GC-LSTM: Graph Convolution Embedded LSTM for Dynamic Link Prediction

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Abstract—Dynamic link prediction is a research hot in complex networks area, especially for its wide applications in biology, social network, economy and industry. Compared with static link prediction, dynamic one is much more difficult since network structure evolves over time. Currently most researches focus on static link prediction which cannot achieve expected performance in dynamic network. Aiming at low AUC, high Error Rate, add/remove link prediction difficulty, we propose GC-LSTM, a Graph Convolution Network (GC) embedded Long Short Term Memory network (LTSM), for end-to-end dynamic link prediction. To the best of our knowledge, it is the first time that GCN embedded LSTM is put forward for link prediction of dynamic networks. GCN in this new deep model is capable of node structure learning of network snapshot for each time slide, while LSTM is responsible for temporal feature learning for network snapshot. Besides, current dynamic link prediction method can only handle removed links, GC-LSTM can predict both added or removed link at the same time. Extensive experiments are carried out to testify its performance in aspects of prediction accuracy, Error Rate, add/remove link prediction and key link prediction. The results prove that GC-LSTM outperforms current state-of-art method.

Index Terms—Link prediction, Dynamic network, GCN, LSTM, Network Embedding

1 Introduction

PNAMIC link prediction in complex network has wide applications, such as social network [1], economy [2], biology [3], and industry [4] etc. Most networks in real-world are dynamic network, whose structure evolves over time [5], [6]. Dynamic network has dynamic pattern, whose nodes or links added and removed over time.

Dynamic link prediction [7], [8] is defined to predict future network structure based on historic network information. It is an efficient feature learning tool for complex networks. Recently, dynamic link prediction has applied to various real-world networks [9], [10]. For instance, in social network, we predict people's relationship like who will be whose friend in near future [11]. In communication network, we predict the future network structure [12], and in scientific network, we study the cooperation of researchers to predict their future co-workers [13]. Besides, dynamic link prediction can help locating the criminal and predicting activity time in social security network [14]. The dynamic pattern of infectious disease transmission is discovered by dynamic link prediction [15]. Protein mutual influence in biological networks is predicted by dynamic link prediction [16] as well.

For better understanding how dynamic network evolves over time, Fig. 1 shows a simple illustration. We take G as a social network, in which each node represents a user and each link represents the friendship between two users. The solid black line indicates the link that originally existes, the black dotted line indicates the link that disappears at a certain moment, the solid red line indicates the new link that

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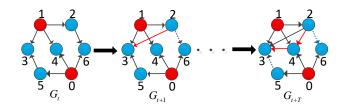


Fig. 1: An evolve pattern illustration of social network.

occurs at a certain moment, and the blue dotted line indicates the link that reappears. At time *t*, two red nodes(User 0 and User 1) have the similar structures, they both have three friends(the blue node), but they don't know each other. The static link prediction method will consider these two subnetworks evolve to the same potential structure, but in fact their evolution patterns are quite different. At time t+1, User 1 will introduce User 2 to one of his friends, User 3. As time passed by, the friends of User 1 gradually become friends of each other. However, the friends of User 0 are not connected to each other, and he may be more willing to maintain his friendship. We can conclude that although User 0 and User 1 have the same network structure at first, their different evolution models reflect different social strategies. These differences are realistic reflection of their social needs, such as whether to develop relationships between others or not. Therefore, in the dynamic link prediction task, how to learn the different evolution modes of each node is particularly important.

The dynamic link prediction problem can be more complex, such as prediction of newly added or removed links [17]. Recently a number of methods have been proposed to predict the potential or future links in dynamic networks [14]–[18]. Most dynamic link prediction methods take advantage of historic network information and compact

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them into one network to predict network of next moment. Similarity based dynamic link prediction is a typical one, in which similarity of nodes is the measurement for link. The larger similarity is, the more likely two nodes link. A bunch of dynamic link prediction technologies [14] utilize the topology information of the network to define the similarity of nodes, named structural similarity indexes, including local indexes and global indexes. The local similarity index only needs the neighborhood information of nodes, a simple but effective one is Common Neighbors (CN) [18]. It uses the number of common neighbors of two nodes as an index. Other common local similarity indexes include Jaccard (JA), Adamic-Adar (AA), Resource allocation (RA), Hub promoted index, Hub-contracted index, and Salton index etc [14]. While the global similarity index [14] makes full use of the global topology information of the network, such as Katz, Random Walk, SimRank, Leicht Holme Newman Index (LHNI) and Matrix Forest Index (MFI) etc.

Besides of similarity based prediction methods, machine learning is also applied to calculate the optimal similarity [19]–[23] for precise link prediction. Catherine A et al. [19] proposed future links prediction by applying the Covariance Matrix Adaptation Evolution Strategy (CMA-ES) to optimize weights which are used in a linear combination of sixteen neighborhood and node similarity indices. Ke-Jia Chen et al. [20] proposed a supervised link prediction method for dynamic network by an ensemble result of classifiers trained for each property. However, the optimization method is computationally expensive and is limited by the existing similarity index.

In order to consider the structural similarity and homogeneity of network nodes in a deeper level, a lot of network embedding methods are proposed for dynamic network link prediction. Inspired by word2vec used in Natural Language Processing (NLP), DeepWalk [24] and node2vec [25] are put forward, which randomly sample sequences of node walks and utilize the skip-gram model to obtain vectors for node and link. Other Random Walk based methods, like Large-scale Information Network Embedding (LINE) [26], learn node representations in a similar way but with different walk strategies. Such methods map the network into the a lower dimension vector space to obtain the feature vectors of each link, and then train a classifier to predict link (two categories, exist or not exist).

The above dynamic link prediction methods are all based on the snapshot network, such as given a snapshot of the network at a given time to predict links at next time. However, these methods only take the network topological information of the previous moment into account, regardless of the dynamic evolution of the network at the previous moment. Therefore, the accuracy of those methods is not as high as expected if the links dynamically change over time.

In addition to spatial features, there are also methods learn temporal information of dynamic networks. Some methods [8], [27]–[31] are designed to utilize a sequence of previous snapshots to predict future links, which integrates both structural information and temporal information to model the dynamic evolution process. Sina Sajadmanesh et al. [27] introduced a Non-Parametric Generalized Linear Model(NP-GLM) to infer the potential probability distribution of the time based on the characteristics of the appear-

ance time of links.

Because of the dynamic feature of network, most recent snapshot is more reliable for the future link prediction. Nahla Mohamed Ahmed [8], [30], [31] proposed a damping coefficient to aggregate the global topology information of the snapshots at T moments(window sizes) so as to obtain better results. Wenchao Yu et al. [28] proposed a link prediction model with spatial and temporal consistency (LIST) to predict links in a sequence of networks over time. LIST characterizes the network dynamics as a function of time, which integrates the spatial topology and the temporal network evolution of the network at each time. Xiaoyi Li et al. [29] proposed a deep model framework based on the Conditional Temporal Restricted Boltzmann Machine (ctRBM) to learn the dynamic characteristics of large-scale evolutionary networks. However, those methods simply take advantage of temporal features (not enough depth) so that they cant effectively learn the evolution of dynamic networks, and most of which are quite complicated.

Since embedding algorithms are applied to each snapshot of the dynamic graph, mostly ignores the temporal dynamic information of the network, therefore many researchers [32]–[36] recently integrated time information into network embedding to make it capable of capturing the dynamic evolution of the network. Palash Goyal et al. [33] proposed an Dynamic Graph Embedding Model(DynGEM) based on depth automatic encoder, which can handle the growing dynamic network. Giang Hoang Nguyen et al. [34] proposed a general framework for learning timerespecting embeddings from continuous-time dynamic networks. Lekui Zhou et al. [35] proposed a novel representational learning method, DynamicTriad, to preserve both the structural information and evolutionary patterns of a given network, so that the model can capture network dynamics and learn the representation vector for each node at different time steps. However, such methods generally focus only on adding links in the future, while ignoring other disappearing or persistent links, thus they can only reflect a part of the dynamic network evolution.

Long short-term memory (LSTM) was first proposed by Sepp Hochreiter and Jrgen Schmidhuber in 1997 [37], which is a specific form of RNN that can process time-dependent data of long-term dependence. It has been successfully used in various fields, such as image field [38], video field [39], language model [40], speech recognition [41], and machine translation [42]. Recently, in dynamic networks, the LSTM module is used to adaptively capture the dependencies among multi-dimensional interactions based on the learned representations for each time slot [43].

Most real-world network data does not have a regular spatial structure, and convolutional neural networks widely used in the image field cannot process these network data. Therefore, Joan Bruna [44] proposed a Graph Convolutional Network (GCN) to process network data in the earliest year of 2014. Recently, some work has adopted GCN to learn the structural characteristics of network data, thereby implementing various tasks, such as network representation learning, node classification [45].

To the best of our knowledge, neither LSTM nor GCN are applied to dynamic network analysis. Motivated by LSTM's excellent performance in handling temporal data

and GCN's feature learning capacity in network, we are interested in propose an unified model which is capable of handling spatio-temporal data. However, how to ensemble GCN and LSTM is tricky. In this paper, we propose a novel end-to-end dynamic link prediction deep model, GC-LSTM, which is capable of handling links that are going to appear or disappear. The main idea of our model is to make full use of GCN to learn network structure in hidden state and cell state, and learn temporal feature of network through LSTM model. GC-LSTM can effectively handle high-dimensional, time-dependent and sparse structural sequence data. We conduct extensive experiments on four real-world data sets. The results show that our model is significantly better than the current state-of-the-art methods. The main contributions of our paper are as follows.

- For dynamic link prediction, we propose a novel endto-end deep learning model, namely GC-LSTM, which extracts the spatial feature of each snapshot network through Graph Convolution, and structure learning through LSTM. The model can effectively learn spatiotemporal features of dynamic networks.
- Since most existing methods can only predict the added links in the network, our method can predict all links that are going to appear, disappear or constant to obtain accurate prediction of the whole dynamic network links.
- We conduct extensive experiments, verifying the effectiveness of GC-LSTM on four dynamic networks compared with four baseline methods. It is shown that our model significantly outperforms the current state-of-the-art methods on various metrics.

2 METHODOLOGY

In this section, we will introduce GC-LSTM model for link prediction in dynamic networks. It's capable of learning both spatial and temporal feature of dynamic networks for future added or removed links.

2.1 Problem Definition

We will give necessary definitions used throughout this paper. Formally, we define dynamic networks as follows

DEFINITION 1 (*Dynamic Networks*). Dynamic networks can be represented as a sequence of discrete snapshots, $\{G_1, \cdots, G_T\}$, where $G_t = (V, E_t, A_t)(t \in [1, T])$ represents a directed and unweighted network at time t. Let V be the set of all vertices and E_t be the temporal edges within the fixed timespan $[t - \tau, t]$. A_t denotes the adjacency matrix of G_t , where the element $A_t(i, j)$ =1 if there is a directed edge from vertex i to j, and $A_t(i, j)$ =0 otherwise.

In a static network, the link prediction problem generally aims to predict the unobserved or future links by the current network. They mainly focus on the spatial feature of the network. Different from static network link prediction, dynamic network link prediction also needs to learn the temporal feature of the network according to the dynamic evolution processes of previous snapshots. Our goal is to accomplish dynamic network link prediction by capturing the structural and evolutionary properties of the network.

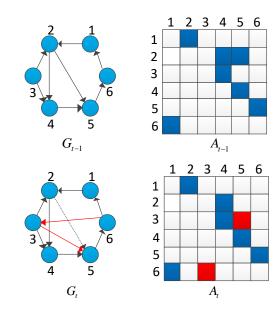


Fig. 2: An illustration of dynamic network evolution and its adjacency matrix. The network changes from time t-1 to t. E(6;3) and E(3;5) emerge while E(2;5) vanishes, the adjacency matrix also changes from A_{t-1} to A_t , with those elements equal to 1 represented by filled squares.

DEFINITION 2 (Link Prediction in Dynamic Networks). Given a sequence of graphs with length T, $\{G_{t-T}, \cdots, G_{t-1}\}$. Considering the dynamic network link prediction as a structural sequence modeling problem, it aims to learn the evolution information of the precious T snapshots to predict the probability of all links at time t, defined as

$$\hat{A}_t = argmaxP(A_t \mid A_{t-T}, \cdots, A_{t-1}) \tag{1}$$

where $\{A_{t-T}, \dots, A_{t-1}\}$ represents the adjacency matrix of precious T snapshots, A_t represent the real adjacency matrix of the snapshot at time t, \hat{A}_t represent the predictive adjacency matrix of the snapshot at time t.

Fig. 2 is an illustration of how dynamic network evolves. Since the adjacency matrix A_t is a precise reflection of how network changes over time, which is adopted as the input of our prediction model. In order to effectively learn the evolution model of the dynamic network, we utilize a sequence of data $\{A_{t-T}, \cdots, A_{t-1}\}$ with length T to predict the adjacency matrix A_t , where $P(A_t \mid A_{t-T}, \cdots, A_{t-1})$ models the probability of links to appear conditioned on the past T adjacency matrixes.

2.2 Overall Framework

We propose a novel deep learning model, GC-LSTM, consisted of an encoder and an decoder shown in Fig. 3. Encoder model is Graph Convolution Network (GCN) embedded LSTM, using GCN to learn network structure of the cell state c and the hidden state h of each moment snapshot, while using LSTM to learn the temporal information of the state of each link. Decoder is a fully connected layer network to convert the extracted features mapping back to the original space. GC-LSTM will output the predicted network and implement link prediction in an unified fashion.

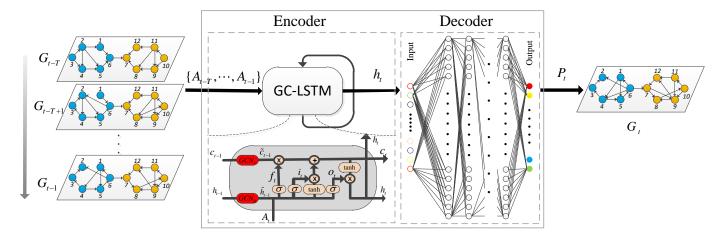


Fig. 3: The overall framework of encoder and decoder model for end-to-end dynamic link prediction, in which encoder model is GCN-LSTM, while decoder model is a fully connected layer network. Given a sequence of networks with length T, $\{G_{t-T}, \cdots, G_{t-1}\}$, each network is transformed into a adjacency matrix A_t as the input. The GC-LSTM is two GCNs embedded into the LSTM to learn temporal and spatio feature h_t from the extracted data. GCN_h and GCN_c denote the graph convolution on long-term information c and h respectively. The decoder projects the received feature h_t maps back to the original space to get G_t . Here, σ in GC-LSTM is an activation function and sigmoid is adopted in this paper.

Before detailed description of the proposed model, we will introduce some terms and notations that will be used in this paper, listed in TABLE 1. Notice that subscript f represent the forget gate, i and c represent the input gate and o represent the output gate.

TABLE 1: Terms and notations used in GC-LSTM

Symbol	Definition
N	number of nodes at each snapshot
A_t	the adjacency matrix at time t as the input data
P_t	the output probability of each link at time t
d	number of hidden layer unit in GC-LSTM
$W_{f,i,o,c}, b_{f,i,o,c}$	weight and bias of three gates in GC-LSTM
K	the order of graph convolution
$\sum_{k=0}^{K} \theta_k$ \tilde{L}_t	weight of graph convolution
$ ilde{L}_t$	the rescaled graph Laplacian matrix at time t
D_t	the degree matrix of A_t at time t
I_N	the identity matrix
λ_{max}	the largest eigenvalue of graph Laplacian matrix
h_t, c_t	hidden and cell state of GC-LSTM
$ ilde{h}_t$, $ ilde{c}_t$	hidden and cell state extracted by GCN
$W_d^{(l)}$, $b_d^{(l)}$	weight and bias of l^{th} layer of decoder

2.3 GC-LSTM Model

We use the proposed GC-LSTM model as an encoder to extract the corresponding temporal and spatial features from the structure sequence data $\{A_{t-T}, \cdots, A_{t-1}\}$, and the hidden layer vector h_t at the last moment will be used as the output of GC-LSTM.

In the task of dynamic link prediction, the link state (exist or non-exist) of each node with others at multiple times can be regarded as a time series, equivalent to the row vector in the adjacency matrix. Generally, LSTM is applied to capture the temporal characteristics of time series data. So in GC-LSTM, we utilize the LSTM to solve long-term dependency problems and effectively learn temporal feature of the dynamic graph. The link states of each node in the dynamic network may use LSTM to implement timing prediction,

when predict links at the next moment. On the other hand, it is necessary to not only utilize the previous link state Information of the node, but also consider the impact of the link states of the neighbors, as well as the network structure characteristics. GCN has been proved efficient in network embedding for learning spatial feature. We propose GC-LSTM model, where the Graph Convolution (GC) models are adopted to extract the structural characteristics of the snapshot at each moment. and LSTM is capable of learning temporal feature of dynamic network.

The GC-LSTM model mainly relies on two state values, the hidden state h which is used to extract the input information at the last time, and the cell state c which is used to save the long-term information. The essential of GC-LSTM is that it has a cell state c throughout the forward process, results in information transmitted over the cell state c for a long time. In the dynamic link prediction task, because of the cell state c and the hidden state d respectively reflect different information, we need to consider not only the influence of the hidden state of the neighbors on the hidden state of the neighbors. Therefore, we propose to use two GCN models to perform convolution operations on the cell layer state and the hidden layer state at the last time.

In GC-LSTM model, the first step is to decide what information will be thrown away from the previous cell state. This decision is performed by a forget gate $f_t \epsilon [0,1]^d$, where 0 means all information will be forgotten, 1 means all information will be reserved, defined as

$$f_t = \sigma(W_f A_t + \sum_{k=0}^{K} \theta_{hkf} T_k(\tilde{L}_{t-1}) h_{t-1} + b_f)$$
 (2)

where $A_t \epsilon R^{N \times N}$ denotes the input of the GC-LSTM at time t, $h_{t-1} \epsilon R^{N \times d}$ denotes the hidden state of the GC-LSTM at time t-1. $W_f \epsilon R^{N \times d}$ and $b_f \epsilon R^d$ are the weight and bias matrix of forget gate. $\sum_{k=0}^K \theta_{hkf} T_k(\tilde{L}_{t-1}) h_{t-1}$ represents the graph convolution on the hidden state h_{t-1} at time t-

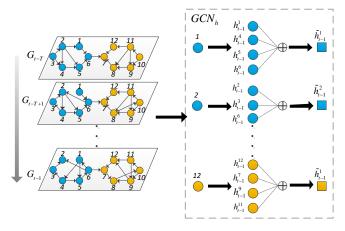


Fig. 4: The framework of 1^{th} GCN on the hidden state h

1. $\tilde{L}_{t-1} = \frac{2}{\lambda_{max}} L_t - I_N$ is a rescaled graph Laplacian, where $L_t = I_N - D_t^{-\frac{1}{2}} A_t D_t^{-\frac{1}{2}}$ is the normalized graph Laplacian. A_t is the adjacency matrix. D_t is the degree matrix of A_t , I_N is the identity matrix, λ_{max} denotes the largest eigenvalue of L_t . $\sum_{k=0}^K \theta_{hkf}$ are the parameter vector, and K is the order of the graph convolution. $\sigma(\cdot)$ denotes the sigmoid function, N denotes the input dimension, d denotes the hidden layer dimension of GC-LSTM. When K=1, the GCN model can use the information of the 1st-order neighbors, so the operation of the 1^{th} GCN on the hidden state h is shown in the Fig. 4. In addition, the operation of the GCN on the hidden state c is same as h, only the input of GCN has changed from h to c.

The next step is to update the cell state. First, a tanh layer generates a new candidate vector of cell layer, $\bar{c}_t \epsilon [-1,1]^d$. Then, \bar{c}_t a sigmoid layer determines how many new candidate vector will be added to the cell state, which named as the input gate $i_t \epsilon [0,1]^d$. Finally, the cell state can be updated by the forget gate and the input gate.

$$\bar{c}_{t} = tanh(W_{c}A_{t} + \sum_{k=0}^{K} \theta_{hkc}T_{k}(\tilde{L}_{t-1})h_{t-1} + b_{c}),$$

$$i_{t} = \sigma(W_{i}A_{t} + \sum_{k=0}^{K} \theta_{hki}T_{k}(\tilde{L}_{t-1})h_{t-1} + b_{i}),$$

$$c_{t} = f_{t} \odot \sum_{k=0}^{K} \theta_{ck}T_{k}(\tilde{L}_{t-1})c_{t-1} + i_{t} \cdot \bar{c}_{t}$$
(3)

where $W_{i,c}\epsilon R^{N\times d}$ and $b_{i,c}\epsilon R^d$ are the weight and bias matrix of input gate. $\sum_{k=0}^K \theta_{hkc}$, $\sum_{k=0}^K \theta_{hki}$ and $\sum_{k=0}^K \theta_{ck}$ are the parameter vector of the graph convolution on h and c.

Therefore, the updated cell layer information can not only save long-term information, but also selectively filter out some useless information. Finally, we need to decide what information will be output, it is implemented by the output gate:

$$o_{t} = \sigma(W_{o}A_{t} + \sum_{k=0}^{K} \theta_{hko}T_{k}(\tilde{L}_{t-1})h_{t-1} + b_{0}),$$

$$h_{t} = o_{t} \odot tanh(c_{t}).$$
(4)

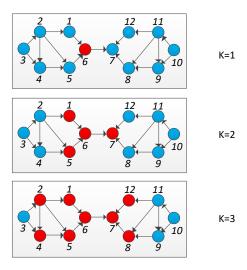


Fig. 5: An illustration of K^{th} GCN.

where $W_o \epsilon R^{N \times d}$ and $b_o \epsilon R^d$ are the weight and bias matrix of output gate. $\sum_{k=0}^K \theta_{hko}$ are the parameter vector of the graph convolution on h.

Above all, the three gates constitute the entire forward process of the GC-LSTM. In this paper, the adjacency matrix of T time $\{A_{t-T},\cdots,A_{t-1}\}$ is used as the input data, so the hidden layer vector $h_t \in R^{N \times d}$ obtained by GC-LSTM already contains both temporal and spatial information of snapshot at the previous T moments. It should be always noticed that the numbers of hidden units d in GC-LSTM varies when the number of nodes N is different for each dynamic network. The larger N is, the more units we need to use in the model. Generally, the numbers of hidden units d is selected from $\{64,128,256,512\}$.

It is worth noting that we use the K-order Chebyshev polynomial to approximate the graph convolution, so that the GC-LSTM model can utilize the information of the node that are at the largest K hop from the central node. So K is a very important hyperparameter. As shown in Fig. 5, when K=1, only the information of the node 6 itself is considered; when K=2, the influence of the information of the 1^{th} neighbor nodes (1, 5, 7) of the node 6 will be considered; when K=3, the information on the 1^{th} neighbor nodes (1, 5, 7) and 2^{th} neighbor nodes (2, 4, 8, 12) will be additionally considered. When K is larger, the more additional structure information form the neighbor nodes of the central node will be considered, but the cost of computing is greatly increased. In general, K is 3.

2.4 Decoder Model

In order to output the final prediction network, we use a fully connected layer network as a decoder to turn the hidden vector h_t at last moment in the sequence data into the final probability matrix.

$$Y_d^{(1)} = ReLU(W_d^{(1)}h_t + b_d^{(1)}),$$

$$Y_d^{(k)} = ReLU(W_d^{(k)}Y_d^{(k-1)} + b_d^{(k)}),$$

$$P_t = o_t \odot tanh(c_t).$$
(5)

where $W_d \in \mathbb{R}^{d \times N}$ and $b_d \in \mathbb{R}^N$ are the weight and bias matrix of the decoder. L denotes the number of hidden layers

in the fully connected layer, and the number of units in each hidden layer may vary according to the dimension of data for better performance. $P_t \epsilon R^{N \times N}$ represents the final probability matrix of links, each $P_t(i,j)$ =[0,1] represents the probability of the link from i to j. The lager P_t is, the larger the probability that the link will exist.

2.5 Loss Function and Model Training

The purpose of training the entire GC-LSTM model is to improve the accuracy of the dynamic link prediction, so the training is designed to make the output probability matrix more similar to the adjacency matrix at time t. In the regression prediction problem, the L_2 distance is usually used to reflect the degree of similarity between the predicted value and the true value.

$$L_2 = ||P_t - A_t||_F^2 = \sum_{i=0}^N \sum_{j=0}^N (P_t(i,j) - A_t(i,j))^2$$
 (6)

where P_t represent the output probability matrix at time t, A_t represent the real adjacency matrix at time t, N represent the number of nodes in the snapshot at time t. However, due to the sparsity of the network, this means that the number of zero elements in the adjacency matrix is much larger than that of non-zero elements. If we only use the L_2 distance as the loss function of the proposed model, it will be possible to lead the loss function to be more biased towards ensuring the prediction accuracy of zero elements, which results in overfitting. In order to ensure that the model can avoid overfitting to a certain extent, we add a regularized loss function. We calculate the sum of the squares of the F norms of all the weights in the GC-LSTM model to calculate the regularized loss.

$$L_{reg} = \|W_f\|_F^2 + \|W_i\|_F^2 + \|W_c\|_F^2 + \|W_o\|_F^2 + \|W_d\|_F^2 + \sum_{k=0}^K \|\theta_{hk}\|_F^2 + \sum_{k=0}^K \|\theta_{ck}\|_F^2$$

$$(7)$$

The total loss in the training process is defined as

$$L = L_2 + \beta L_{reg} \tag{8}$$

where β is a parameter to trade-off the importance of L_2 and L_{reg} , and the best β will be found in the model training process.

In order to minimize Eq. 8, we adopt the Adam optimizer to optimize our model.

3 EXPERIMENTS

The proposed GC-LSTM model is compared with widely used baseline methods on several real benchmark dynamic network datasets to testify its performance. All experiments are implemented on 12G NVIDIA GPU, 32G DDR running memory server, which are coded by Python.

3.1 Datasets

We carry out the experiments on four real-world datasets, with each one representing a dynamic network. Most networks are human relation networks, with nodes representing humans and links showing their connections. The contacts can be face-to-face, phone, emailing, and other kinds of

contact. The data sets adopted are described in detail listed as follows.

- CONTACT [46] and HYPERTEXT09 [47]: They are human contact dynamic networks of face-to-face proximity. The data are collected through wireless devices carried by people who attended corresponding activity. If a person contacts a person under a certain timestamp, a corresponding link will occur. The data are recorded every 20 seconds.
- ENRON and RADOSLAW [48]: They are email networks, each node represents an employee of a medium-sized company, a link occurs each time such as an email sent from one employee to another. ENRON recorded email data for nearly three years, and RADOSLAW lasted nearly nine months.

TABLE 2 provides a summary of the four dynamic networks and their statistics for evaluation. $|E_T|$ shows the number of dynamic links, \bar{d} represents the average dynamic node degree, d_{max} represents the maximum dynamic node degree.

TABLE 2: Dynamic network data and statistics

Dataset	V	$ E_T $	\overline{d}	d_{max}	Timespan(days)
CONTACT	274	28.2K	206.2	2092	3.97
HYPERTEXT09	113	20.8K	368.5	1483	2.46
ENRON	151	50.5K	669.8	5177	1137.55
RADOSLAW	167	82.9K	993.1	9053	271.19

Before training, we generate snapshots for each dataset at fixed intervals, and then sort them in an ascending order of time to generate dynamic network structure sequence data. Considering that the connection between people may be temporary, we remove the link that does not reappear within 8 intervals. In order to get enough samples, we split each dataset into 331 snapshots according to an ascending order of time, then continuous 11 snapshots are used as one sample, where the first 10 snapshots are divided into inputs and the last snapshot network is used as output, equal to the sampling period T=10. Therefore, we can get a total of 320 samples. Then, we group the first 240 samples as a training set and the remaining 80 samples as a test set.

3.2 Baseline Methods

CN [18], node2vec [25] and LINE [26] are popular used baseline methods in dynamic link prediction tastk. CN is one of the similarity-based prediction methods, while node2vec and LINE are classic network embedding methods. The above three methods can both applied to static and dynamic link prediction tasks. For solving dynamic problem only, Temporal Network Embedding (TNE) [36] is a state-of-art baseline method that can handle time dependencies.

The four baseline methods are introduced as follows.

- CN [18]: It is a widely used link prediction method, whose main idea is that a link is more likely to exist between two nodes with more common neighbors.
- node2vec [25]: It is a network embedding method by mapping the nodes of a network from a high dimensional space to a lower dimensional vector space. If there is a shorter distance between the vectors of a pair

- of nodes, they are more similar and the link tend to connect with higher probability.
- LINE [26]: It integrates local and global information to learn node representations, similar to node2vec. It is widely applied to all types of networks, especially for large-scale network embedding.
- TNE [36]: It models network evolution as a Markov process and then uses the matrix factorization to learn the embedding vectors for all nodes.

CN only gives scores for potential links, therefore, we adopt average of the scores as the threshold to decide whether there should be a link or not. For node2vec, we set the dimension of the embedded vector to 80, and find the optimal values of the hyperparameters p and q from the scope $\{0.5,1,1.5,2\}$. Weighted-L2 [25] is used to obtain a embedding vector $e^{u,v}$ for the link from node u to v. Each element in the vector is defined as

$$e_i^{u,v} = |u_i - v_i|^2 (9)$$

where u_i and v_i are i^{th} element of embedding vectors of nodes u and v, respectively. Then we use a pretrained logistic regression classifier to classify the links. For LINE, we set the dimension to 80 with 2nd-order proximityand, and the probability of all links are calculated in the same way as node2vec. For TNE, we also set the dimension to 80 and regard the inner products of embedding matrix and its transpos. When we calculate the embedded vector matrix Z for each node, then $Z \cdot Z^T$ is used to calculate the probability of all links and the threshold τ =0.9 is used to divide the link is existing or not. For our proposed model, GC-LSTM, we set the hidden unit d to 256, and the order K=3. In extensive experiments, we also analyze the parameter sensitivity of GC-LSTM model.

3.3 Evaluation Metrics

Usually, metrics evaluating link prediction in static networks are employed for dynamic ones. Area Under the ROC Curve (AUC) is brought up to measure dynamic link prediction method. Based on AUC, the Area Under the Precision-Recall Curve (PRAUC) [49] is designed to evaluate the sparsity of networks. Different from predicting links added to network, there are also links removed from network in future dynamic networks. AUC and PRAUC may be not qualified to evaluate both added and removed links. Junuthula et al. [17] restricted the measurements to only part of node pairs and proposed the Geometric Mean of AUC and PRAUC (GMAUC) for the added and removed links. Li et al. [29] use SumD that caculates the differences between the predicted network and the true one, evaluating link prediction methods in a more strict way. But the absolute difference could be misleading. For example, the SumD of the two dynamic link prediction models are all equal to 5, however, one prediction model is 5 errors in a total of 10 links, and the other prediction model is 5 errors in a total of 100 links. Obviously the latter performed better than the former, but SumD could not distinguish the two cases

In our experiment, AUC, GMAUC, and Error Rate are chosen as metrics to evaluate our GC-LSTM model compared with other baseline methods.

• AUC: among n independent comparisons, there are n' times that the existent link gets a higher probability sore than the non-existent link and n'' times they get the same score, then the AUC is defined as

$$AUC = \frac{n' + 0.5n''}{n} \tag{10}$$

Before calculating the AUC index, we will select all existing links and randomly sampling the same number of links that do not exist to reduce the impact of sparsity.

 GMAUC: is a metric proposed to evaluate dynamic link prediction, which combines both PRAUC and AUC by taking geometric mean of the two quantities, and the GMAUC is dened as

$$GMAUC = \left(\frac{PRAUC_{new} - \frac{L_A}{L_A + L_R}}{1 - \frac{L_A}{L_A + L_R}}\right)$$

$$\cdot 2(AUC_{prev} - 0.5)^{1/2}$$
(11)

where L_A and L_R represent the numbers of added and removed links respectively, $PRAUC_{new}$ represents the PRAUC value calculated among the new links and AUC_{prev} represents the AUC for the originally existed links

• Error Rate: is dened as the ratio of the number of mispredicted links N_{false} to the total number of truly existent links N_{true} , which is dened as

$$ErrorRate = \frac{N_{false}}{N_{true}} \tag{12}$$

Unlike the SumD which only calculates the absolute link difference in two networks, Error Rate considers relative link difference for precise evaluation.

In particular, we divide the Error Rate into two parts as an effective supplement, Error Rate+ and Error Rate-. Error Rate+ indicates the ratio of the number of mispredicted links in truly existent links to the total number of truly existent links. Error Rate- indicates the ratio of the number of mispredicted links in truly non-existent links to the total number of truly existent links.

3.4 Experimental Results

During the training of the model, we input 10 consecutive snapshots $\{G_{t-10},\cdots,G_{t-1}\}$ as a sample into our GC-LSTM model to predict the snapshot at next time G_t . For the TNE model, it has the same input as our model. For traditional methods CN, node2vec and LINE, which cannot handle time dependencies. There are two typical methods to process the data: 1) using only information of G_{t-1} to predict G_t [50]; 2) integrating the previous 10 snapshots $\{G_{t-10},\cdots,G_{t-1}\}$ into one network to predict G_t [51]. Because there may be insufficient information if only the information of the last snapshot is used for link prediction and our GC-LSTM model takes 10 consecutive snapshot networks as input, we choose the second method to ensure the similarity of the input data with our method.

Since the evolution pattern of the network may change over time, we select the average of the three evaluation metrics of the first 20 test samples and all 80 samples to reflect

TABLE 3: Dynamic link prediction performances on AUC, GMAUC, Error Rate, Error Rate+ and Error Rate- for the first 20 samples and all the 80 samples.

Metric	Method	CONTACT		HYPERTEXT09		ENRON		RADOSLAW	
		20	80	20	80	20	80	20	80
AUC	CN	0.8541	0.8457	0.6696	0.7266	0.7247	0.8102	0.8342	0.8408
	node2vec	0.5212	0.5126	0.6348	0.6591	0.7659	0.6806	0.6103	0.7676
	LINE	0.6064	0.4239	0.5416	0.5357	0.5294	0.5042	0.5292	0.5231
	TNE	0.9442	0.9371	0.9076	0.8517	0.8096	0.8314	0.9053	0.8801
	GC-LSTM	0.9797	0.9741	0.9583	0.9758	0.8909	0.8731	0.9862	0.9859
	CN	0.8445	0.8330	0.6010	0.6749	0.6818	0.7929	0.8279	0.8343
	node2vec	0.1805	0.1398	0.4891	0.5163	0.4069	0.5417	0.7241	0.7203
GMAUC	LINE	0.4502	0.3875	0.4686	0.3724	0.2642	0.2358	0.3341	0.3105
	TNE	0.9083	0.8958	0.8856	0.8392	0.8233	0.7974	0.8282	0.8251
	GC-LSTM	0.9823	0.9748	0.9905	0.9366	0.9156	0.8867	0.9979	0.9982
	CN	0.8596	0.7836	3.7763	5.2674	2.1111	3.3025	4.8880	5.6093
	node2vec	29.343	25.207	24.398	12.826	68.808	31.971	20.713	17.113
ER	LINE	11.327	11.425	16.690	6.788	23.257	12.158	1.5488	3.0576
	TNE	1.8169	1.6656	1.6453	1.9675	2.0468	2.9335	4.7635	4.3204
	GC-LSTM	0.2051	0.2831	0.1801	0.2090	0.3632	0.4340	0.1783	0.1881
	CN	0.2885	0.3051	0.5610	0.3419	0.5351	0.3388	0.2528	0.2201
	node2vec	0.3001	0.2989	0.4087	0.3595	0.1743	0.3493	0.2225	0.2867
ER+	LINE	0.2119	0.2291	0.2730	0.3483	0.2117	0.1958	0.3760	0.2655
	TNE	0.9436	0.9437	0.7598	0.5800	0.6702	0.4518	0.1795	0.1829
	GC-LSTM	0.1491	0.1845	0.1665	0.1504	0.2733	0.3347	0.1069	0.1154
ER-	CN	0.5711	0.4785	3.2153	4.9255	1.5760	2.9637	4.6351	5.3892
	node2vec	29.043	24.908	23.990	12.466	68.633	31.622	20.490	16.826
	LINE	11.115	11.196	16.417	6.439	23.046	11.962	1.1729	2.7921
	TNE	0.8733	0.7219	0.8855	1.3874	1.3766	2.4817	4.5841	4.1375
	GC-LSTM	0.0560	0.0985	0.0136	0.0586	0.0899	0.0993	0.0714	0.0727

the short-term and long-term prediction performance of predictive model. The results are shown in TABLE 3. We can conclude that the GC-LSTM model outperforms all baseline methods in all dynamic networks for both the short-term and long-term prediction capabilities. From the results, the performance obtained by CN, node2vec and LINE explains that these methods designed for static networks are not suitable for dynamic link prediction. In contrast, TNE and GC-LSTM achieve much better performance due to their ability of capturing dynamic characteristics. Our GC-LSTM model still performs better than TNE on all data sets, especially on the GMAUC metrics that reflect the predictive performance of added and removed links in dynamic networks.

In addition, for the test samples at each moment, we also compare the difference of links between the predicted network and the real network to calculate the Error Rate. The significant difference in the Error Rate indicates that this metric is a good complement to fully measure the performance of dynamic link prediction.

As shown in TABLE 3, we found that most of the baseline methods may predict more invalid links than the number of links that actually exist, resulting in a relatively large Error Rate. The traditional methods of network embedding, node2vec and LINE, perform the worst in terms of Error Rate. They can almost predict a large number of invalid links, which is 10 times or even 70 times the number of links actually exist. This is because the link of the dynamic network evolves over time, but the pre-trained linear regression

model used in the network embedding method cannot capture the dynamic changes of the link, thereby they misclassify many links. TNE also has a poor effect on the Error Rate. This may be because the matrix decomposition method used by TNE cannot balance the positive and negative samples on the sparse adjacency matrix, which makes it impossible to deal with the sparse dynamic network we adopt. GC-LSTM is significantly better than all baseline algorithms in Error Rate. The results prove once again that our GC-LSTM model has better performance in dynamic link prediction accuracy. Moreover, our model has far more advantages in Error Rate compared with other models than AUC and GMUUC, it means that the newly defined Error Rate metric compared with AUC and GMUUC is more discernible when evaluating the dynamic link predictions. This is because other comparison algorithms directly predict the next snapshot network based on the first 10 snapshot networks, , but our method requires pre-training models to learn the evolution pattern of dynamic networks more effectively from the first 240 samples. Our GC-LSTM model not only uses LSTM to learn the timing characteristics of the sequence network but also uses GCN to learn the network characteristics of each snapshot. Therefore, in the test process, our model can predict future links more accurately, with lower Prediction error.In the four data sets, ENRON is the most unsatisfactory in each evaluation index. This may be because the evolutionary model of ENRON has changed greatly during the evolution process, so the evaluation results of our pretrained GC-LSTM model on the test set are relatively poor.

Interestingly, in most cases, the Error Rate- of the comparison method is much larger than Error Rate+, especially node2vec and LINE. They are more likely to predict non-existing links as existing links. Because the dynamic network data we experimented basically are sparse network, the pre-trained classifier in the embedded method cannot effectively classify sparse networks. For our GC-LSTM method, although Error Rate+ is slightly larger than Error Rate-, our method's Error Rate+ is still the smallest of all comparison experiments. It is further shown that our method not only has very high prediction accuracy on the non-existent link, but also has better predict the dynamic link of the network.

It can be seen from the TABLE 3 that the prediction effect of Error Rate+ is very significant and Error Rate+ can be well applied to the joint prediction in the gene regulatory network. In the gene regulatory network, the node represents the gene, and the directed edge of the directed gene indicates the regulatory relationship between the genes. Our model can be applied to the link prediction of the gene regulatory network, On the one hand, it can further explore the potential regulatory relationship of known regulatory networks, and on the other hand, it can provide research directions for unknown gene regulation. In addition, In the research cooperation network, it is generally predicted which researchers will work together, but the relationship of the researchers who do not cooperate in practice is also very important, we cannot make too many mistakes to predict the relationship between researchers who will not cooperate. Therefore, ER- is very important in the research cooperation network, and the smaller the Error Rate- is, the better the performance of the prediction model is.

In addition, in most cases, the short-term prediction performance of our method is better than the long-term prediction performance, this is because the evolution pattern in the second half part of the test set is different from the evolution pattern in the first half part, and our model tends to fit the evolution pattern of the first half part.

Next, for test samples G_t , t changes from 1 to 80, we plot the AUC, GMAUC, and Error Rate metrics curves over time obtained by our GC-LSTM model at four datasets as a function of time t to reflect the dynamic link prediction performance. The results are shown in Fig. 6. As time goes by, AUC and GMUUC are gradually decreasing, and the Error Rate is gradually increasing, which indicates that longterm links prediction for dynamic network is relatively difficult due to the uncertainty of dynamic network evolution over a long period of time. Interestingly, the predictive performance of the dataset RADOSLAW is relatively stable. This may be due to its network structure evolves periodically, so it has a good long-term predictive performance. In order to further explain this phenomenon, we studied the trend of the two most common structural properties (ie, the average degree and the average clustering coefficient) of the four dynamic networks with time t increasing, the results are shown in Fig. 7. We can see that the average degree and average clustering coefficients of the three datasets, CONTACT, HYPERTEXT09 and ENRON, have changed significantly over time, while RADOSLAW is relatively stable. These results reflect why we can get better long-term predictive performance on the last dynamic network.

In summary, although some methods have superior performance in the statistical metric AUC, they are not satisfactory in terms of Error Rate and wrong predict many invalid links. But in most real-world scenarios, we may only care whether the most important links are predicted correctly. Therefore, we further evaluated the predictive performance of all models on a particularly important part of the link. Here, we use two metrics to measure the importance of each link: degree centrality (DC) and edge intermediate centrality (EBC). At the beginning, the central DC is to measure the importance of the node according to the number of neighbors. In this paper, we use the sum of the degree centrality of two nodes to measure the importance of the link. In this paper, we select the top 10% important links based on DC and EBC, then we calculate the predicted Error Rate for these important links. The results are shown in TABLE 4. In most cases, our GC-LSTM model has the lowest Error Rate on all four data sets, both for short-term and long-term prediction. This further proves that our GC-LSTM model still performs very well in predicting the important links. Furthermore, comparing the results of TABLE 3 and TABLE 4, we find that the Error Rate on the top 10% of the important links is much smaller than the Error Rate on all links. This shows that the prediction performance on those important links of our model are better than the prediction performance on unimportant links.

4 CONCLUSION

In this paper, we propose a new deep learning model, GC-LSTM, which is an encoder-decoder architecture for dynamic link prediction. The entire GC-LSTM model combines the characteristics of the two models of LSTM and GCN, using LSTM to learn the timing characteristics from continuous snapshots, and using GCN to learn the structural characteristics of the snapshot at each moment, and finally using the fully connected layer network as a decoder to convert the extracted spatiotemporal features back to the original space. The proposed model not only captures the time dependence between a sequence of snapshots, but also considers the impact of the network structure. Therefore, it can better capture the pattern of network evolution. Finally, we conducted a number of experiments to compare our model with traditional link prediction methods on various dynamic network datasets. The results show that our model is not only superior to other models in terms of AUC, GMUUC and Error Rate, but also shows excellent performance in important link prediction tasks.

Our future research will focus on link prediction for large-scale dynamic networks, and we will work to reduce the computational complexity of the GC-LSTM model to make it suitable for large networks. Compared to other dynamic link prediction methods, our model needs pretraining, so the time complexity of the model is still high, so in the future we need to study the work of reducing the time complexity of the model.In addition, we are also preparing to study the mobility of our models on various other tasks, such as dynamic network embedding, node classification, and so on.

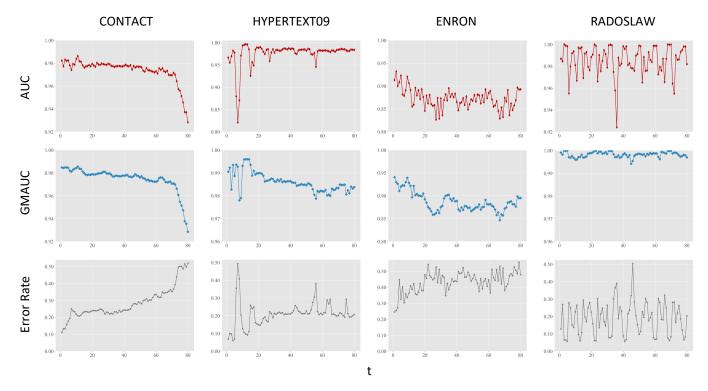


Fig. 6: The curves of AUC, GMUUC, and Error Rate as a function of time t.

TABLE 4: Prediction error rate of the top 10% important links in terms of DC and EBC

Metric	Method	CONTACT		HYPERTEXT09		ENRON		RADOSLAW	
		20	80	20	80	20	80	20	80
DC	CN	0.0378	0.0449	0.5288	0.5806	0.4130	0.4148	0.4910	0.5466
	node2vec	0.5974	0.5976	0.4397	0.4837	0.6296	0.4991	0.4931	0.5037
	LINE	0.7382	0.7520	0.4297	0.4230	0.3983	0.3789	0.5186	0.4691
	TNE	0.8235	0.7843	0.2869	0.3360	0.2411	0.2138	0.2342	0.2450
	GC-LSTM	0.0299	0.0661	0.0652	0.0766	0.1172	0.1305	0.0394	0.0467
ЕВС	CN	0.4868	0.5374	0.6865	0.4198	0.3433	0.2088	0.5347	0.5076
	node2vec	0.6375	0.6295	0.5602	0.5064	0.5174	0.4963	0.5032	0.5361
	LINE	0.8165	0.7952	0.7195	0.7874	0.7237	0.8049	0.9079	0.8541
	TNE	0.9746	0.9846	0.6655	0.4705	0.6402	0.4669	0.3658	0.3543
	GC-LSTM	0.2786	0.4146	0.1932	0.2046	0.2706	0.3439	0.1629	0.1708

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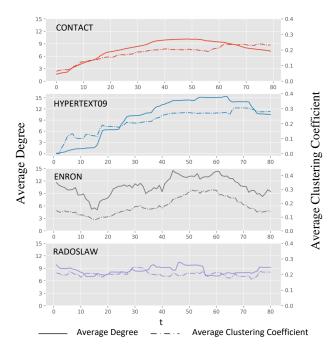


Fig. 7: The trends curves over time of network structure attributes (average value and average cluster coefficient)

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