A Tutorial on Hypergraph Neural Networks: An In-Depth and Step-by-Step Guide

Part 1. Introduction


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Part 1. Introduction

The slides are available at https://sites.google.com/view/hnn-tutorial

SCAN ME

Presenter

Kijung Shin.

Associate Professor @

KAIST

Higher-Order Interactions are Everywhere

- **[Example 1]** Group chats on social messaging apps

Higher-Order Interactions are Everywhere (cont.)

- **[Example 2]** Co-authorship of researchers

dblp
computer science bibliography

Google Scholar

ResearchGate

A Survey on Hypergraph Neural Networks: An In-Depth and Step-by-Step Guide

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HYPEBOY: GENERATIVE SELF-SUPERVISED REPRESENTATION LEARNING ON HYPERGRAPHS

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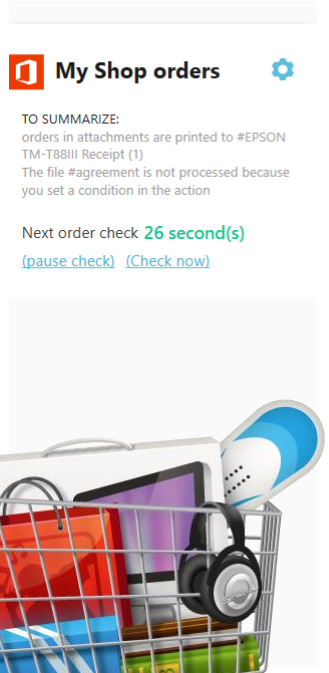
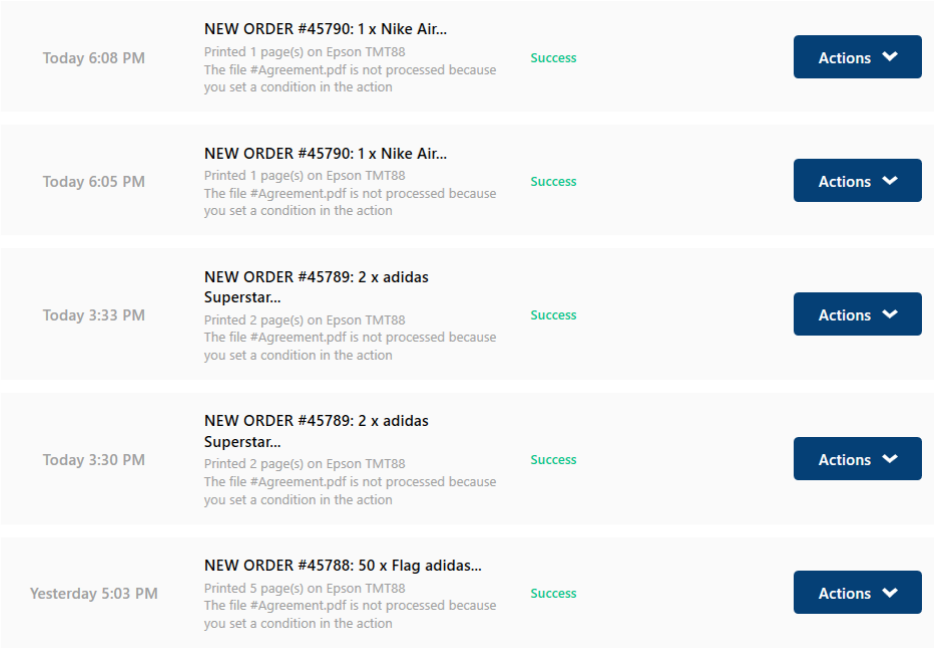
Higher-Order Interactions are Everywhere (cont.)

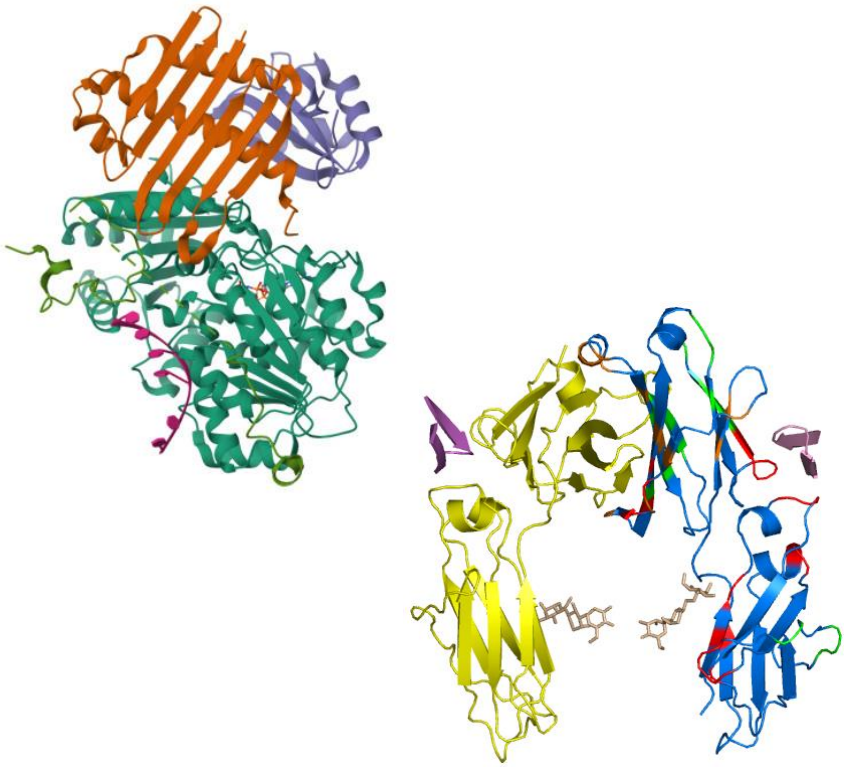
- **[Example 3]** Co-purchase of items





Higher-Order Interactions are Everywhere (cont.)

- **[Example 4]** Interactions of proteins



Hypergraphs Model Higher-Order Interactions

- Higher-order interactions are commonly modeled as a **hypergraph**.
  - A hypergraph consists of a **node** set and a **hyperedge** set.
  - A **hyperedge** (i.e., a subset of nodes) models a higher-order interaction.

Co-Authorship

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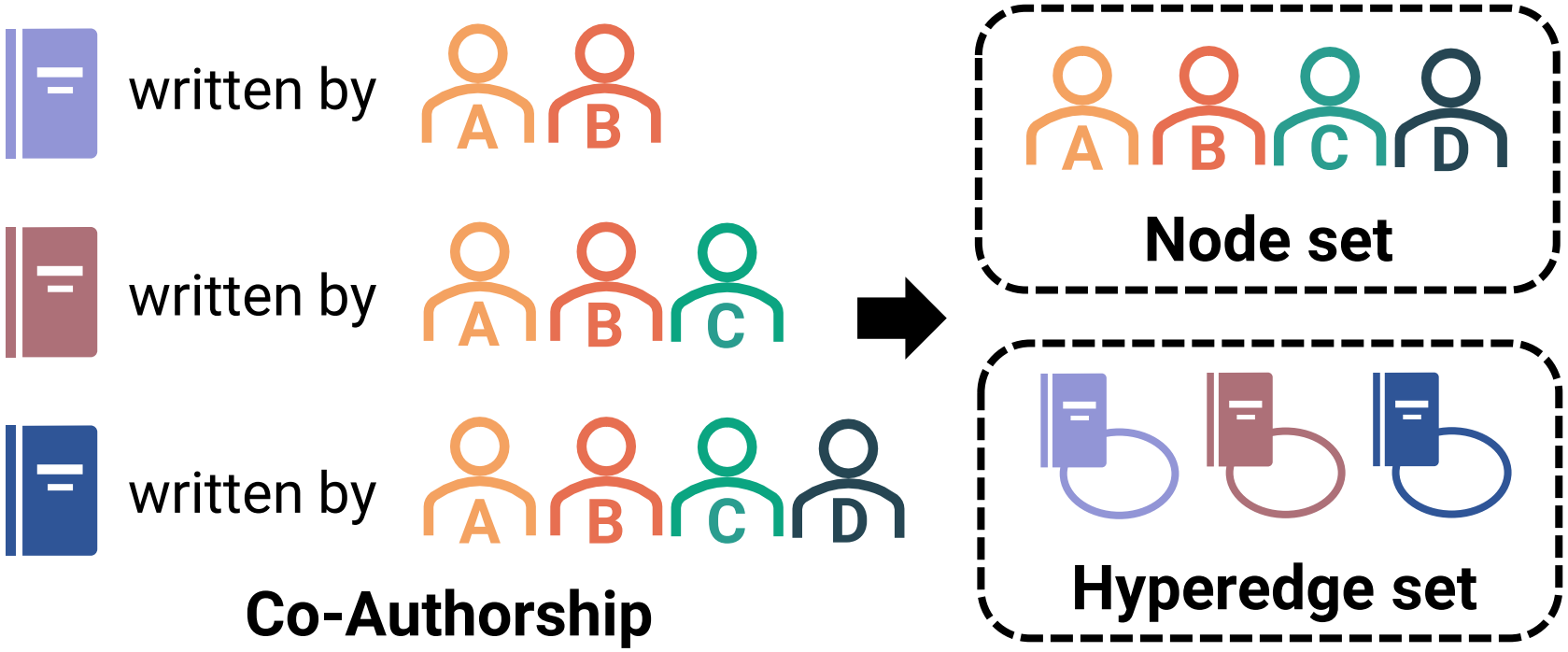

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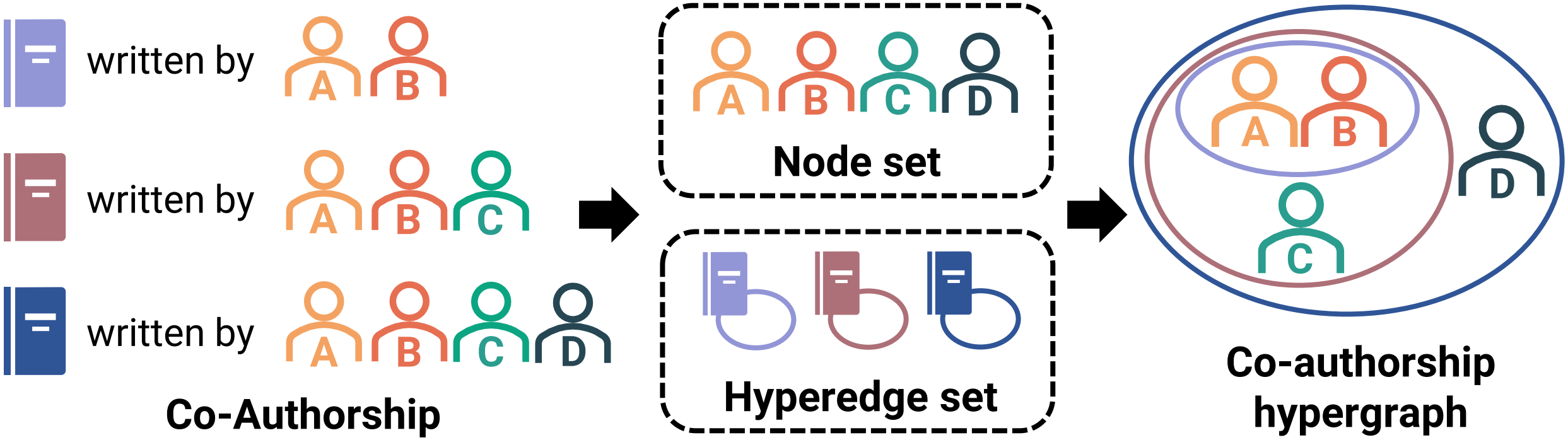
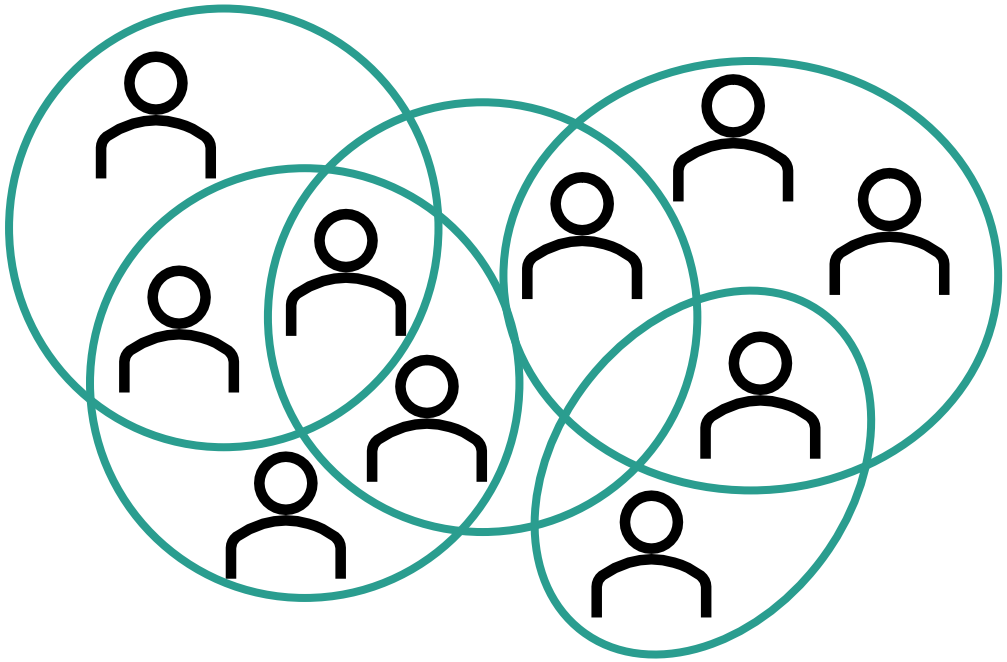
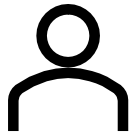


Machine Learning Tasks on Hypergraphs

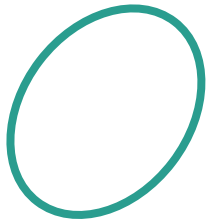
- There are various machine learning tasks on hypergraphs.
  - The first example is a **node classification** task.



Messaging app hypergraphs



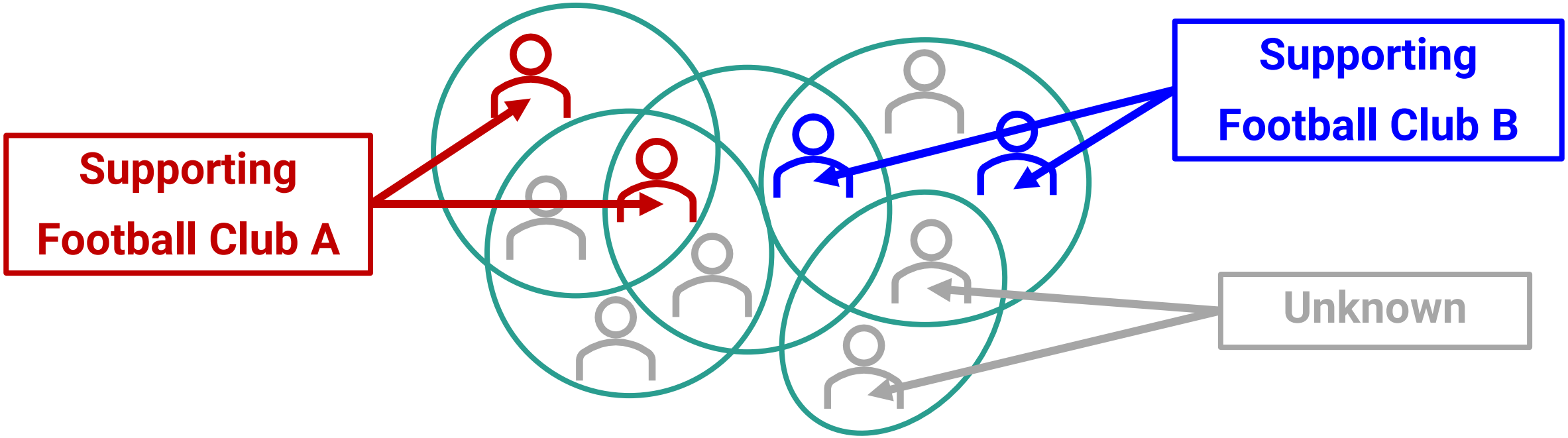
[Nodes] Messaging app users



[Hyperedge] A group of users involving in the same group chat

Machine Learning Tasks on Hypergraphs (cont.)

- There are various machine learning tasks on hypergraphs.
  - The first example is **node classification**.



Which club does each user support?

Machine Learning Tasks on Hypergraphs (cont.)

- There are various machine learning tasks on hypergraphs.
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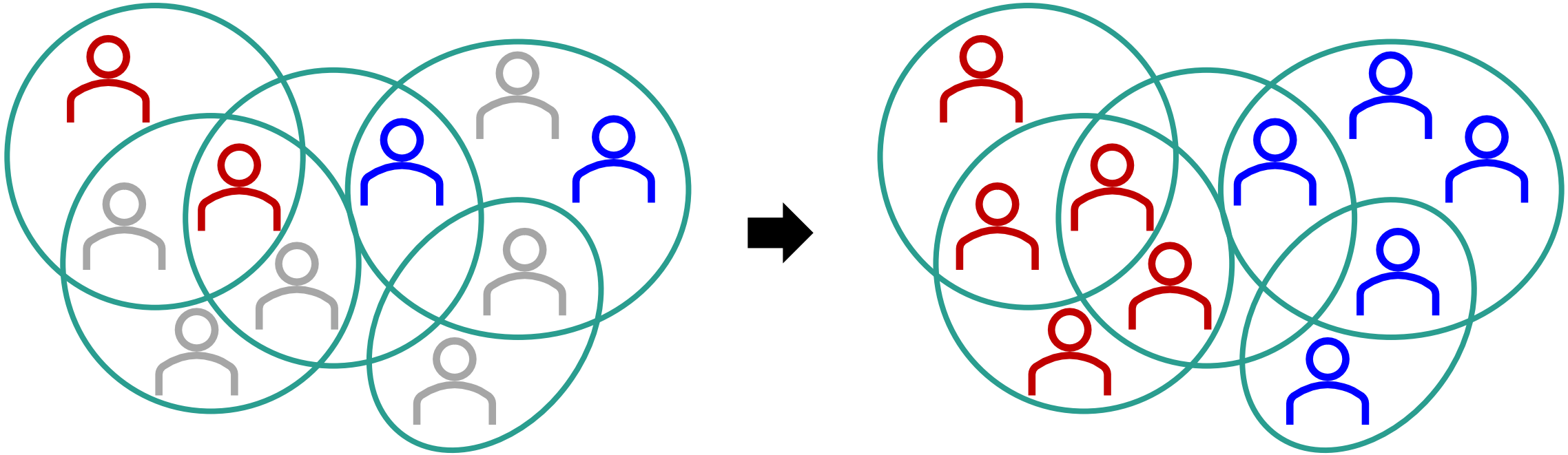
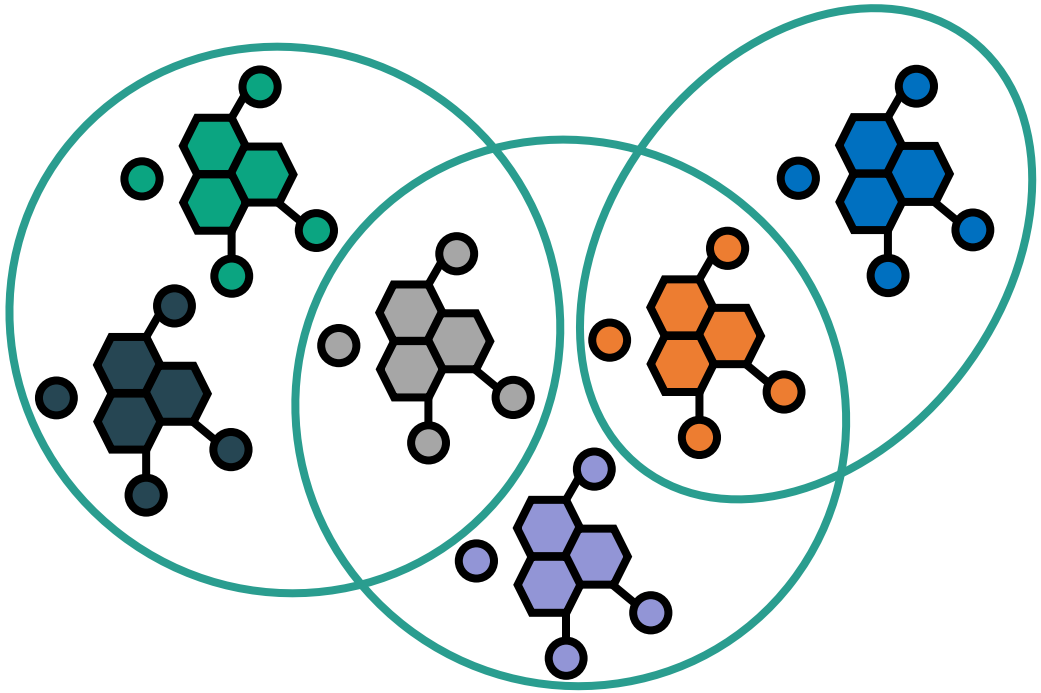


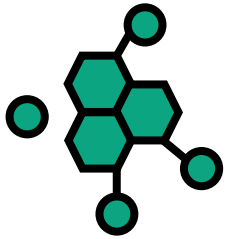
The node classification task formalizes this user profiling.

Machine Learning Tasks on Hypergraphs (cont.)

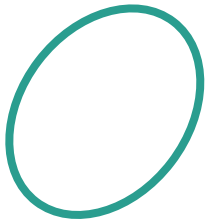
- There are various machine learning tasks on hypergraphs.
  - The second example is **hyperedge prediction**.



Metabolic reaction hypergraph



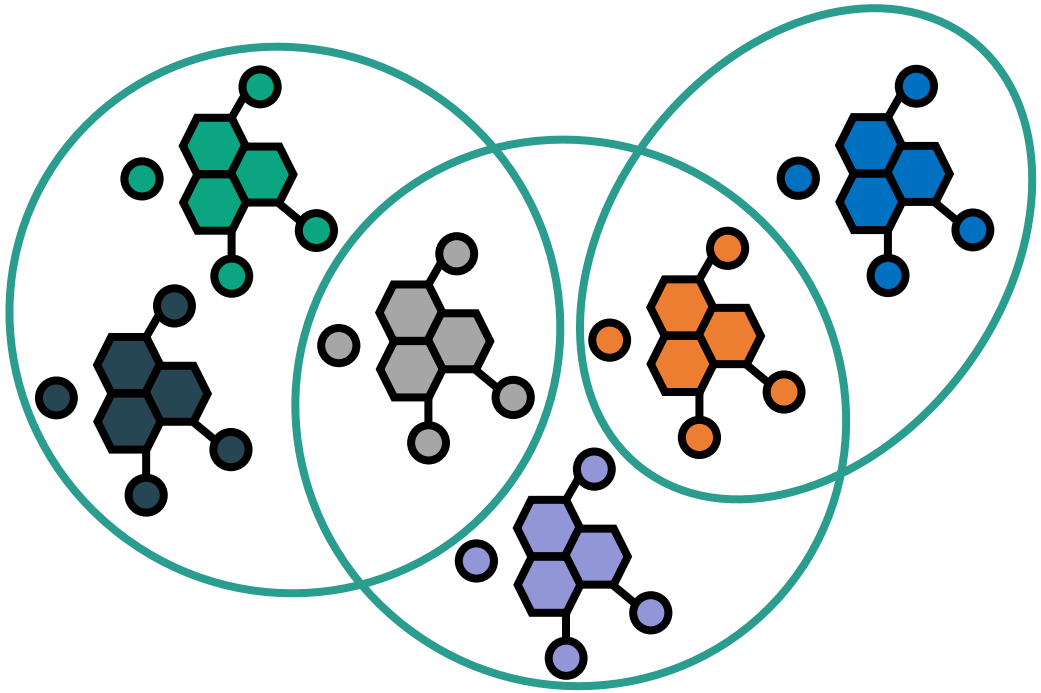
[Nodes] Metabolites



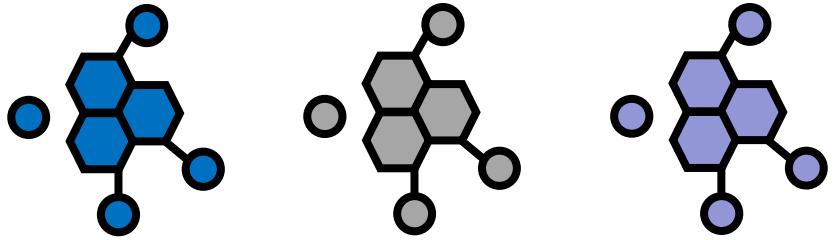
[Hyperedge] A set of metabolites involved in the same chemical reaction.

Machine Learning Tasks on Hypergraphs (cont.)

- There are various machine learning tasks on hypergraphs.
  - The second example is **hyperedge prediction**.



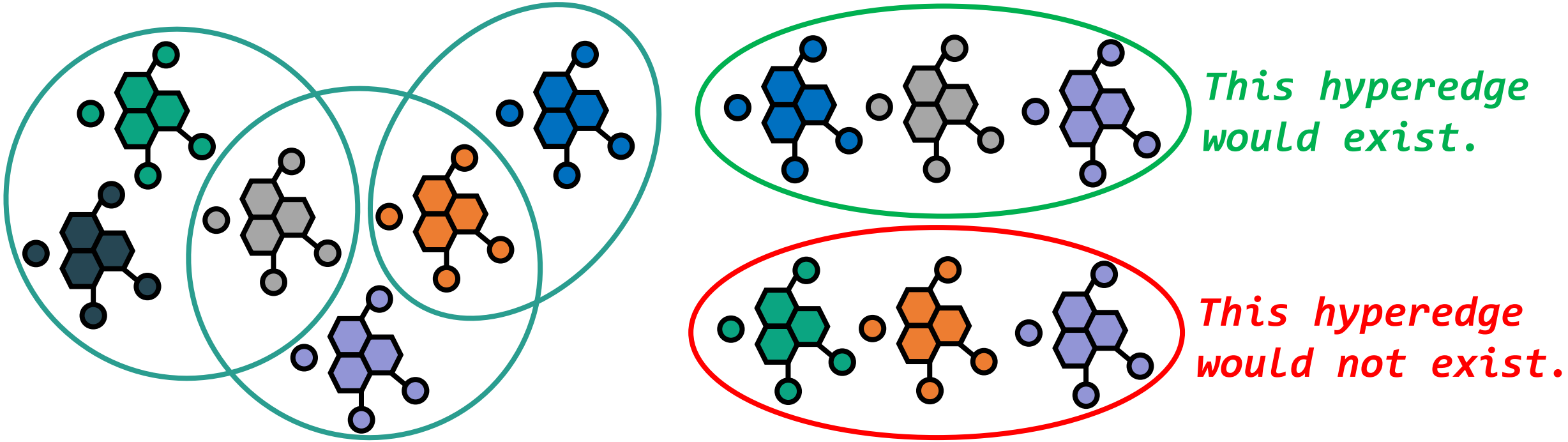
Metabolic reaction hypergraph



Would these three metabolites react together?

Machine Learning Tasks on Hypergraphs (cont.)

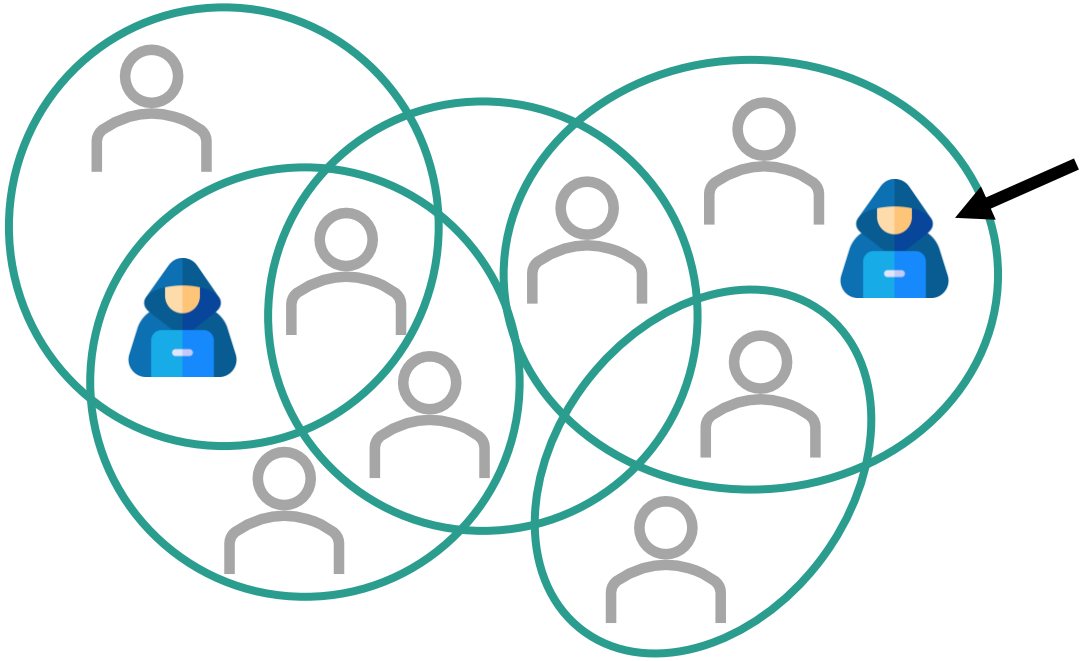
- There are various machine learning tasks on hypergraphs.
  - The second example is **hyperedge prediction**.



The hyperedge prediction task formalizes this reaction prediction.

Machine Learning Tasks on Hypergraphs (cont.)

- There are various machine learning tasks on hypergraphs.
  - More examples include **anomaly detection**, **ranking**, and **alignment**.



*E.g., **fraud** in social messaging apps*

Messaging app hypergraphs

Machine Learning Tasks on Hypergraphs (cont.)

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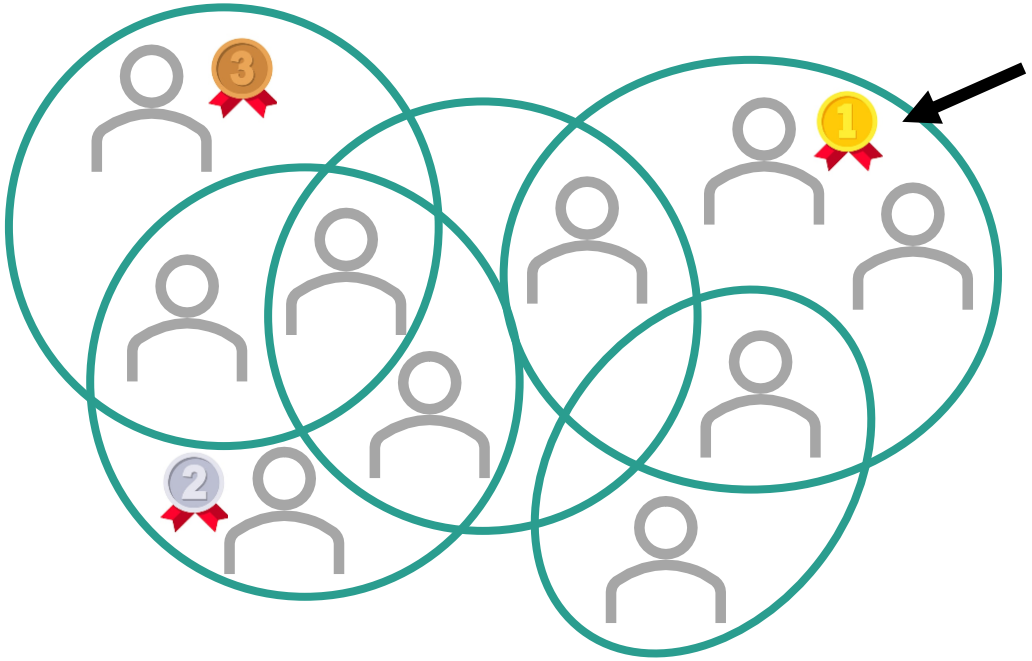

*E.g., **most influential user** in social messaging apps*

Messaging app hypergraphs

Machine Learning Tasks on Hypergraphs (cont.)

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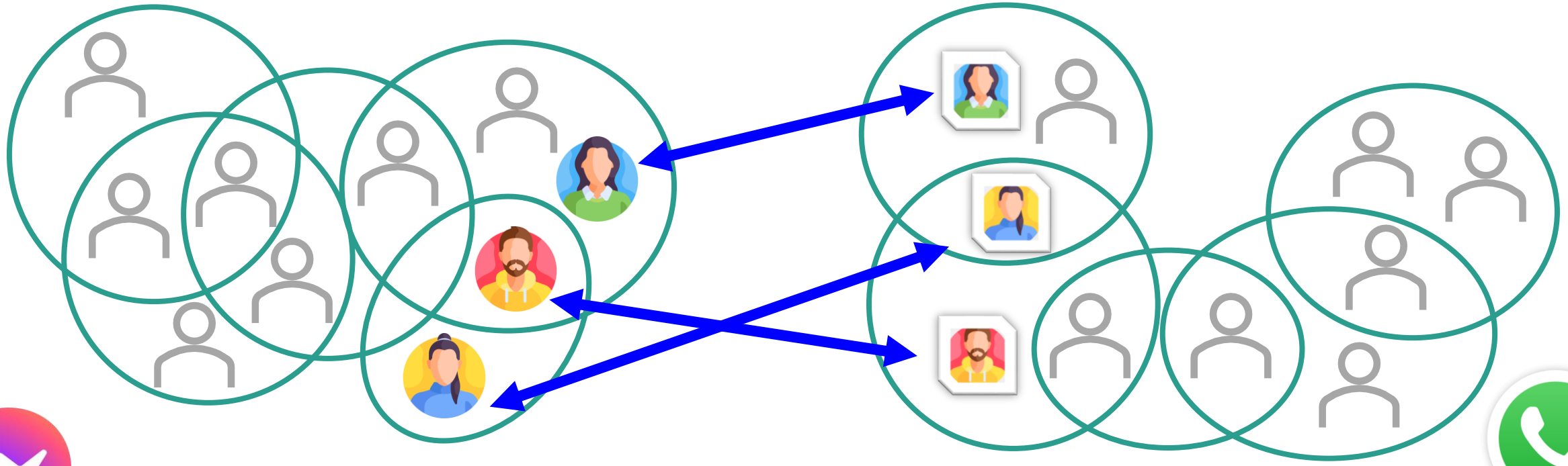
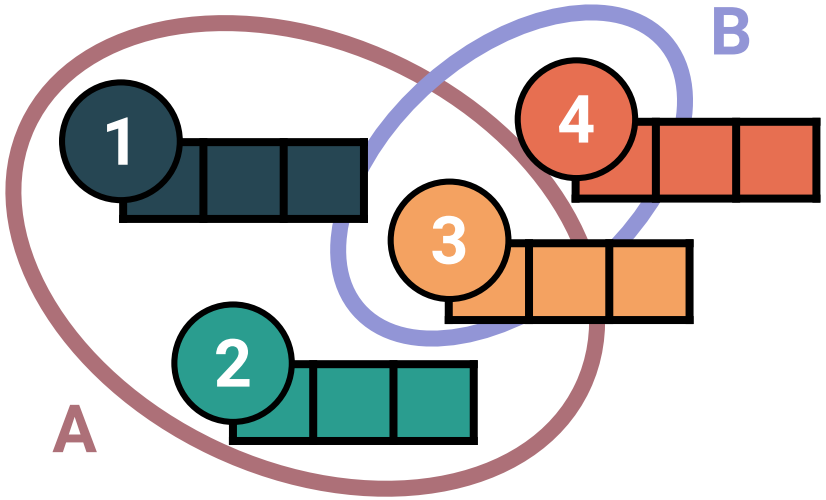
  - More examples include **anomaly detection**, **ranking**, and **alignment**.



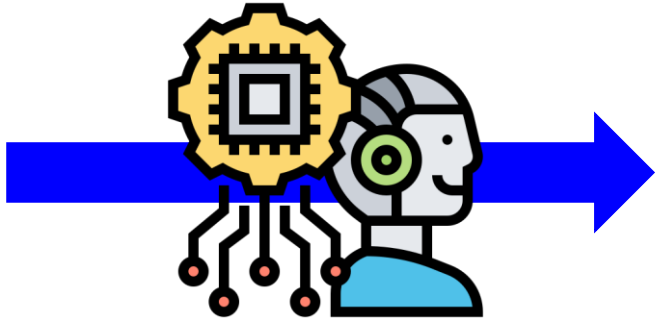
Facebook messenger hypergraph **WhatsApp hypergraph**

Hypergraph Neural Network (HNN)

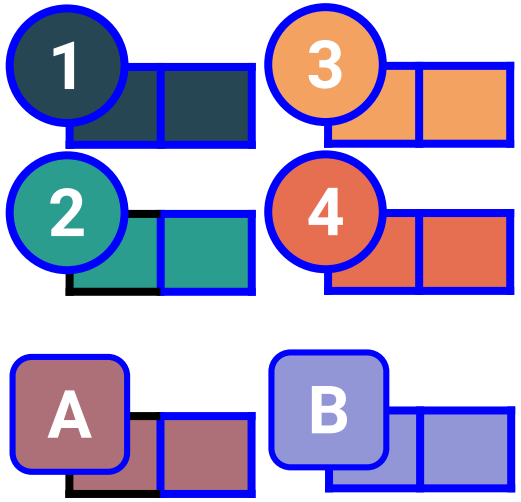
- **Hypergraph neural networks (HNNs)** are family of neural networks specialized for machine learning on hypergraphs.



Hypergraph and node (and hyperedge) features



Hypergraph neural network (HNN)



Node (and hyperedge) embeddings

Hypergraph Neural Network (cont.)

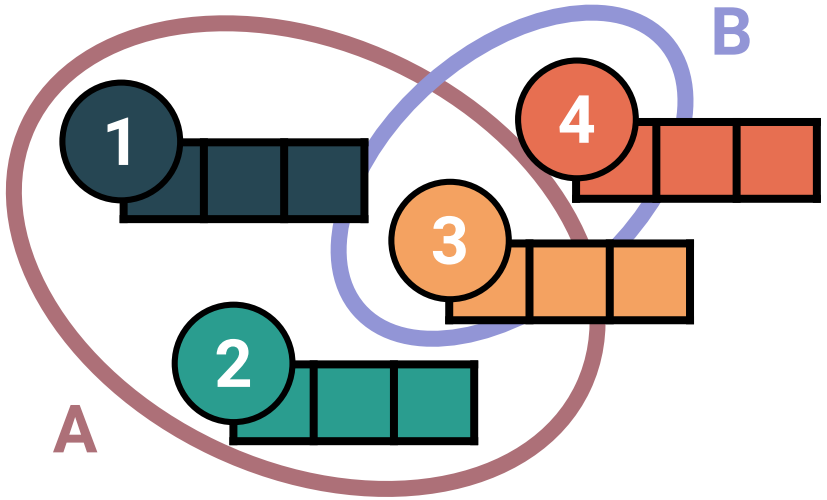
- **Hypergraph neural networks (HNNs)** have achieved state-of-the-art performance in many machine learning tasks on hypergraphs.

Hypergraph Node Classification Leader Board

Dataset: DBLP	Dataset: Trivago	Dataset: House
1. HNN	1. HNN	1. HNN
2. GNN	2. SVM	2. GNN
…	…	…

Why Hypergraph Neural Networks?

- For hypergraph learning, one might consider using **graph neural networks**:
  - **[Step 1]** Represent higher-order interactions as a pairwise graph.
  - **[Step 2]** Apply graph neural networks to the pairwise graph.



Hypergraph

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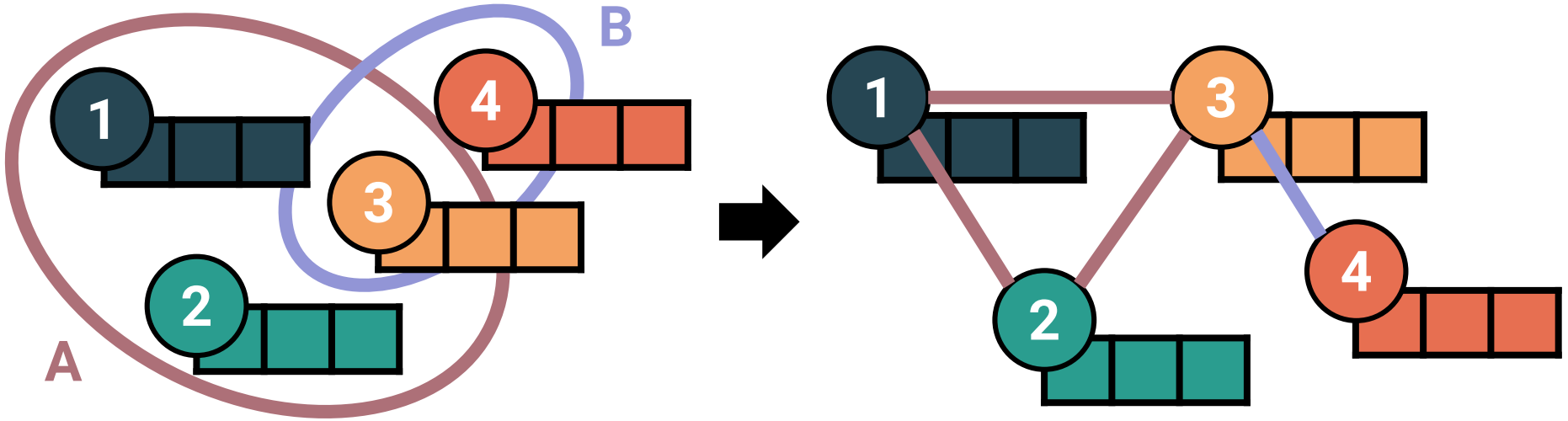

Hypergraph **Pairwise graph**

Why Hypergraph Neural Networks? (cont.)

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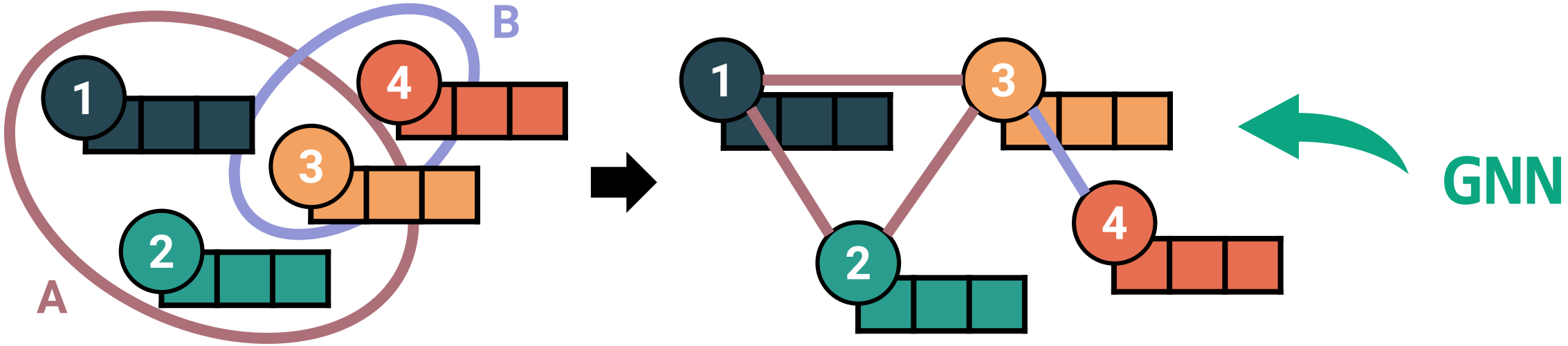
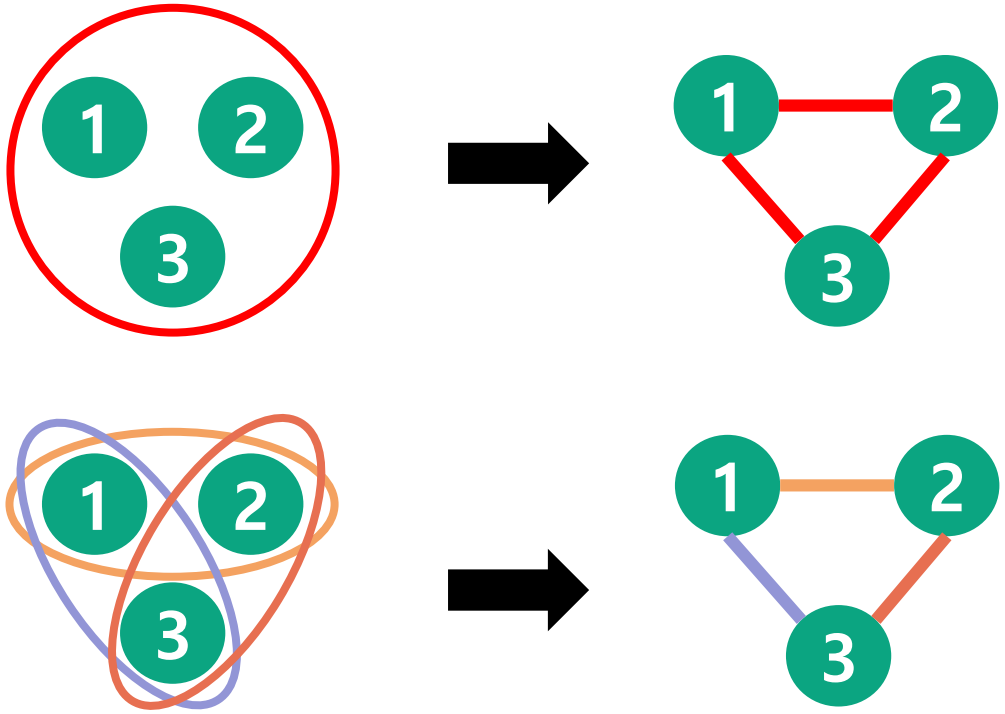


Hypergraph **Pairwise graph**

Why Hypergraph Neural Networks? (cont.)

- However, expressing higher-order interactions with a pairwise graph may cause an **information loss** [Zhou et al., 2006].



Resulting in the

Resulting in the

same structure.

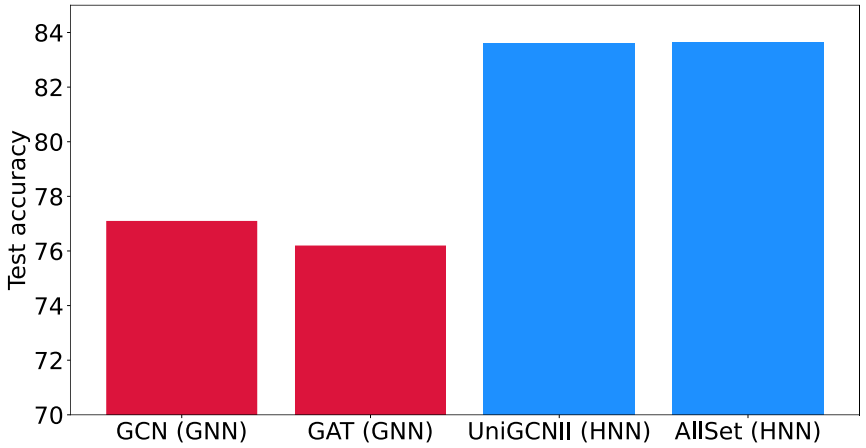
same structure.

Why Hypergraph Neural Networks? (cont.)

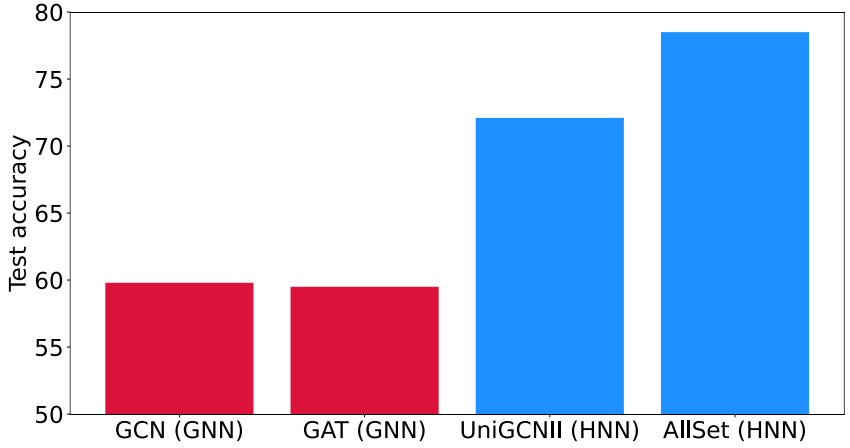
- Such information loss can result in a significant performance degradation.

→ **Hypergraph neural networks are crucial for hypergraph learning.**

Cora-CA dataset



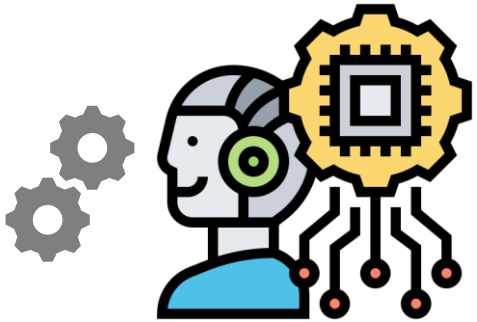
Walmart dataset



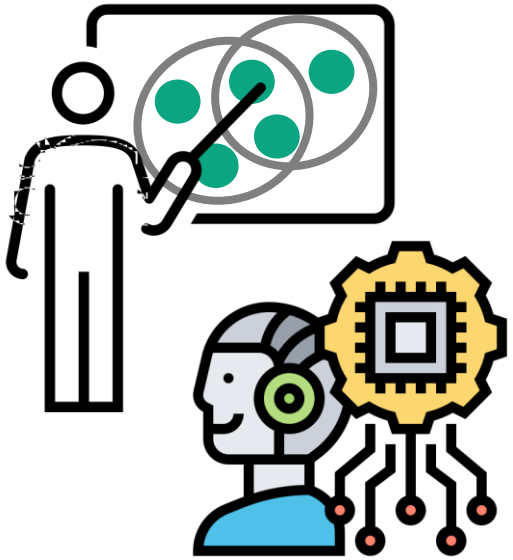
Node classification performance on hypergraph benchmark datasets

Tutorial Overview

- In this tutorial, we provide an overview of how hypergraph neural networks are **designed, trained, and utilized for various applications.**



Design choice



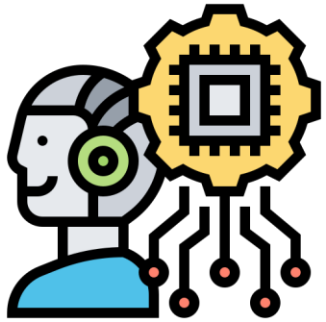
Training strategy

Application

Tutorial Overview (cont.)

- The remainder of our tutorial is divided into the five parts.

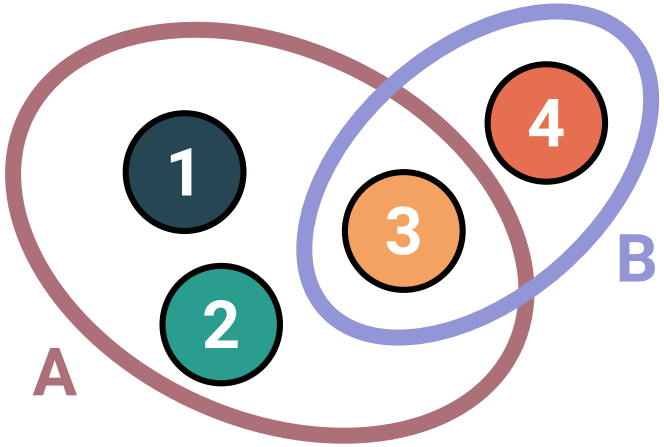
We are now here!



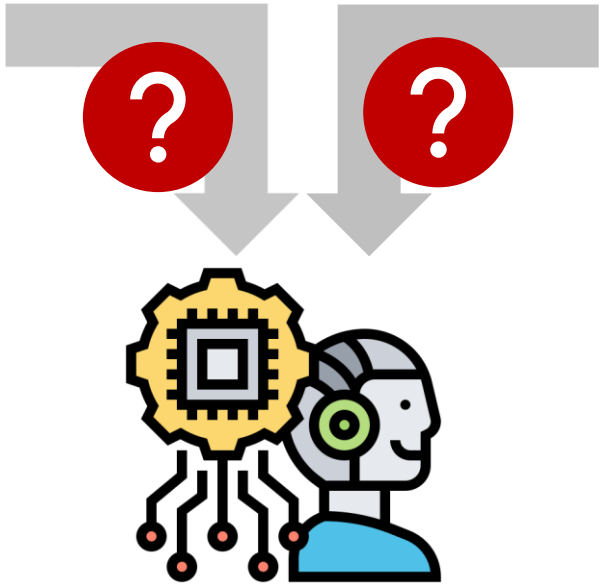
Part 1. Introduction	Part 2. Inputs	Part 3. Message Passing	Part 4. Training Strategies	Part 5. Applications	Part 6. Discussion

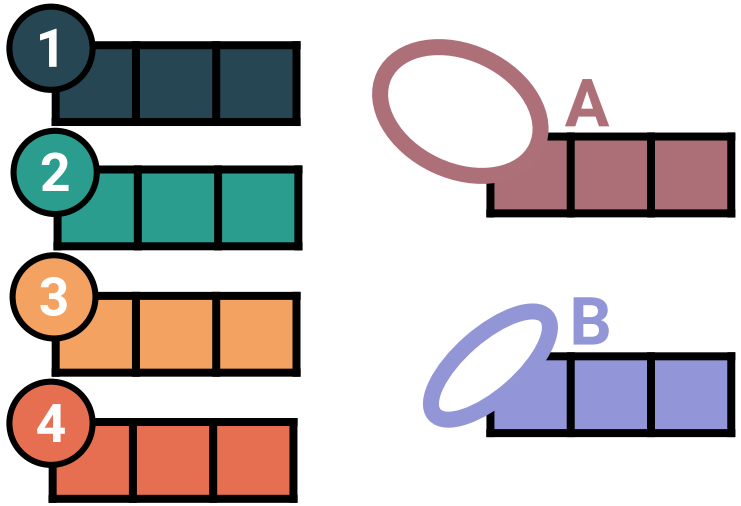
Tutorial Overview (cont.)

- **[Part 2]** We cover inputs of hypergraph neural networks.
  - **2.1.** How can hypergraph structures be represented?
  - **2.2.** What input features can be used for nodes and hyperedges?



Hypergraph structure

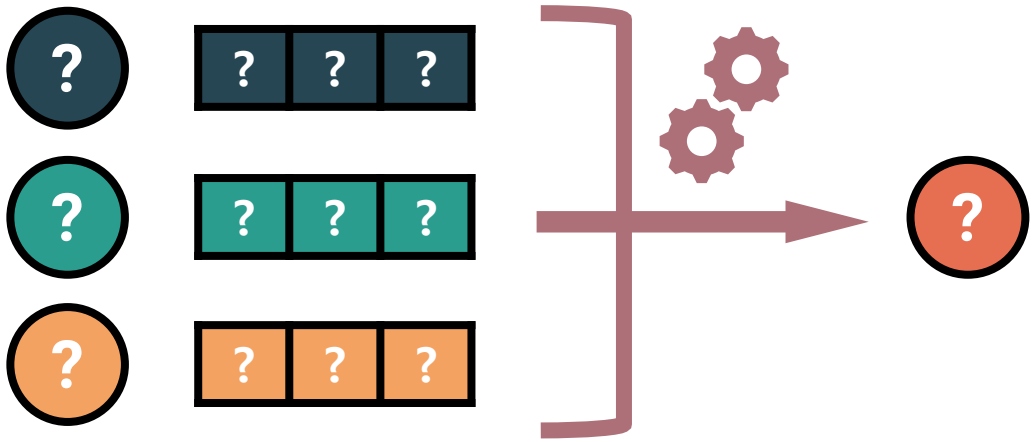




Node and hyperedge features

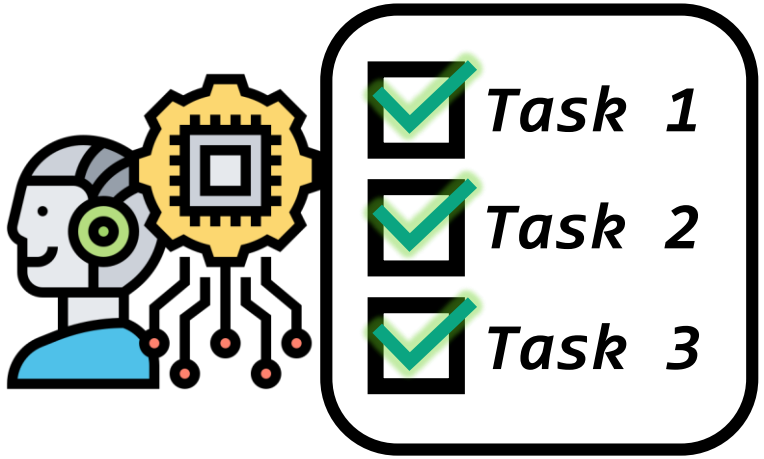
Tutorial Overview (cont.)

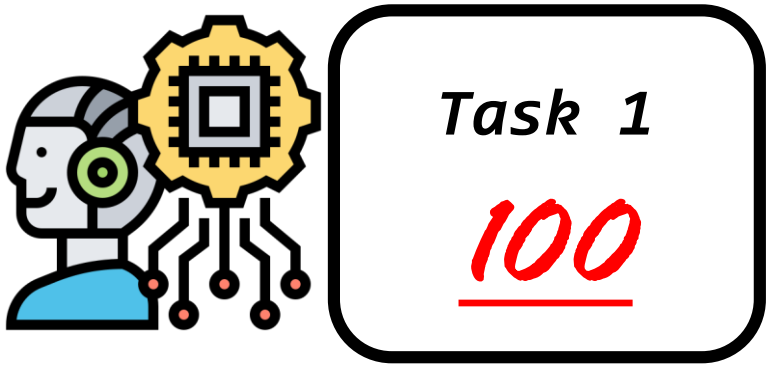
- **[Part 3]** We cover message passing in hypergraph neural networks.
  - **3.1.** Whose messages to aggregate
  - **3.2.** What messages to aggregate
  - **3.3.** How to aggregate messages



Tutorial Overview (cont.)

- **[Part 4]** We cover training strategies for hypergraph neural networks.
  - **4.1.** Task-agnostic training
  - **4.2.** Task-targeted training





Tutorial Overview (cont.)

- **[Part 5]** We cover practical applications of hypergraph neural networks.
  - **5.1.** Recommender systems
  - **5.2.** Bioinformatics and medical science
  - **5.3.** Time series analysis
  - **5.4.** Computer vision




Tutorial Overview (cont.)

- **[Part 6]** We discuss open questions related to hypergraph neural networks.
  - **6.1.** What are theoretical foundation of HNNs in hypergraph learning?
  - **6.2.** When is using HNNs especially advantageous?
  - **6.3.** How should HNNs encode more complex hypergraphs?
  - **6.4.** How to utilize large language models to empower HNNs.

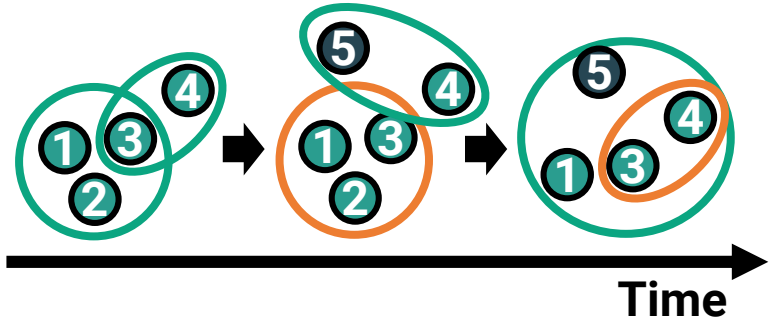
HNN Theory

When?

GNNs
Transformers
MLPs

HNNs

Advantages of HNNs



Complex Hypergraphs

+

HNNs