Artificial Intelligence: Foundations, Theory, and Algorithms

Series Editors

Barry O'Sullivan, Department of Computer Science, University College Cork, Cork, Ireland

Michael Wooldridge, Department of Computer Science, University of Oxford, Oxford, UK

Artificial Intelligence: Foundations, Theory and Algorithms fosters the dissemination of knowledge, technologies and methodologies that advance developments in artificial intelligence (AI) and its broad applications. It brings together the latest developments in all areas of this multidisciplinary topic, ranging from theories and algorithms to various important applications. The intended readership includes research students and researchers in computer science, computer engineering, electrical engineering, data science, and related areas seeking a convenient way to track the latest findings on the foundations, methodologies, and key applications of artificial intelligence.

This series provides a publication and communication platform for all AI topics, including but not limited to:

- Knowledge representation
- · Automated reasoning and inference
- Reasoning under uncertainty
- Planning, scheduling, and problem solving
- · Cognition and AI
- Search
- Diagnosis
- Constraint processing
- Multi-agent systems
- · Game theory in AI
- Machine learning
- Deep learning
- · Reinforcement learning
- Data mining
- Natural language processing
- Computer vision
- · Human interfaces
- Intelligent robotics
- Explanation generation
- · Ethics in AI
- Fairness, accountability, and transparency in AI

This series includes monographs, introductory and advanced textbooks, state-of-the-art collections, and handbooks. Furthermore, it supports Open Access publication mode.

More information about this series at https://link.springer.com/bookseries/13900

Heterogeneous Graph Representation Learning and Applications



Chuan Shi School of Computer Science Beijing University of Posts and Telecommunications Beijing, China

Philip S. Yu Department of Computer Science University of Illinois at Chicago Chicago, IL, USA Xiao Wang School of Computer Science Beijing University of Posts and Telecommunications Beijing, China

© The Editor(s) (if applicable) and The Author(s), under exclusive license to Springer Nature Singapore Pte Ltd. 2022

This work is subject to copyright. All rights are solely and exclusively licensed by the Publisher, whether the whole or part of the material is concerned, specifically the rights of translation, reprinting, reuse of illustrations, recitation, broadcasting, reproduction on microfilms or in any other physical way, and transmission or information storage and retrieval, electronic adaptation, computer software, or by similar or dissimilar methodology now known or hereafter developed.

The use of general descriptive names, registered names, trademarks, service marks, etc. in this publication does not imply, even in the absence of a specific statement, that such names are exempt from the relevant protective laws and regulations and therefore free for general use.

The publisher, the authors, and the editors are safe to assume that the advice and information in this book are believed to be true and accurate at the date of publication. Neither the publisher nor the authors or the editors give a warranty, expressed or implied, with respect to the material contained herein or for any errors or omissions that may have been made. The publisher remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.

This Springer imprint is published by the registered company Springer Nature Singapore Pte Ltd. The registered company address is: 152 Beach Road, #21-01/04 Gateway East, Singapore 189721, Singapore

Foreword

Graphs and networks are ubiquitous in today's interconnected world. Among complex network models, a specific one, called *heterogeneous network* (or *heterogeneous graph*), which models real-world systems as interactions among a massive set of multi-modal and multi-typed objects, is of particular importance because the explicit modeling of the inherent structure of complex networks facilitates powerful, in-depth network analysis. In recent years, *representation learning* (which is also known as *embedding learning*), which represents high-dimensional data with lower dimensional distributions by various deep learning or embedding methods, has been rapidly developed as a powerful tool for high-dimensional data analysis. Similarly, *graph representation learning* (also called *network embedding*), which learns representations of nodes/edges in a lower-dimensional space, has demonstrated its effectiveness for various graph mining and graph analysis tasks.

This book is the first book dedicated to *heterogeneous graph representation learning*, which learns node/edge representations in a lower dimensional space while preserving the heterogeneous structures and semantics for downstream tasks (e.g., node/graph classification and link prediction). Heterogeneous graph representation learning has become a powerful, realistic, and general network modeling tool in recent years and has attracted increasing attention in both academia and industry.

This book serves as a comprehensive and extensive introduction to heterogeneous graph representation learning and its applications, including a survey of current developments and the state of the art in this booming field. It not only extensively introduces the mainstream techniques and models, including structure-preserved, attribute-assisted, and dynamic graph, but also presents wide applications in recommendation, text mining, and industry. In addition, the book provides a platform and practice of heterogeneous graph representation learning. As the first book on the theme, it summarizes the latest developments and presents cutting-edge research on heterogeneous graph representation learning. It may have double benefits: (1) providing researchers with an understanding of the fundamental issues and a good entry point for working in this rapidly expanding field, and (2) presenting the latest research on applying heterogeneous graphs to model real systems and learning structural features of interaction systems.

vi Foreword

The authors of this book have done substantial research on heterogeneous graph representation learning and the related themes. Philip S. Yu is one of the leading experts on data mining and heterogeneous information networks. Chuan Shi is a long-term collator with Philip on research into heterogeneous information networks. Chuan has systematically studied the recommendation and representation learning based on heterogeneous graphs, applied heterogeneous information network modeling to e-commerce and text mining, and dived recently into heterogeneous graph representation learning. Wang Xiao is a rising-star scholar in network embedding community. The book systematically summarizes their contributions in the direction of heterogeneous graph representation learning. This book can be used not only as a guidebook for academia and industry but also as a textbook for undergraduate and graduate students. I hope you enjoy reading it.

Michael Aiken Chair Professor University of Illinois at Urbana-Champaign Jiawei Han

Preface

Heterogeneous graph, containing different types of nodes and links, is ubiquitous in the real world, ranging from bibliographic networks and social networks to recommendation systems. Currently, heterogeneous graph representation learning, which learns node/edge representations in a lower dimensional space while preserving the heterogeneous structures and semantics for downstream tasks (e.g., node/graph classification and link prediction), has attracted considerable attentions, and we have witnessed the impressive performance of heterogeneous graph representation learning methods on various real-world applications (e.g., recommender systems). The increasing number of works on heterogeneous graph representation learning indicates a global trend in both academic and industrial communities. Thus, there is a pressing demand for comprehensively summarizing and discussing heterogeneous graph representation learning methods.

Compared with homogeneous graph representation learning, heterogeneous graph representation learning shows different challenges because of the heterogeneity. For example, heterogeneous graph has more complex structures caused by multiple relations, where the node attributes are also heterogeneous. The heterogeneous graph representation learning is highly related with real-world applications from the heterogeneous graph construction to learning, which may need more advanced domain knowledge. All these factors heavily affect the performance of heterogeneous graph representation learning, which should be carefully considered. Therefore, researches on heterogeneous graph representation learning are of great scientific and application value.

This book serves the interests of specific reader groups. Generally, the book is intended for anyone who wishes to understand the fundamental problems, techniques, and applications of heterogeneous graph representation learning. In particular, we hope that students, researchers, and engineers will find this book inspiring.

This book is divided into four parts, and the readers are able to quickly understand this field through the first part, deeply study the techniques and applications with the second and third parts, and perform typical algorithms with a platform in the fourth part.

viii Preface

• In the first part, we first present an overview of recent heterogeneous graph representation learning methods from different aspects, including both of the methodology and technique levels. Open sources are also summarized so as to facilitate future research and applications in this area. This part will help readers rapidly understand the overall development of this field. In particular, in Chap. 1, the basic concepts and definitions, as well as the background of homogeneous and heterogeneous graph representation learning, will be introduced. The method taxonomy and open sources will be summarized in Chap. 2.

- In the second part, we then provide an in-depth and detailed introduction of representative heterogeneous graph representation learning techniques. This part will help readers understand the fundamental problems in this field and illustrate how to design the state-of-the-art heterogeneous graph representation learning methods for these problems. In particular, the structure-preserved heterogeneous graph representation learning methods are discussed in Chap. 3, including the meta-path structure and network schema structure. In Chap. 4, the heterogeneous graph representation learning methods with attributes are presented, mainly focusing on the heterogeneous graph neural networks. After that, we introduce the dynamic heterogeneous representation learning methods in Chap. 5, which consider the incremental learning, sequence information, and temporal interaction. Then, in Chap. 6, we discuss some emerging topics of heterogeneous graph representation learning, covering the adversarial learning, sampling, and hyperbolic representation learning.
- In the third part, we summarize the real-world applications based on heterogeneous graph representation learning. This part enables readers to know the successful applications of heterogeneous graph representation learning and the way of applying the advanced techniques to the real-world scenarios. Specifically, in Chap. 7, we show how the heterogeneous graph representation learning improves different recommender systems, e.g., the top-N recommendation, cold-start recommendation, and author-set recommendation. The application on text mining is introduced in Chap. 8, focusing on the short text classification and the news recommendation scenarios. In Chap. 9, we present the heterogeneous graph representation learning in industry applications, e.g., the cash-out user detection, intent recommendation, share recommendation, and friend-enhanced recommendation.
- In the fourth part, we introduce a platform of heterogeneous graph representation learning and conclude this book. Considering the importance of deep learning platforms, we introduce the foundation platforms on graph machine learning, especially the platform of heterogeneous graph representation learning in Chap. 10. Also, we take three representative heterogeneous graph neural networks as examples, showing how we can perform them using the platform. Finally, the future research directions and open problems are discussed in Chap. 11.

Writing a book always involves more people than just the authors. We would like to express our sincere thanks to all those who worked with us on this book. They are Deyu Bo, Jiawei Liu, Ruijia Wang, Yugang Ji, Houye Ji, Yiding Zhang, Mengmei

Preface

Zhang, Tianchi Yang, Shaohua Fan, Chunchen Wang, Hui Han, Qi Cui, Qi Zhang, Nian Liu, Yuanxin Zhuang, Zhenyi Wang, Guanyi Chu, Hongrui Liu, Chen Li, Tianyu Zhao, Xinlong Zhai, Donglin Xia, and Fengqi Liang. We also give our thanks to many students of Prof. Philip S. Yu for their careful proofreading. They are Yuwei Cao, Yingtong Dou, Ziwei Fan, He Huang, Xiaohan Li, Zhiwei Liu, and Congying Xia. In addition, the work is supported by the National Natural Science Foundation of China (No. U20B2045, U1936220, 61772082, 61702296, 62002029, 62172052). It is also supported in part by NSF under grants III-1763325, III-1909323, III-2106758, and SaTC-1930941. We also thank the supports of these grants. Finally, we thank our families for their wholehearted support throughout this book.

About the Book

Representation learning in heterogeneous graphs (HGs) is intended to provide a meaningful vector representation for each node so as to facilitate downstream applications, such as link prediction, personalized recommendation, node classification, etc. This task, however, is challenging not only because of the need to incorporate heterogeneous structural (graph) information consisting of multiple types of node and edge but also because of the need to consider heterogeneous attributes or types of content (e.g., text or image) associated with each node. Although considerable advances have been made in homogeneous (and heterogeneous) graph embedding, attributed graph embedding, and graph neural networks, few are capable of simultaneously and effectively taking into account the heterogeneous structural (graph) information as well as the heterogeneous content information of each node.

In this book, we provide a comprehensive survey of the current developments in HG representation learning. More importantly, we present the state-of-the-art in this field, including theoretical models and real applications that have been showcased at the top conferences and journals, such as TKDE, KDD, WWW, IJCAI, and AAAI. This book has two major objectives: (1) to provide researchers with an understanding of the fundamental issues and a good point of departure for working in this rapidly expanding field and (2) to present the latest research on applying heterogeneous graphs to model real systems and learning structural features of interaction systems. To the best of our knowledge, it is the first book to summarize the latest developments and present cutting-edge research on heterogeneous graph representation learning. To gain the most from it, readers should have a basic grasp of computer science, data mining, and machine learning.

Contents

1	Intr	oduction	1		
	1.1	Basic (Concepts and Definitions		
	1.2	Graph	Representation Learning		
	1.3				
			hallenges		
	1.4	Organi	ization of the Book		
	Refe				
2	The	State of	f the Aut of Heterogeneous Creph		
4		The State-of-the-Art of Heterogeneous Graph Representation			
	2.1		d Taxonomy		
	2.1	2.1.1	Structure-Preserved Representation		
		2.1.2	Attribute-Assisted Representation		
		2.1.3	Dynamic Representation		
		2.1.3	Application-Oriented Representation		
	2.2		ique Summary		
	2.2	2.2.1	Shallow Model		
		2.2.2	Deep Model		
	2.3		Sources		
	2.3	2.3.1	Benchmark Datasets		
		2.3.2			
		2.3.3	Available Tools		
	Refe		Available 10015		
	Ittic	1011005			
Pa	rt I	Гесhniqu	ies		
3	Stru	cture-Pr	reserved Heterogeneous Graph Representation		
	3.1		uction		
	3.2	.2 Meta-Path Based Random Walk			
		3.2.1	Overview		
		3.2.2	The HERec Model		
		3.2.3	Experiments		

xiv Contents

	3.3	Meta-P	Path Based Decomposition	41
		3.3.1	Overview	41
		3.3.2	The NeuACF Model	42
		3.3.3	Experiments	47
	3.4	Relatio	on Structure Awareness	48
		3.4.1	Overview	48
		3.4.2	Preliminary	51
		3.4.3	The RHINE Model	53
		3.4.4	Experiments	56
	3.5	Netwo	rk Schema Preservation	58
		3.5.1	Overview	58
		3.5.2	The NSHE Model	59
		3.5.3	Experiments	64
	3.6	Conclu	isions	65
	Refer	ences		66
	A 44 •		'A III A COLD A A	7.1
4			sisted Heterogeneous Graph Representation	71
	4.1		action	71
	4.2		geneous Graph Attention Network	72
		4.2.1	Overview	72
		4.2.2	The HAN Model	74
	4.0	4.2.3	Experiments	78
	4.3		geneous Graph Propagation Network	83
		4.3.1	Overview	83
		4.3.2	Semantic Confusion Analysis	85
		4.3.3	The HPN Model	87
		4.3.4	Experiments	90
	4.4		geneous Graph Structure Learning	93
		4.4.1	Overview	93
		4.4.2	The HGSL Model	94
		4.4.3	Experiments	100
	4.5		isions	102
	Refer	ences		103
5	Dvna	mic Het	terogeneous Graph Representation	107
	5.1		iction	107
	5.2		ental Learning	108
		5.2.1	Overview	108
		5.2.2	The DyHNE Model	109
		5.2.3	Experiments	116
	5.3		nce Information	122
		5.3.1	Overview	122
		5.3.2	The SHCF Model	124
		5.3.3	Experiments	129
	5.4		ral Interaction	132
		5.4.1	Overview	132

Contents xv

		5.4.2	The THIGE Model	132
		5.4.3	Experiments	138
	5.5	Conclu	ision	140
	Refe	rences		140
6	Eme	rging To	ppics of Heterogeneous Graph Representation	145
	6.1		action	145
	6.2			146
		6.2.1	Overview	146
		6.2.2	The HeGAN Model.	147
		6.2.3	Experiments	151
	6.3		ance Sampling	154
	0.0	6.3.1	Overview	154
		6.3.2	The HeteSamp Model	155
		6.3.3	Experiments	160
	6.4		bolic Representation	162
		6.4.1	Overview	162
		6.4.2	The HHNE Model	163
		6.4.3	Experiments	166
	6.5	Conclu	ision	170
	Refe			170
Par	t II	Applicat	tions	
7	Hete	rogeneo	us Graph Representation for Recommendation	175
	7.1	Introdu	action	175
	7.2	Top-N	Recommendation	176
		7.2.1	Overview	176
		7.2.2	The MCRec Model	177
		7.2.3	Experiments	182
	7.3	3 Cold-Start Recommendation		
		7.3.1	Overview	185
		7.3.2	The MetaHIN Model	186
		7.3.3	Experiments	192
	7.4	Author	r Set Recommendation	195
		7.4.1	Overview	195
		7.4.2	The ASI Model	197
		7.4.3	Experiments	202
	7.5	Conclu	isions	206
	Refe	rences		206
8	Heterogeneous Graph Representation for Text Mining			
	8.1		action	209
	8.2 Short Text Classification			210
	0.2	Short	icat Classification	
	0.2	8.2.1	Overview	210

xvi Contents

		8.2.3	The HGAT Model	212
		8.2.4	Experiments	216
	8.3	News I	Recommendation with Long/Short-Term Interest	
		Modeli	ing	220
		8.3.1	Overview	220
		8.3.2	Problem Formulation	220
		8.3.3	The GNewsRec Model	221
		8.3.4	Experiments	227
	8.4	News I	Recommendation with Preference Disentanglement	229
		8.4.1	Overview	229
		8.4.2	The GNUD Model	231
		8.4.3	Experiments	235
	8.5	Conclu	sion	237
	Refer	ences		238
9	Hoto		us Cranh Danussantation for Industry Application	241
9	9.1	_	us Graph Representation for Industry Application	241
	9.1		Out User Detection	241
	9.2	9.2.1	Overview	242
		9.2.1	Preliminaries	243
		9.2.2	The HACUD Model	243
		9.2.3	Experiments	247
	9.3		Recommendation	250
	9.3	9.3.1	Overview	250
		9.3.1	Problem Formulation	251
		9.3.3	The MEIRec Model	251
		9.3.4	Experiments	256
	9.4		Recommendation	259
	∕. ⊤	9.4.1	Overview	259
		9.4.2	Problem Formulation	261
		9.4.3	The HGSRec Model	262
		9.4.4	Experiments	266
	9.5		Enhanced Recommendation	270
	7.0	9.5.1	Overview	270
		9.5.2	Preliminaries	272
		9.5.3	The SIAN Model	272
		9.5.4	Experiments	276
	9.6		isions	281
				282
4.0				_02
10	Platforms and Practice of Heterogeneous Graph			
	-		on Learning	285
	10.1		action	285
	10.2		ation Platforms	286
		10.2.1	Deep Learning Platforms	286

Contents xvii

		10.2.2 Platforms of Graph Machine Learning	290
		10.2.3 Platforms of Heterogeneous Graph	
		Representation Learning	292
	10.3	Practice of Heterogeneous Graph Representation Learning	293
		10.3.1 Build a New Dataset	294
		10.3.2 Build a New Model	299
		10.3.3 Practice of HAN	301
		10.3.4 Practice of RGCN	305
		10.3.5 Practice of HERec	307
	10.4	Conclusion	309
	Refer	ences	310
11	Future Research Directions.		
	11.1	Introduction	311
	11.2 Preserving HG Structures11.3 Capturing HG Properties		312
			313
	11.4	Deep Graph Learning on HG Data	313
	11.5	Making HG Representation Reliable	314
	11.6	Technique Deployment in Real-World Applications	315
	11.7	Others	315
	References		

About the Authors

Chuan Shi is a professor in the School of Computer Sciences of Beijing University of Posts and Telecommunications and the deputy director of the Beijing Key Lab of Intelligent Telecommunication Software and Multimedia. His main research interests include data mining, machine learning, artificial intelligence, and big data analysis. He has published more than 100 refereed papers, including top journals and conferences in data mining, such as IEEE TKDE, ACM TKDD, KDD, WWW, NeurIPS, AAAI, and IJCAI. In the meanwhile, his first monograph about heterogeneous information networks has been published by Springer. He has been honored with the best paper award in ADMA 2011 and ADMA 2018 and has guided students to the world championship in the IJCAI Contest 2015, the premier international data mining competition. He is also the recipient of "the Youth Talent Plan" and "the Pioneer of Teacher's Ethics" in Beijing.

Xiao Wang is the associate professor in the School of Computer Sciences of Beijing University of Posts and Telecommunications. He was a postdoc in the Department of Computer Science and Technology at Tsinghua University. He got his Ph.D. in the School of Computer Science and Technology at Tianjin University and a joint-training Ph.D. at the Washington University in St. Louis. His main research interests include data mining, machine learning, artificial intelligence, and big data analysis. He has published more than 70 refereed papers, including top journals and conferences in data mining, such as IEEE TKDE, KDD, NeurIPS, AAAI, IJCAI, and WWW. He also serves as SPC/PC member and Reviewer of several high-level international conferences, e.g., KDD, AAAI, IJCAI, and journals, e.g., IEEE TKDE.

Philip S. Yu's main research interests include big data, data mining (especially on graph or network mining), social network, privacy-preserving data publishing, data stream, database systems, and Internet applications and technologies. Dr. Yu is a distinguished professor in the Department of Computer Science at UIC and also holds the Wexler Chair in Information and Technology. Before joining UIC, he was with the IBM Thomas J. Watson Research Center, where he was the manager of

xx About the Authors

the Software Tools and Techniques department. He has published more than 1,300 papers in refereed journals and conferences with more than 149,000 citations and an H-index of 176. He holds or has applied for more than 300 U.S. patents. He is a fellow of the ACM and the IEEE. He is a recipient of the ACM SIGKDD 2016 Innovation Award and the IEEE Computer Society's 2013 Technical Achievement Award.