

UNIVERSITY OF TECHNOLOGY SYDNEY
Faculty of Engineering and Information Technology

**Local Information and Structures in Analysis and
Modelling of Complex Networks**

by

Mingshan Jia

A THESIS SUBMITTED
IN PARTIAL FULFILLMENT OF THE
REQUIREMENTS FOR THE DEGREE

Doctor of Philosophy

Sydney, Australia

July 2022

Certificate of Authorship/Originality

I, Mingshan Jia, declare that this thesis, is submitted in fulfilment of the requirements for the award of Doctor of Philosophy, in the Faculty of Engineering and Information Technology at the University of Technology Sydney.

This thesis is wholly my 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.

Mingshan Jia

Signature: Production Note:
Signature removed
prior to publication.

Date: July 2022

ABSTRACT

Local Information and Structures in Analysis and Modelling of Complex Networks

by

Mingshan Jia

Abstracting entities and their interactions as nodes and links, networks are a general representation for modelling and studying complex systems. Modelling relational structures of the underlying data, rather than only a set of isolated entities, allows us to build more accurate models for various types of domain data, such as social relationships, molecular interactions, program executions, and many more. Despite being powerful and ubiquitous, networks are also difficult to process, mainly due to their complex topological structures. Therefore, the study of network structure, especially local structure, has been the core theme of studying complex networks. This dissertation aims to provide new understandings of how local structure information is extracted and utilised in studying different types of complex networks.

The dissertation includes three original works in the direction of local structure and information on top of a comprehensive survey. In the review, we propose new taxonomies for graph structures that bring together the notions of centrality measures, motifs, and other local-level metrics. For theoretical understanding, we propose new metrics to quantify the formation of 3-node and 4-node subgraphs and develop new motif patterns that are distinctive features in both network- and node-level analysis. For methodological approaches, we propose the framework to effectively encode edge attributes into the typed-edge graphlet degree vector, for both sociocentric and egocentric networks. Moreover, for practical applications, the proposed metrics and approaches are applied in many different types of complex net-

works and case studies. They are not only proven to be effective in multiple learning and analytical tasks but also lead to new insights and interesting discoveries.

Dissertation directed by Professor Katarzyna Musial-Gabrys and Professor Bogdan Gabrys

School of Computer Science, Data Science Institute, Complex Adaptive Systems Lab, UTS

Acknowledgements

Although pursuing a PhD is not an easy path to take, looking back on the past three years and nine months, it might be one of the best decisions I have ever made. I am grateful that I did not give up in some very tough situations. It eventually led me to meet my current supervisors and other wonderful people, who have advised me, supported me, worked with me and motivated me.

First and foremost, I am eternally grateful to my supervisors, — Professor Katarzyna Musial-Gabrys and Professor Bogdan Gabrys, for all the support and guidance they have provided throughout my PhD study. They gave me the opportunity to continue my PhD at my most difficult time, and they have supported me, encouraged me and trusted me ever since. They introduced me to the world of network science and provided me with all kinds of advice, from idea selection and experiment design to paper writing and rebuttal. They not only helped me improve in academics, but also recommended me to participate in collaborative research projects with other universities, and gave me multiple opportunities to participate in teaching activities. Without them, I could not have achieved such an all-round growth. Thank you, Professor Katarzyna Musial-Gabrys and Professor Bogdan Gabrys.

Moreover, I would like to thank all the people who have advised me, worked with me and helped me along my PhD journey. I want to thank my co-authors, Maité Van Alboom, Liesbet Goubert and Piet Bracke. Thanks to you and my supervisors, we have conducted an exciting cross-disciplinary study about chronic pain. I want to thank Professor Wei Liu and Dr Yi Zhang for being on my candidature assessment panel. I also thank Professor Pasquale De Meo for the interesting and insightful discussions on multiple research topics.

Next, I want to express my gratitude to my colleagues and friends, who have

always been so kind and helpful whenever I seek advice or help. Their knowledge, diligence and perseverance are also what motivate me to move forward. Thank you, Joakim Skarding, Mohamad Barbar, Guanping Xiao, Bin Wang, Xiaolin Zhang, Yanbin Liu, Xiaohan Zhang, and Yu-Xuan Qiu.

Finally and most importantly, I would like to thank my family. It is your everlasting love and support that allow me to start this wonderful journey and make me fearless in the face of all difficulties. Thank you, my parents Lingxiang Feng, Zilai Jia, my wife Yuanyuan Liu, and my son Yiqian Jia. This is dedicated to you.

Mingshan Jia
Sydney, Australia, 2022

List of Publications

Journal Papers

- J-1. **M. Jia**, B. Gabrys and K. Musial, "Directed closure coefficient and its patterns," in Plos one 16.6 (2021): e0253822.
- J-2. **M. Jia**, B. Gabrys and K. Musial, "Measuring Quadrangle Formation in Complex Networks," in IEEE Transactions on Network Science and Engineering, vol. 9, no. 2, pp. 538-551, 1 March-April 2022.

Conference Papers

- C-1. **M. Jia**, B. Gabrys and K. Musial, "Closure Coefficient in Complex Directed Networks." International Conference on Complex Networks and Their Applications. Springer, Cham, 2020.
- C-2. **M. Jia**, M. Van Alboom, L. Goubert, P. Bracke, B. Gabrys, K. Musial. "Analysing Ego-Networks via Typed-Edge Graphlets: A Case Study of Chronic Pain Patients." International Conference on Complex Networks and Their Applications. Springer, Cham, 2021.
- C-3. **M. Jia**, M. Van Alboom, L. Goubert, P. Bracke, B. Gabrys, K. Musial. "Analysing Egocentric Networks via Local Structure and Centrality Measures: A Study on Chronic Pain Patients." 2022 International Conference on Information Networking (ICOIN). IEEE, 2022.

Contents

| | |
|---|----------|
| Certificate | ii |
| Abstract | iii |
| Acknowledgments | v |
| List of Publications | vii |
| List of Figures | xii |
| 1 Introduction | 1 |
| 1.1 Aim, Objectives and Significance | 3 |
| 1.2 Methodology | 6 |
| 1.3 Thesis Organisation | 7 |
| 2 Literature Review | 9 |
| 2.1 Motivation | 9 |
| 2.2 Preliminaries and Background | 11 |
| 2.2.1 Local vs. Global | 11 |
| 2.2.2 Motifs vs. Graphlets | 13 |
| 2.3 Graph structural measures | 15 |
| 2.3.1 Subgraph Count Based Approaches | 17 |
| 2.3.2 Subgraph Formation Based Approaches | 25 |
| 2.3.3 Global Path Based Approaches | 33 |
| 2.3.4 Message Passing Based Approaches | 39 |

| | | |
|----------|---|-----------|
| 2.3.5 | Hybrid Approaches | 42 |
| 2.4 | Discussion and Outlook | 47 |
| 2.5 | Conclusion | 50 |
| 3 | Directed Closure Coefficient | 52 |
| 3.1 | Introduction | 52 |
| 3.2 | Preliminaries | 56 |
| 3.2.1 | Clustering coefficient | 56 |
| 3.2.2 | Directed clustering coefficient | 57 |
| 3.2.3 | Closure coefficient | 59 |
| 3.3 | Closure Coefficient in Directed Networks | 61 |
| 3.3.1 | Closure coefficient in binary directed networks | 61 |
| 3.3.2 | Closure coefficients of particular patterns | 63 |
| 3.3.3 | Closure coefficient in weighted networks | 66 |
| 3.3.4 | Computational efficiency | 68 |
| 3.4 | Experiments and Analysis | 68 |
| 3.4.1 | Directed closure coefficient in real-world networks | 69 |
| 3.4.2 | Link prediction in directed networks | 72 |
| 3.4.3 | Case study in a weighted signed network | 76 |
| 3.5 | Additional Related Work Discussion | 78 |
| 3.6 | Conclusion | 78 |
| 4 | Measuring The Formation of Quadrangles | 80 |
| 4.1 | Introduction | 80 |
| 4.2 | Background and Motivating Example | 84 |
| 4.2.1 | Measuring Triangle Formation | 85 |

| | | |
|----------|--|------------|
| 4.2.2 | A motivating example | 86 |
| 4.3 | Two Quadrangle Coefficients | 87 |
| 4.3.1 | I-quad coefficient | 87 |
| 4.3.2 | O-quad coefficient | 90 |
| 4.3.3 | Quadrangle coefficients in weighted networks | 91 |
| 4.3.4 | Computational cost | 94 |
| 4.4 | Experiments and Analysis | 94 |
| 4.4.1 | Quadrangle coefficients in real-world networks | 94 |
| 4.4.2 | Correlation with node degree | 97 |
| 4.4.3 | Network classification | 101 |
| 4.4.4 | Link prediction | 104 |
| 4.4.5 | Limitations and Future Directions | 107 |
| 4.5 | Related Work | 109 |
| 4.6 | Conclusion | 111 |
| 5 | Typed-Edge Graphlets | 113 |
| 5.1 | Introduction | 113 |
| 5.2 | Background and Preliminaries | 115 |
| 5.2.1 | Graphlets and orbits | 116 |
| 5.2.2 | Egocentric graphlets | 117 |
| 5.3 | Typed-Edge Graphlet Degree Vector | 117 |
| 5.4 | Typed-Edge Degree, Colored Graphlets and Heterogeneous Graphlets . | 121 |
| 5.5 | Experiments and Analysis | 124 |
| 5.5.1 | Dataset | 125 |
| 5.5.2 | Analysing pain grades via GDV and TyE-GDV | 127 |

| | |
|--|------------|
| 5.5.3 Predicting pain grades | 130 |
| 5.6 Conclusion | 132 |
| 6 Conclusion and future works | 134 |
| Bibliography | 137 |

List of Figures

| | | |
|-----|---|----|
| 1.1 | Methodology | 5 |
| 1.2 | Three verification steps in methodology | 6 |
| 2.1 | Structural measures on graphs. | 9 |
| 2.2 | Graphlets and their orbits [160] | 13 |
| 2.3 | Motifs vs. Graphlets | 13 |
| 2.4 | Subgraph count based measures. | 15 |
| 2.5 | Subgraph formation based measures. | 23 |
| 2.6 | Global path based measures. | 31 |
| 2.7 | Message passing based approaches. | 37 |
| 2.8 | Hybrid Approaches. | 41 |
| 3.1 | Classification diagram of local clustering measures. | 52 |
| 3.2 | Taxonomy of directed triangles. | 53 |
| 3.3 | Dealing with bidirectional edges. | 55 |
| 3.4 | Directed open triads. | 62 |
| 3.5 | Scatter plots of the local directed closure coefficient and the local directed clustering coefficient, with the Pearson correlation coefficient. | 68 |

| | | |
|------|--|-----|
| 3.6 | Average normalized closure coefficients of four patterns: head-of-path (HoP), mid-of-path (MoP), end-of-path (EoP) and cyclic (CYC). The dominant pattern in each network is labelled with its value. | 69 |
| 3.7 | Two scatter plots of the network BTC-ALPHA. | 73 |
| 3.8 | Two local enlarged scatter plots between weighted signed directed closure coefficient and node strength in the network BTC-ALPHA. . . | 74 |
| 4.1 | The i-quad coefficient and the o-quad coefficient in comparison with the clustering coefficient and the closure coefficient. | 78 |
| 4.2 | An example of the i-quad coefficient and the o-quad coefficient in a movie recommender network. | 79 |
| 4.3 | A motivating example. | 83 |
| 4.4 | Two types of open quadriads in a quadrangle. | 86 |
| 4.5 | Correlation of quadrangle coefficients and weighted quadrangle coefficients in three different networks. | 90 |
| 4.6 | Cumulative distribution curve of the i-quad coefficient $I(i)$ (in green colour) and the o-quad coefficient $O(i)$ (in purple colour) in six real-world networks of different types. | 94 |
| 4.7 | Correlation of two quadrangle coefficients with node degree in six real-world networks. | 95 |
| 4.8 | Two types of quadrangle formation via stub matching. | 97 |
| 4.9 | Two-dimensional visualisation of K-means clustering on PCA-reduced data, without and with quadrangle coefficients (left figure and right figure respectively). | 97 |
| 4.10 | Critical difference diagram of four classifiers with different feature sets. | 104 |

| | | |
|------|---|-----|
| 4.11 | An example of the coefficients proposed in related works, compared with our proposed quadrangle coefficients. | 107 |
| 5.1 | Graphlets of size 2–4 nodes with enumeration of orbits. | 111 |
| 5.2 | 7 egocentric graphlets of 2 to 4 nodes. Ego node is painted in black. | 113 |
| 5.3 | Degree distribution and edge type distribution of all patients. | 122 |
| 5.4 | Parallel coordinates plot of average GDV of different GCPS grades. Each coordinate represents the average number of graphlets belonging to that type. | 123 |
| 5.5 | Parallel coordinates plot of average TyE-GDV of different GCPS grades for two graphlets. Each coordinate represents the average number of edges belonging to that type. | 125 |
| 5.6 | Prototypes of GCPS grade-1 and GCPS grade-4. | 126 |