining brain-like cognitive mechanisms, breaking the bottleneck of traditional neural network in practical applications, especially in image recognition, semantic understanding and speech recognition [37,38,39,40,41,42].

## 5. Combination of Complex Network Theory and Deep learning

To explore the complexity in complex systems, combining complex network theory and deep learning techniques is becoming an effective and powerful strategy, attracting extensive attention. The combination of two cross-disciplines are twofold. On the one hand, the network scale goes increasingly large due to the dramatic growth in the data volume, leading to the need for rapid information mining that cannot be achieved solely through complex network analysis. With the rapid development of artificial intelligence, it is possible to mine the information in complex networks, such as topological structure, the statistical characteristics of our concern (e.g., key nodes, degree distribution, path) by means of machine learning algorithms, especially deep learning techniques.

On the other hand, the key issue is how the complex network theory can be applied to tackle the problems of supervised and unsupervised learning in deep learning. It is well known that data is regarded as the "fuel" of machine learning. The operation of various models in machine learning strongly relies on datasets that is a collection of many samples. In the algorithms of machine learning, we usually use vectors to store information about a sample of data. Therefore, the response to the key issue is to convert the commonly used vector-based data to the network-based data. In this way, a variety of models in complex networks can be used in machine learning. As a consequence, the data represented in the form of networks effectively captures the relationships between spatial structure, topology, and function of datasets. In this work, we will focus on the research advances and applications regarding deep learning based on complex network theory.

In recent decades, there have been many achievements in studying the complex systems through the combination of complex network theory and deep learning technology. In the following sections, we will address the research process in terms of above two aspects.

## 5.1. Applications of Deep Learning in Complex Networks

In the area of many large-scale complex systems, such as social systems, biological systems, etc., the features and topology are becoming difficult to be described and captured only through complex network theory. In this case, the advances of machine learning, especially deep learning techniques, provides ideas for mining the network information. There have been many achievements for deep learning algorithms applied in complex networks, including structural metrics or other network information extraction. One popular aspect of application is to identify the key nodes and key links. In this area, machine learning has achieved notable success. For instance, Pereda et al. developed a new way to identify clusters in networks which is applied through a Euclidean hyper-dimensional representation of relational data, belonging to a geometric unsupervised learning paradigm [43]. Adam et al. proposed the ARACNE algorithm to detect the non-directly connected links and delete them which is helpful to obtain the simple correlated subgraphs. The core of this algorithm is to analyze the links between three nodes in each group and iteratively delete the links that are below the given threshold of mutual information [44]. Of course, the more superior technology, i.e., deep learning performs well in this respect. In Ref. [45], authors proposed a

framework FINDER with reinforce learning and deep neural networks to find an optimal set of nodes. The framework could automatically optimize the goal relying on the small synthetic graphs which are constructed by toy models. Surprisingly, it can be generalized in a wide variety of real-world systems, improving their robustness and resilience.

Table 2. Summary of applications of deep learning in complex networks

Application	Area	Reference	
Key nodes identification	Many real-world systems	Fan et al. [45]	
Statistical features extraction	Brain networks, Social networks	Gao et al. [46]	
		Ha et al. [47]	
Security issues	Cellular networks	Hussain et al. [48	
		Lv et al. [49]]	
Community detection	Social networks	Dhilber et al. [50], Cao et al. [51], Li et al. [52], Zhang et al. [53]	
Link prediction	Social dynamic networks	Chen et al. [54], Wang et al. [55], Chiu et al. [56]	

Another wide application for deep learning techniques in complex networks is to extract the statistical characteristics. For example, the time series recorded by Electroencephalogram (EEG) signals obtained from complex brain systems can detect the synchronization characteristics between neurons in the brain. The intricate connections between structure and function of brain systems reveal that brain networks are considerably complicated so that the feature extraction and complex classification problems need deep learning approach to provide solutions. Gao et al. proposed a framework to recognize the fatigue driving. The convolutional neural networks are helpful to conduct the analysis of EEG signals to realize a better feature extraction [46]. The authors proposed a generalized framework with deep learning methods (i.e., graph attention networks), called AgentNet, used to model the hidden interactions between agents in complex networks [47].

In addition, deep learning methods show the preeminence in exploring the popular generation of cellular systems (5G) which are considered as cellular signaling networks. Hussain et al. leveraged the deep neural network to detect the anomalies and conduct mobile edge computing (MEC) paradigm. The framework utilizes real call detail record data to achieve a very high accuracy up to 98.8% [48]. In Ref. [49], authors considered deep learning technology to deal with security problems in 5G cellular networks and greatly reduce the calculation complexity. The superiority of the unsupervised deep learning algorithm can contribute to meeting security needs in 5G heterogeneous networks.

There are two other areas where deep learning plays an important role on complex networks, especially in social networks, namely community detection and link prediction. In the case of community detection, Dhilber et al. developed a deep learning framework with multiple autoencoders stacked. They also applied parameter sharing to detect community and obtained successful results [50]. The authors devised an approach by applying autoencoder into community detection after the discovery the similarity between autoencoders and spectral clustering [51]. In Ref. [52], they proposed an algorithm for community detection based on the sparse autoencoder which operates in an unsupervised deep learning way. The authors get the similarity matrix by combining weighted adjacent paths of node and the path weight matrix, improving detection accuracy. Zhang et al. developed a framework involving a generative adversarial network in a semi-supervised way for community detection. The training data is composed of several communities in a network [53]. On the other hand, deep learning technology has appeared superior in terms of link prediction in complex networks. Chen et al. proposed a deep learning architecture, called E-LSTM-D, to solve long-term link prediction problems in dynamic networks [54]. In Ref. [55], they devised a relational deep learning framework following Bayesian method. They also used the product of Gaussians (PoG) structure in the RDL model to predict links. Chiu et al. applied weak estimators used in deep learning algorithm to generate an efficient feature vector for link prediction in dynamic networks [56].

## 5.2. Applications of Complex Network Theory in Deep Learning

In the research direction of deep learning technology based on complex network theory, the key lies in how to represent the commonly used vector-based data with network-based data. The vector-based data are one by one points, while network-based data are composed of nodes and links. The local relevance between two data sample points and the global structure derived from the local information can be represented in a way of networks. Then, the problem is transferred to how to generate the relations between pairs of points. Therefore, we consider network construction techniques to convert the input sample set into a network, mainly including three ways: (1) leveraging the information of a small portion of nodes information, that is the local geometric information of data [57,58], (2) utilizing not only the local one, but also the long distance information, such as a shortest path trajectory [59,60], (3) considering the aggregate information from all data [61].

The major breakthroughs in deep learning technology are mainly in the field of natural language, (e.g., speech, audio) processing, and image recognition in the way of unsupervised learning, semi-supervised learning, and supervised learning as well. [35,37,62,63,64,65,66]. The fruitful performance in the field of image and language reveals that the biggest advantage

of deep learning is to automatically mine the "structure" of systems at a higher level. Then, the direction of utilizing deep learning technology to automatically extract hidden features from large-scale network data lies in how to interpret the language and image into the representative networks.

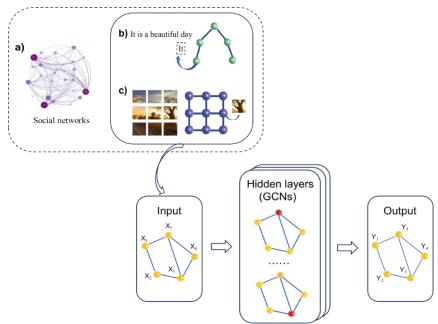


Figure 3. Framework of Graph Convolutional neural network (GCN). (a) A social networks that consists of 35 countries where 22 soccer teams had contacts, extracted from Pajek datasets (<a href="http://vlado.fmf.uni-lj.si/pub/networks/data/sport/football.htm">http://vlado.fmf.uni-lj.si/pub/networks/data/sport/football.htm</a>). (b) A sentence is a sequence, which can be considered as a tree graph or a line graph. (c) An image that can be regarded as grid graphs with size fixed.

In terms of complex network theory, the characteristic of a node or link is naturally determined by its network. As long as each node is assigned to an N-dimensional vector, we can get a cloud of nodes in N-dimensional space to represent the entire network. Therefore, in the case of language, the words that appear in the same sentence can be linked to each other to form a co-occurrence network in which each word is indicated by each node and a link represents the simultaneous occurrence. In 2013, Miklov pioneered a vector representation of English words, called Word2Vec that can quickly construct a point in N-dimensional space for each word [67].

The image belongs to a static two-dimensional array with very standard data structure, while a network is an irregular data type between a two-dimensional array and a one-dimensional sequence. Consequently, we cannot consider a network as an image since the nodes of the network do not have the same regular adjacent relationship between pixels of an image. Meanwhile, we also cannot regard a network as a one-dimensional sequence of nodes and links (see comparisons between them in the above panel of Fig. 3). The reason is that the network keeps unchanged when we arbitrarily reverse the order between nodes. Nevertheless, deep learning can be deployed in the complex network related tasks due to its outstanding performance in image identification. For example, the Graph classification problem related to identify or classify what kind of network the system belongs to can be addressed by the Graph Convolutional neural network (GCN) which is an extension of Convolutional neural network (CNN) [68]. The GCN is of course one of deep neural networks while the input is graph-based data as shown in Fig. 3 where the input data can be a text or an image. It can leverage the structure of networks and aggregate node information from adjacent nodes in a convolutional way by defining the graph convolutions from a spectral and spatial perspective [69,70].

Table 3. Summary of applications of complex network theory in deep learning

Area	Applications	Reference	
Natural language processing	Documents classification in two ways	Leverage node classification [71,72]	
		Model text as a network (graph) [73,74]	
Computer vision	Image and video classification	Garcia et al. [78], Zhang et al. [79], Marino et al. [80]	
Science (chemistry, biology, physics) Chemical reaction prediction.		Li et al. [81]	
	Protein interface prediction,	Fout et al. [82]	
	Physics prediction	Mrowca et al. [83]	
		Kipf et al. [84]	

The GCN models have achieved a great success in many related areas. In the field of natural language processing, there are two ways for documents classification, i.e., leveraging node classification to classify texts into different categories [71,72] and classifying the documents through graph classification once texts are modelled as a network (graph) [73,74]. The GCN models are used for event detection and extraction in sentences in which the CNN is based on a kind of graph, called dependency trees [75,76]. Yao et al. applied the GCN into the task of text classification by constructing the document relational network [77].

In the domain of images and videos classification, authors in Ref. [78] defined a graph neural network framework where nodes represent images and links are the similarity between input images to study the few-shot learning problems. The GCN models are used to encode nodes, taking advantage of the association structure information between images. In addition, Zhang et al. developed a framework to extend the few-shot learning with GCN models which perform superior in audio classification [79]. Marino et al. employ the GCN models in the task of image classification by using prior knowledge from knowledge graphs to gain improvements on the multi-label classification task of the dataset [80].

The graph convolutional network models are not only used in natural language processing and image recognition, but also in the domain of science, such as chemistry, biology, and physics. For instance, the authors in Ref. [81] proposed a attention-based GCN architecture used to predict the chemical stability in drug discovery. Fout et al. applied GCN in the prediction of Protein interface where protein is represented as node [82]. The GCN models are also used in physics prediction for classifying IceCube signal [83]. Kipf et al. proposed an unsupervised model, namely neural relational inference (NRI) to learn relational structure inference and learn dynamics simultaneously for the prediction in interacting systems [84].

#### 6. Discussion and Conclusion

To gain a deep insight into the complexity of real-world complex systems, we proceed this work from a complex network perspective combined with deep learning technology. In modern research, complex network has become a standard universal language to describe complex systems. It allows us to interpret systems as the essential abstraction of their interaction structures. In other words, complex networks can be regarded as the skeleton of complex systems. Although there have been abundant descriptors and feature metrics in networks developed, artificial intelligence performs better in the face of huge amounts of data. More specifically, the large number of achievements in deep learning in the field of image recognition show that once machines can learn to extract features automatically, we can make predictions and recognition with a high level of accuracy that is unimaginable to humans, such as its excellent application in face recognition.

Meanwhile, deep learning can be combined with traditional techniques, including multi-subject simulation and system dynamics, increasing the possibility to achieve automatic modeling of complex systems. In addition, the study about complexity can also help us better understand deep learning models. For example, a group of physicists has recently been trying to understand deep neural networks by using Variational renormalization group, where neuron nodes in each layer is performed a higher level of coarse granulation based on the original problem [85].

In conclusion, there is an inevitable trend to integrate complex network theory and deep learning into the study of complex systems. However, there is still a lot of work that deserves further exploration, such as the development of new models for feature extraction and effective learning paradigms in deep learning. Moreover, the large amount of data in networks (graph), such as social networks, cannot be easily represented by vectors because its size and structure are changeable. In real-world systems, the networks tend to show dynamic properties, including those that have nodes and edges that constantly change over time. Therefore, developing a deep learning framework that can model network dynamics is an important research direction. In addition, researchers design deep learning technology only for one property in complex networks, such as characteristics of links, nodes, clustering, etc. The problem of developing a generalized deep learning model to express many complexity properties of networks is worthy of deep investigation in the future.

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