

Very Quick Overview

What are graphs?

Simply, a collection of sets of size two!

{Apple, Orange} {Apple, Banana} {Mango, Peach}

{Suter, Xian} {Xian, Xidian}

Order of the subsets doesn't matter. Order of items within the subsets doesn't matter. (There are *directed* graphs where the order in the subsets DOES matter – then we would be better to use the ordered pair notation... (Suter, Xian) (Suter, Perth) (Suter, Adelaide) etc.)

What are hypergraphs?

Simply a collection of sets of any size (not necessarily two but can be...)

{Apple,Orange,Pear}, {Banana, Peach}, {Mango, Grape, Blueberry}

Sometimes we will consider *special* types of hypergraphs – e.g., hypergraphs where all subsets are of a fixed size – e.g., 3-uniform hypergraphs, 7-uniform hypergraphs.

Note 2-uniform hypergraphs are graphs...

Course finished...no need for any more lectures

Pretty well everything known about graphs and hypergraphs is *deducible* from the definitions!

Well....

Perhaps...we ought to help you out and tell you/show you some of the deducible facts...

Are hypergraphs “new”

- Yes and No.....
- Yes because the study of them – in certain ways – is definitely quite new...about 1960 (about as old as me...). Graph theory as a study goes back at least a 100 years earlier.
- Yes because what is essentially the same idea has only more recently gone under the term “hypergraph” in areas like machine learning and AI
- Yes because dealing with other than “trivially small” hypergraphs requires modern computing resources

Are hypergraphs “new”

- Yes and No.....
- No because the study of essentially the same idea (which goes under many different names “tuple”, “triplet”, “pair”, is of course ubiquitous – and been around for centuries
- No because “Database theory” is essentially about hypergraphs..and other examples abound...
- Indeed, its pretty easy to find hypergraphs wherever you look and most often they are not called hypergraphs in the relevant description...

So what *is* “new” apart from the name?

- Well just looking at a list/collection/set of sets doesn’t help you think about them in useful and powerful ways
- It makes it hard to ”see” the *structure*
- Graphs and hypergraphs (well the ways we associate “pictures”/interpretations of these in the theories that go under the names graph and hypergraph theory – that DOES help us to see/exploit/understand the *structure* inherent in various collections of sets – the “patterns” if you like.
- And it starts with the concept of an edge....(well vertices then edges...)

So what *is* "new" apart from the name?

- And it starts with the concept of an edge....(well vertices then edges...)

Well..before we get on to that...

Since we are interested in the *structure* of collections of sets (of objects/things) – it doesn't matter what we CALL those objects.

(it does for the application of course...but not for the general/abstract theory).

So what *is* “new” apart from the name?

Since we are interested in the *structure* of collections of sets (of objects/things) – it doesn’t matter what we CALL those objects.

So...why not just label them with integers...1,2,3,4.....n

(we will usually deal with situations where the “objects” are finite in number)

Sometimes mathematicians denote this $[n]$ – the sequence of integers starting at 1 and ending at n....

Thus vertices (the objects) will be given labels from $[n]$.

For a graph – edges are pairs of integers...e.g, $\{1,3\}, \{7,10\}$

For a hypergraph edges are subsets of $[n]$ of any size.

For a k-uniform hypergraph – edges are subsets of $[n]$ of size k.

OK – but before we go on...surely it's more interesting than collections of numbers, or of fruit, of places Suter has been?

Yes!

Examples:

Chemistry – molecules and higher structure are a collection of atoms (the 118(?) elements of the periodic table – ignoring isotopes...). So chemistry is about subsets of $[n]=[118]$. Well,...elements can occur multiple times to really about multi-sets, and order matters...directed graphs and hypergraphs). Graph concepts & techniques are used in drug/compound discovery,DNA etc.

Hierarchical structures – special type of graph – a tree. Trees (and hypertrees) are “everywhere”. Theory of evolution. Human organizational charts. Folders/directories in a computing system. Your ancestry.

Social and computer networks...

Etc. etc. wherever you look, almost always a graph or hypergraph viewpoint tells at lease some important part of what you are interested in.

For me...the realization that hypergraphs is an important way to view the world, goes back around 10 years...

Clustering with Hypergraphs: The Case for Large Hyperedges

Pulak Purkait¹, Tat-Jun Chin¹, Hanno Ackermann², and David Suter¹

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D. Fleet et al. (Eds.): ECCV 2014, Part IV, LNCS 8692, pp. 672–687, 2014.
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(Pulak was then a postdoc on my grant, Hanno was a visitor who I invited because I spent sabbatical at Leibniz University). Hanno now works for Qualcomm research. Pulak worked at Toshiba research Cambridge England and other places and...by coincidence now works for Amazon and was recently posted to Perth. I visited Leibnitz university a second time last year....and another student from there will visit “my lab” this month.)

For me...the realization that hypergraphs is an important way to view the world, goes back around 10 years...

Clustering of data is a pretty fundamental task in data analysis, machine learning, AI

Typically clustering is done on pairwise distances...i.e., a graph type notion – affinity/distance between points/samples/objects

That paper looked at k-wise measures of affinity...i.e, based on uniform hypergraph notions...

Applied to face clustering, image trajectory clustering,

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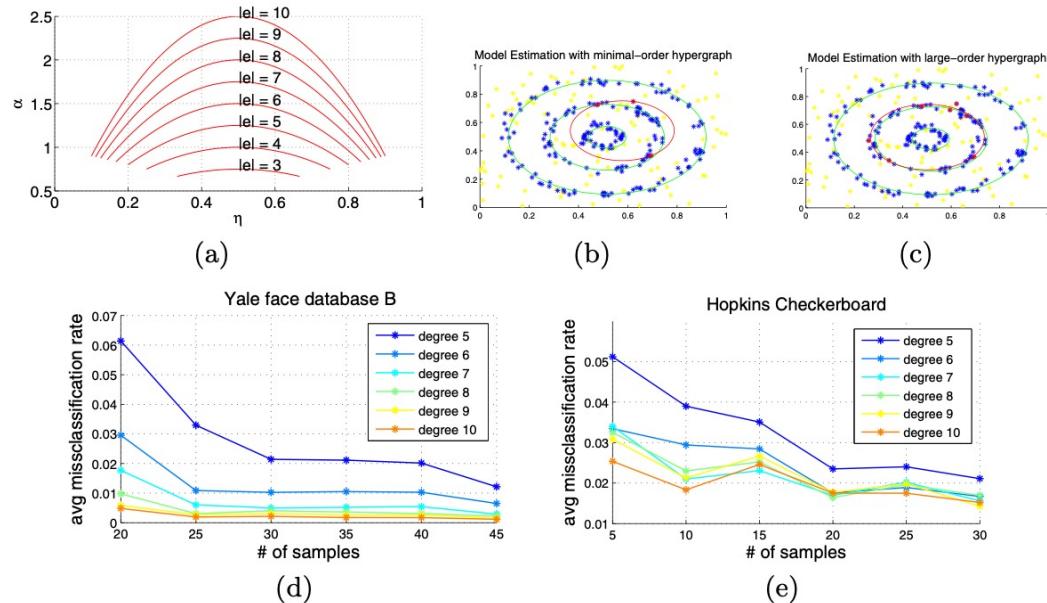


Fig. 1. (a) Plot of $\alpha(e|\eta)$ against η for e 's of different degrees. (b–c) NCut segmentation (first cluster only) on a 4-uniform and 8-uniform hypergraph, respectively. (d–e) Average misclassification rate plotted against number of samples and size of hyperedges on Yale Face Database B and the 3-motion checkerboard sequences from Hopkins 155.

Since then I've had several works where hypergraph was so central it featured in the title...

- Erchuan Zhang, David Suter, Giang Truong, and Syed Zulqarnain Gilani. “Sparse Hypergraph Community Detection Thresholds in Stochastic Block Model”. In: Advances in Neural Information Processing Systems. Ed. by S. Koyejo, S. Mohamed, A. Agarwal, D. Belgrave, K. Cho, and A. Oh. Vol. 35. Curran Associates, Inc., 2022, pp. 34012–34023.
https://proceedings.neurips.cc/paper_files/paper/2022/file/dbdea7859f1d2fc10f2c9e79b8f5ae54-Paper-Conference.pdf
- Shuyuan Lin, Guobao Xiao, Yan Yan, David Suter, and Hanzi Wang. “Hypergraph Optimization for Multi-structural Geometric Model Fitting”. In: The AAAI Conference on Artificial Intelligence (AAAI), Hawaii, USA. Vol. 33. 01. 2018, pp. 8730–8737. doi: [10.1609/aaai.v33i01.33018730](https://doi.org/10.1609/aaai.v33i01.33018730). 16% acceptance rate.
- H. Wang, G. Xiao, Y. Yan, and D. Suter. “Mode-Seeking on Hypergraphs for Robust Geometric Model Fitting”. In: 2015 IEEE International Conference on Computer Vision (ICCV). Dec. 2015, pp. 2902–2910. doi: [10.1109/ICCV.2015.332](https://doi.org/10.1109/ICCV.2015.332).

And many where it perhaps should have featured in the title...particularly recently

- Dzung Doan, Michele Sasdelli, Tat-Jun Chin, and David Suter. “A Hybrid Quantum-Classical Algorithm for Robust Fitting”. In: 2022 IEEE/CVF Conference on Computer Vision and Pattern Recognition (CVPR). 2022, pp. 417–427. doi: 10.1109/CVPR52688.2022.00051.
- Erchaun Zhang, David Suter, Ruwan Tennakoon, Tat-Jun Chin, Alireza Bab-Hadiashar, Giang Truong, and Syed Zulqarnain Gilani. “Maximum Consensus by Weighted Influences of Monotone Boolean Functions”. In: 2022 IEEE/CVF Conference on Computer Vision and Pattern Recognition (CVPR). 2022, pp. 8954–8962. doi: 10.1109/CVPR52688.2022.00876.
- Ruwan Tennakoon, David Suter, Erchuan Zhang, Tat-Jun Chin, and Alireza Bab-Hadiashar. “Consensus Maximisation Using Influences of Monotone Boolean Functions”. In: 2021 IEEE/CVF Conference on Computer Vision and Pattern Recognition (CVPR). Oral Presentation (17% of accepted papers, roughly 3% of submitted papers). 2021, pp. 2865–2874. doi: 10.1109/CVPR46437.2021.00289.
- Tat-Jun Chin, David Suter, Shin-Fang Ch’ng, and James Quach. “Quantum Robust Fitting”. In: Computer Vision – ACCV 2020. Ed. by Hiroshi Ishikawa, Cheng-Lin Liu, Tomas Pajdla, and Jianbo Shi. Cham: Springer International Publishing, 2021, pp. 485–499. isbn: 978-3-030-69525-5. doi: 10.1007/978-3-030-69525-5_29.

But of course MANY machine learning/AI people are using hypergraph concepts to innovate/solve problems

Proceedings of the Thirty-Second International Joint Conference on Artificial Intelligence (IJCAI-23)

Basket Representation Learning by Hypergraph Convolution on Repeated Items for Next-basket Recommendation

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Abstract

Basket representation plays an important role in the task of next-basket recommendation. However, existing methods generally adopt pooling operations to learn a basket's representation, from which two critical issues can be identified. First, they treat a basket as a set of items independent and identically distributed. We find that items occurring in the same basket have much higher correlations than those randomly selected by conducting data analysis on two real datasets. Second, although some works have recognized the importance of items repeatedly purchased in multiple baskets, they ignore the correlations among the repeated items in the same basket, whose importance is shown by our data analysis. In this

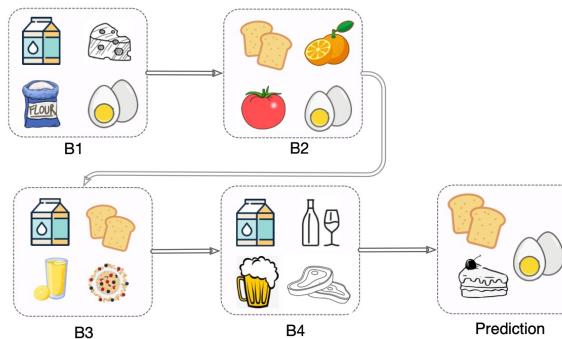


Figure 1: A toy example to explain our assumptions, where a user purchased four baskets and we make recommendations accordingly.

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Proceedings of the Thirty-Second International Joint Conference on Artificial Intelligence (IJCAI-23)

Towards Hierarchical Policy Learning for Conversational Recommendation with Hypergraph-based Reinforcement Learning

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Abstract

Conversational recommendation systems (CRS) aim to timely and proactively acquire user dynamic preferred attributes through conversations for item recommendation. In each turn of CRS, there naturally have two decision-making processes with different roles that influence each other: 1) **director**, which is to select the follow-up **option** (*i.e.*, ask or recommend) that is more effective for reducing the action space and acquiring user preferences; and 2) **actor**, which is to accordingly choose **primitive actions** (*i.e.*, asked attribute or recommended item)

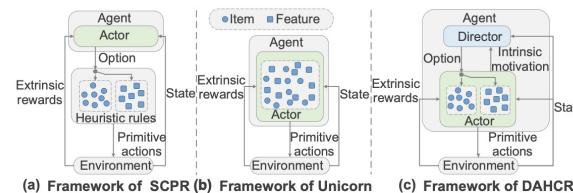


Figure 1: Illustration of policy learning frameworks for CRS, including a framework of the outsourcing strategy (SCPR), a unified framework (Unicorn), and our proposed Director-Actor framework.

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Proceedings of the Thirty-Second International Joint Conference on Artificial Intelligence (IJCAI-23)

Sorting and Hypergraph Orientation under Uncertainty with Predictions

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Proceedings of the Thirty-First International Joint Conference on Artificial Intelligence (IJCAI-22)

Hypergraph Structure Learning for Hypergraph Neural Networks

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Proceedings of the Thirty-Second International Joint Conference on Artificial Intelligence (IJCAI-23)
Sister Conferences Best Papers Track

Learning Causal Effects on Hypergraphs (Extended Abstract)*

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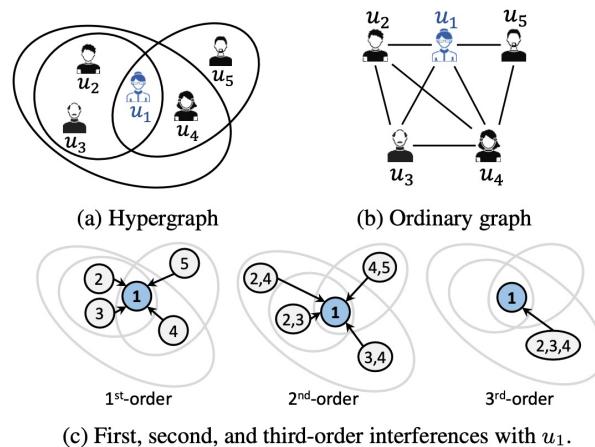
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Abstract

Hypergraphs provide an effective abstraction for modeling multi-way group interactions among nodes, where each hyperedge can connect any number of nodes. Different from most existing studies which leverage *statistical dependencies*, we study hypergraphs from the perspective of *causality*. Specifically, we focus on the problem of individual treatment effect (ITE) estimation on hypergraphs, aiming to estimate how much an intervention (e.g., wearing face covering) would causally affect an outcome (e.g., COVID-19 infection) of each individual node. Existing works on ITE estimation either assume that the outcome of one individual should not be influenced by the treatment of other individuals (i.e., no *interference*), or assume



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Proceedings of the Thirty-Second International Joint Conference on Artificial Intelligence (IJCAI-23)

Multi-view Contrastive Learning Hypergraph Neural Network for Drug-Microbe-Disease Association Prediction

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Abstract

Identifying the potential associations among drugs, microbes, and diseases is of great significance in exploring the pathogenesis and improving precision medicine. There are plenty of computational methods for pair-wise association prediction, such as drug-microbe and microbe-disease associations, but few methods focus on the higher-order triple-wise drug-microbe-disease (DMD) associations. Driven by the advancement of hypergraph neural networks (HGNNS), we expect them to fully capture high-order interaction patterns behind the hypergraph formulated by DMD associations and realize sound prediction performance. However, the

with them separately and fail to provide in-depth insights into intricate drug-microbe-disease (DMD) interaction patterns. Indeed, recent studies in human metabolic systems pointed out the importance of identifying triple-wise DMD associations [Wu *et al.*, 2022; Wang *et al.*, 2022a]. For that reason, it is necessary to develop effective methods for predicting DMI associations that have been few investigated before.

Predicting triple-wise associations is a fundamental issue in multiple domains, e.g., recommendation systems [Wang *et al.*, 2022b; Cheng *et al.*, 2022], knowledge graphs [Qiao *et al.*, 2018; Guan *et al.*, 2018] and bioinformatics [Sidorov *et al.*, 2019; Chen and Li, 2019; Chen and Li, 2020; Liu *et al.*, 2022]. For example, [Chen and Li, 2019] developed a tensor decomposition model to predict which target a drug

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Proceedings of the Thirty-Second International Joint Conference on Artificial Intelligence (IJCAI-23)

Totally Dynamic Hypergraph Neural Network

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Abstract

Recent dynamic hypergraph neural networks (DHGNNs) are designed to adaptively optimize the hypergraph structure to avoid the dependence on the initial hypergraph structure, thus capturing more hidden information for representation learning. However, most existing DHGNNs cannot adjust the hyperedge number and thus fail to fully explore the underlying hypergraph structure. This paper proposes a new method, namely, totally hypergraph neural network (TDHNN), to adjust the hyperedge number for optimizing the hypergraph structure. Specifically, the proposed method first captures hyperedge feature distribution to obtain dynamical hyperedge features rather than fixed ones, by conducting the sampling from the learned distribution. The hypergraph is then constructed based on the attention coefficients of both sam-

Previous hypergraph methods can be divided into two categories, *i.e.*, static hypergraph neural networks (SHGNNs) and dynamic hypergraph neural networks (DHGNNs). SHGNNs conduct representation learning by using the initialized hypergraph structure to capture the relationships among nodes. To do this, HGNN [Feng *et al.*, 2019] employed the convolution method and HGNN⁺ [Gao *et al.*, 2022] introduced a spatial-based hypergraph convolution. However, SHGNNs are highly dependent on the initialized hypergraph structure, which usually has redundant information and cannot discover hidden relationships among nodes. To address these issues, DHGNNs were proposed to learn latent connections from features and can mine more useful information. For instance, [Jiang *et al.*, 2019] proposed to reconstruct the hypergraph using both k NN and k -means. [Bai *et al.*, 2021] proposed using continuous values to construct the incidence matrix and the attention mechanism to learn the connection weights. DeepHGSL [Zhang *et al.*, 2022] uses hidden representations in multiple hypergraph convolutional layers to

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Proceedings of the Twenty-Ninth International Joint Conference on Artificial Intelligence (IJCAI-20)

Knowledge Hypergraphs: Prediction Beyond Binary Relations*

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Abstract

Knowledge graphs store facts using relations between two entities. In this work, we address the question of link prediction in knowledge hypergraphs where relations are defined on *any number* of entities. While techniques exist (such as reifica-

In these studies, knowledge graphs are defined as directed graphs having nodes as entities and labeled edges as relations; edges are directed from the *head* entity to the *tail* entity. The common data structure for representing knowledge graphs is a set of triples $relation(head, tail)$ that represents information as a collection of binary relations. There exist a large number of knowledge graphs that are publicly available, such

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Link Prediction with Relational Hypergraphs

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Abstract

Link prediction with knowledge graphs has been thoroughly studied in graph machine learning, leading to a rich landscape of graph neural network architectures with successful applications. Nonetheless, it remains challenging to transfer the success of these architectures to *relational hypergraphs*, where the task of link prediction is over *k-ary relations*, which is substantially harder than link prediction with knowledge graphs. In this paper, we propose a framework for link prediction with relational hypergraphs, unlocking applications of graph neural networks to *fully relational* structures. Theoretically, we conduct a thorough analysis of the expressive power of the resulting model architectures via corresponding relational Weisfeiler-Leman algorithms and also via logical expressiveness. Empirically, we validate the power of the proposed model architectures on various relational hypergraph benchmarks. The resulting model architectures substantially outperform every baseline for inductive link prediction, and lead to state-of-the-art results for transductive link prediction.

1 Introduction

Knowledge graphs consist of facts (or, edges) representing different relations between *pairs of nodes*. Knowledge graphs are inherently incomplete [17, 30] which motivated a large literature on link prediction with knowledge graphs [31, 24–26, 28, 19, 41]. This task amounts to predicting missing facts in the knowledge graph and has led to a rich landscape of graph neural network architectures [24, 26, 28, 41]. Our understanding of these architectures is supported by theoretical studies quantifying their expressive power [4, 38, 16].

In this work, we are interested in link prediction on *fully relational* data, where every relation is between *k* nodes, for any *relation-specific* choice of *k*. Relational data can encode rich relationships between entities; e.g., consider a relationship between *four* entities: “Hawking went

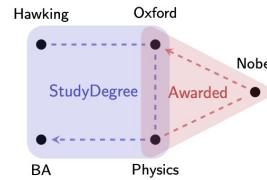


Figure 1: A relational hypergraph over the relations StudyDegree and Awarded. The facts StudyDegree(Hawking, Oxford, Physics, BA) and Awarded(Physics, Nobel, Oxford) are ordered hyperedges, where the order of entities in each fact is denoted by dashed arrows.