Spatial-Temporal Data Modeling with Graph Neural Networks

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Doctor of Philosophy

by

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under the supervision of

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to

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Faculty of Engineering and Information Technology

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CERTIFICATE OF ORIGINAL AUTHORSHIP

I, *Zonghan Wu* declare that this thesis, submitted in fulfilment of the requirements for the award of Doctor of Philosophy, in the *Australian Artificial Intelligence Institute*, *Faculty of Engineering and Information Technology* at the University of Technology Sydney, Australia. This thesis is wholly my own work unless otherwise referenced or acknowledged. In addition, I certify that all information sources and literature used are indicated in the thesis. This document has not been submitted for qualifications at any other academic institution. This research is supported by the Australian Government Research Training Program.

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Abstract

Spatial-temporal graph modeling is an important task to analyze the spatial relations and temporal trends of components in a system. It aims to model the dynamic node-level inputs by assuming inter-dependency between connected nodes. A basic assumption behind spatial-temporal graph modeling is that a node's future information is conditioned on its historical information as well as its neighbors' historical information. Therefore how to capture spatial and temporal dependencies simultaneously becomes a primary challenge. Current studies on spatial-temporal graph modeling face four major shortcomings: 1) Most graph neural networks only focus on the low frequency band of graph signals; 2) Current studies assume the graph structure of data reflects the genuine dependency relationships among nodes; 3) Existing studies on spatial-temporal graph neural networks are not applicable to pure multivariate time series data due to the absence of a predefined graph and lack of a general framework; 4) Existing approaches either model spatial-temporal dependencies locally or model spatial correlations and temporal correlations separately. The aim of this thesis is to study spatial-temporal data from the perspective of deep learning on graphs. I have studied the research objective in deep depth with four research questions: (1) How to coordinate the low, middle, and high frequency band of graph signals in graph convolution networks. (2) How to model spatial-temporal graph data effectively and efficiently; (3) How to handle spatial dependencies when a graph is totally missing, incomplete or inaccurate in spatial-temporal graph modeling; (4) In contrast to traditional spatial-temporal graph neural networks that handle spatial dependencies and temporal dependencies in separate, how to unify space and time as a whole in message passing. To address the aforementioned four research problems, I proposed four algorithms or models that can achieve satisfactory results. Specifically, I proposed an Automatic Graph Convolutional Network to learn graph frequency bands for graph convolution filters automatically; I introduced an efficient and effective framework that integrates diffusion graph convolution and dilated temporal convolution to capture spatial-temporal dependencies simultaneously. I developed a novel joint-learning algorithm that can capture spatial-temporal dependencies and learn latent graph structures at the same time; I designed a unified graph neural network that captures the inner spatial-temporal dependencies without compromising space-time integrity. To validate the proposed methods, I have conducted experiments on real-world datasets with a range of tasks including node classification, graph classification, and spatial-temporal graph forecasting. Experimental results demonstrate the effectiveness of the proposed methods.

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List of Publications

Journal Papers

J-1. Wu Z., Pan S., Chen F., Long G., Zhang C. and Philip S.Y., 2020. A comprehensive survey on graph neural networks. IEEE Transactions on Neural Networks and Learning Systems. [CORE A*, Google Citations: 1,969]

J-2. Wu Z., Pan S., Long G., Jiang J. and Zhang C., 2021. Beyond low-pass filtering: graph convolutional networks with automatic filtering. Submitted to IEEE Transactions on Knowledge and Data Engineering. [CORE A*, Under Review]

J-3. Wu Z., Zheng D., Pan S., Gan G., Long G. and Karypis G., 2021. TraverseNet: Unifying Space and Time in Message Passing. Submitted to IEEE Transactions on Neural Networks and Learning Systems. [CORE A*, Under Review]

Conference Papers

C-1. Wu Z., Pan S., Long G., Jiang J. and Zhang C., 2019. Graph wavenet for deep spatial-temporal graph modeling. In Proceedings of the 28th International Joint Conference on Artificial Intelligence (pp. 1907-1913). [CORE A*, Google Citations: 190]

C-2. Wu Z., Pan S., Long, G., Jiang J., Chang X. and Zhang C., 2020, August. Connecting the dots: Multivariate time series forecasting with graph neural networks. In Proceedings of the 26th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining (pp. 753-763). [CORE A*, Google Citations: 53]

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