On Topology Evolution of Temporal Networks

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Background

- A growing interest on graph and **graph neural networks** in recent years.
- Most of them concentrate on **static graphs**.
- The very few studies on dynamic graphs tend to focus only on **one specific temporal information**.

Research Questions

It is a fundamental task in graph mining to predict graph evolution and is barely explored by the current study of graph neural networks.

- What is the **"general" temporal information** on graph evolution?
- How can we model this information?
- How can we **measure** the effectiveness of our model?

Objectives

We address the above challenge by

- proposing a model that can capture **simultaneously topological and temporal features** of dynamic graphs
- using the model to **predict the topological evolution** of snapshots graphs
- proposing an effective metric to measure the predictive performance

Definition

Dynamic Graph: A sequence of directed or undirected snapshot graphs $\{G_t\}$, with $G_t = (V_t, E_t)$. V_t and E_t are subsets of V and E which represent all the nodes and edges appearing within the time range. $|V_t|$ and $|E_t|$ are not necessarily monotone.

Materials

Message-Passing Graph Network (topological information)

- $x_i = \Theta x_i + \sum_{j \in \mathcal{N}_i} x_j h_\theta(e_{i,j})$ (Aggregation)
- $q = Set2Set(X)$ (Readout)

Recurrent Neural Network (temporal information)

- $q'_t = LSTM(\{q_{t-w}, \dots q_{t-1}\})$

Graph Generative Model

- $\tilde{G} = \arg\max \mathcal{P}(\tilde{A}/\{\tilde{a_1}, \dots, \tilde{a_n}\}|q'_t)$
- $h_i = LSTM(\tilde{a_{i-1}}, h_{i-1})$, where $h_0 = \Theta q'_t$
- $\tilde{a}_i = \sigma(h_i)$

References

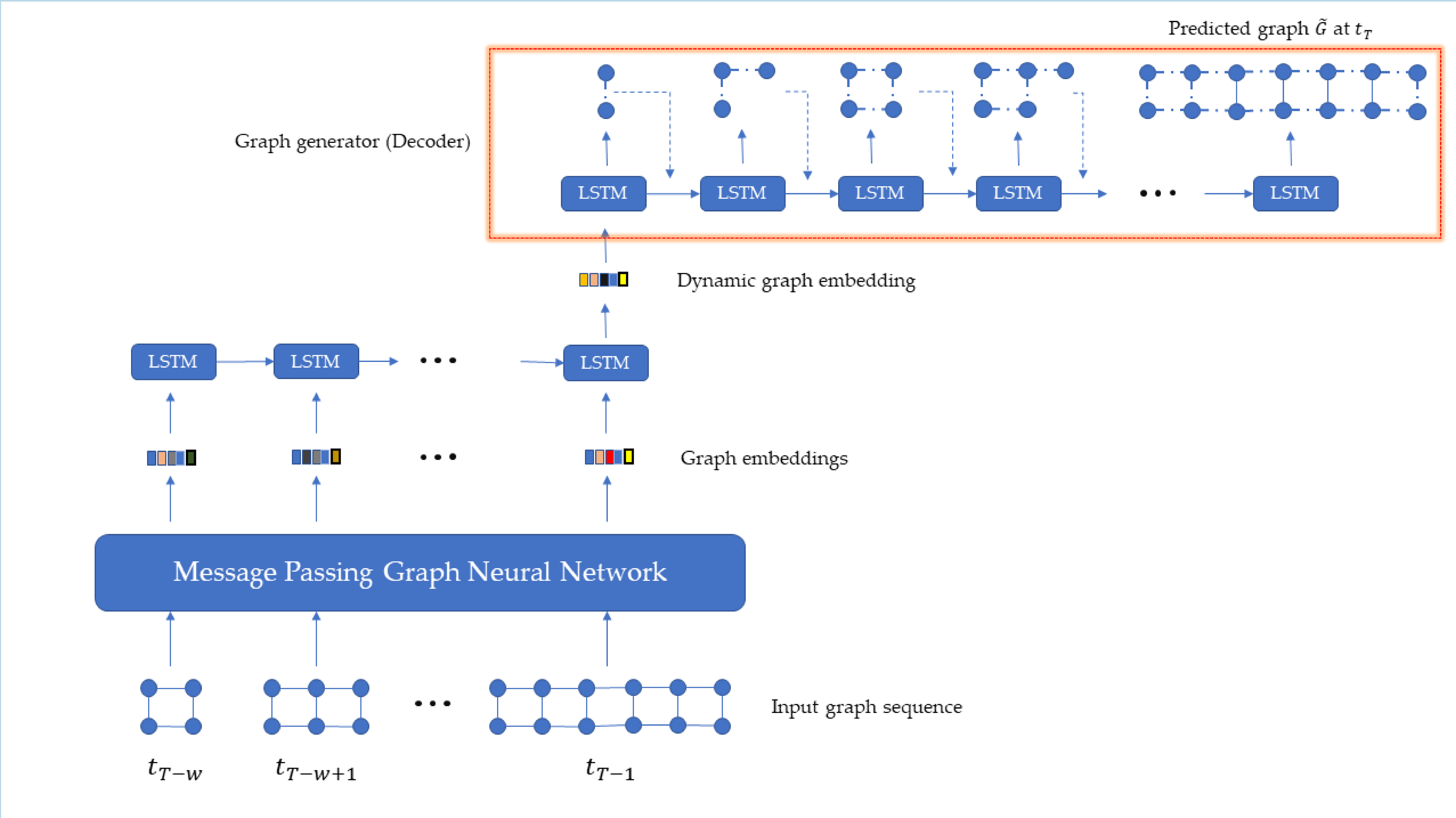
[1] You, Jiaxuan, Rex Ying, Xiang Ren, William L. Hamilton, and Jure Leskovec: *Graphrnn: Generating realistic graphs with deep auto-regressive models*, arXiv preprint arXiv:1802.08773 (2018)

[2] Justin Gilmer, Samuel S. Schoenholz, Patrick F. Riley, Oriol Vinyals, and George E. Dahl: *Neural message passing for Quantum chemistry*, In Proceedings of the 34th International Conference on Machine Learning - ICML 2017

Methods

Proposed Architecture:

As illustrated, the input graph sequence (length w) is feed into a graph neural network to extract their topological feature (graph embedding). They are then passed through a recurrent neural network to couple with temporal information. The output at final timestep is considered containing simultaneously topological and temporal information, thus a good representation modelling network dynamics. It is then feed into a graph generator network to generate graph prediction at expected timestep.



Evaluation:

Metric: Graph kernels $K(G, \tilde{G})$ that measure topological similarity between real graphs and their prediction. (Weisfeiler-Leman Subtree kernel)

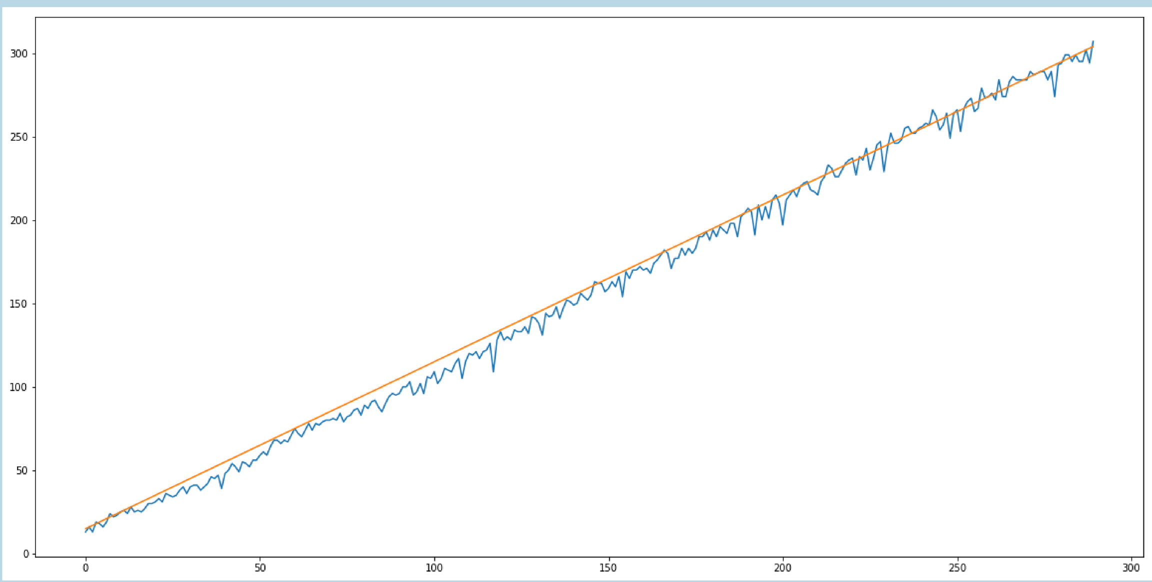
Baseline methods: Erdős–Rényi model, Stochastic block model, Barabási–Albert model, Kronecker graph model, Forest Fire Model.

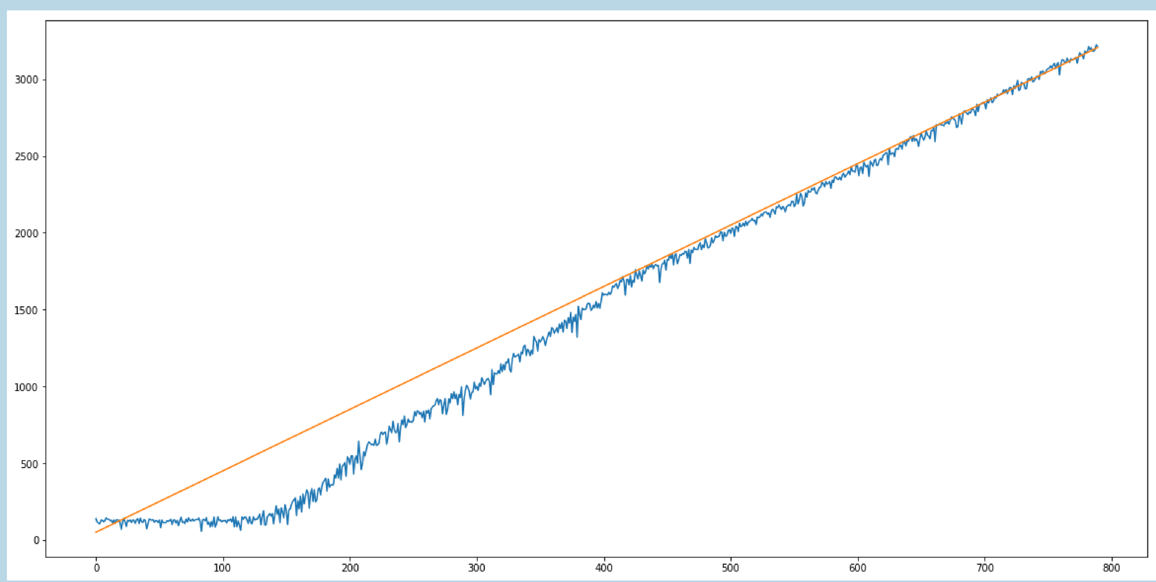
Important Results

Datasets:

- Synthetic dataset: Path graph / Ladder graph with evolving size (add or remove nodes)
- Realworld dataset: Bitcoin-Alpha, Bitcoin-OTC, DNC emails graph

Charts below show the comparison between predicted graph sizes (Blue) and real graph sizes (Orange). *Left: Path graph; Right: Ladder graph.* It seems to be difficult for a relatively complex structure as ladder graph at the beginning but both have good predictions eventually.





The two charts below show the distribution of similarities between predicted graphs and real graphs measured by graph kernel. Histogram in blue is from predictions of proposed model while histogram in orange is from Erdős–Rényi model. *Left: Bitcoin-Alpha; Right: Bitcoin-OTC.*