Abstract on Generative Modelling and Representation Learning in Temporal Graphs

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1 Motivation

Graphs are everywhere in real world systems like geographical networks,social networks, routing networks, biological networks, computer networks, routing networks, geographical weather network, interaction networks, co-citation networks, traffic networks and knowledge graphs. A graph represents the relation between various entities. They are useful in various tasks like node classification, link classification, routing problems, cliques detection, community detection and many more. These tasks have applications in recommendation systems, anomaly detection, pricing models, information retrieval using knowledge graphs, drug discovery. Graph generative modelling [7] and graph representation learning [2] have achieved state of art results on such tasks.

More often, such graphs are dynamic. A new entity can get added or deleted over time. Similarly, a new relationship can form between two entities in future or can cease to exist as well. Even the node features can evolve over time. For example in a university network of faculty and students, a role of faculty will change from assistant professor to associate professor. Static graphs are often aggregation of such temporal graphs observed over a time window. So, it is pertinent to address the temporal nature of these graphs and model the dynamic nature in the learning process. Recent works like jodie [3], dyrep [5], tgn [4], tgat [6] have achieved state of the art results on future link prediction tasks in temporal graphs. Similarly generative models tag-gan [9] and dymond [8] have achieved state of art results on temporal graph generative modelling.

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2 Contribution of the thesis

Most of these works are preliminary in nature especially in the area of temporal graph generative modelling. This problem is even more challenging than static graph generative modelling because the number of graph for training is often one. Moreover, we observe that the future link prediction tasks in temporal graph representation learning involves only predicting the future link but not the time of the link formation. This is mainly due to the fact that temporal graph representation learning methods lack the capacity to learn the generative process of the underlying graph. In this thesis, our contribution will be manifold -

- Learning a generative model of large scale temporal graph(s). This generative model will jointly learn the structural properties of the network as well their dynamism along the temporal axis. Furthermore, it will enable efficient sampling of synthetic graph from this learnt distribution.
- Extend this generative modelling approach to improve upon the future link prediction state of the art results and enable the task of predicting time of future link formation. These tasks originate many significant applications like temporal anomaly detection, privacy preserving data sharing and recommendations.
- Fine-tuning the above methodologies for various kinds of temporal graphs like temporal interaction networks, bi-partite networks, heterogeneous networks and knowledge graphs. Note that in some networks, links are not instantaneous but have start time and end time associated with them.

3 Key challenges in temporal graph generative models

Recent work like tag-gan [9] has proposed a methodology to learn a generative model on temporal interaction network. They transform the temporal graph into a static network by combining the node identity and its interaction time as a new node. Now on this static network, they have sampled actual random walks and synthetic random walks from this network. Finally, they trained a discriminator model to classify between synthetic and random walks. Finally, they assembled the synthetic walks which were mis-classified by the discriminator into the temporal network. Dymond [8] provides a non-neural generative method to learn the underlying distribution. They first mine the size 3 motifs from the temporal graph at each time stamp. For each motif, they estimate arrival rate and inter-event time distribution using exponential distribution. Now during temporal graph generation, they sample the motifs based on their arrival rate and inter-event time distribution and assemble the final graph. We now summarize the limitations of recent works.

- Tag-gan [9] doesn't have the upper bound on the graph sampling complexity since in the worst case, discriminator might not mis-classify any synthetic walk. Moreover, since they are treating each node and its interaction time as unique node, method is not scalable for real worlds networks like reddit where there are over 60K unique timestamps. Moreover, graphs sampled from tag-gan contains very high edge overlap with input graph. This makes sampled graph redundant.
- Dymond [8] suffers from simplistic modelling capability and expensive computation due to mining of 3 size motifs $O(N^3)$ at each time stamps.
- These methods also do not utilize the node features and can sample the graph only containing the nodes seen during training thus lacking inductive capability.

4 Preliminary work and future road map

Initial exploration of current baselines led us to realize that major limitation of these models is to model time along with node embeddings. Temporal point process [1] provides a tool to model the distribution over time of next event given the past information. TPPs are defined using a conditional intensity functions $\lambda(t)$. $\lambda(t)$ denotes the expected no. of events in infinitesimally time window $[t, t+dt]$. Probability distribution over the time given the past information can be written in terms of λ as follows.

$$p(t \mid h_{t_n}) = \lambda(t \mid h_{t_n}) \exp(-\int_{t_n}^{t} \lambda(\tau \mid h_{t_n}) d\tau) \qquad (1)$$

Here h_{t_n} denotes the past information of events till time t_n and t_n is the last event observed. To add the event information, a λ is defined for each event type k.

$$p_k(t \mid h_{t_n}) = \lambda_k(t \mid h_{t_n}) \exp(-\int_{t_n}^{t} \lambda_k(\tau \mid h_{t_n}) d\tau) \qquad (2)$$

The future event and corresponding time is calculated by computing the expected time from time distribution of each event $p_k(t \mid h_{t_n})$. Corresponding to the least expected time, future event is selected. Assuming each node in the graph is an event, TPPs are the natural instrument for node and time modelling. But major limitation of temporal point process is that they are ineffective against large number of events. So, our current focus is to scale the TPP to enable time modelling on large scale graph ($\sim 10K+$ nodes) by transforming nodes into continuous domain instead of modelling them as discrete events. Moreover, our near future road-map is as follows-

- Building upon the above approach to incorporate inductive capability.
- Improve the future link prediction efficiency using this approach and introduce the novel task of predicting the time of future link between any two nodes.
- Learning temporal generative model for graphs with attributes. This implies that the sampled graph will need to have the attributes as well on the nodes and edges.

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