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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]** Social media group chatting

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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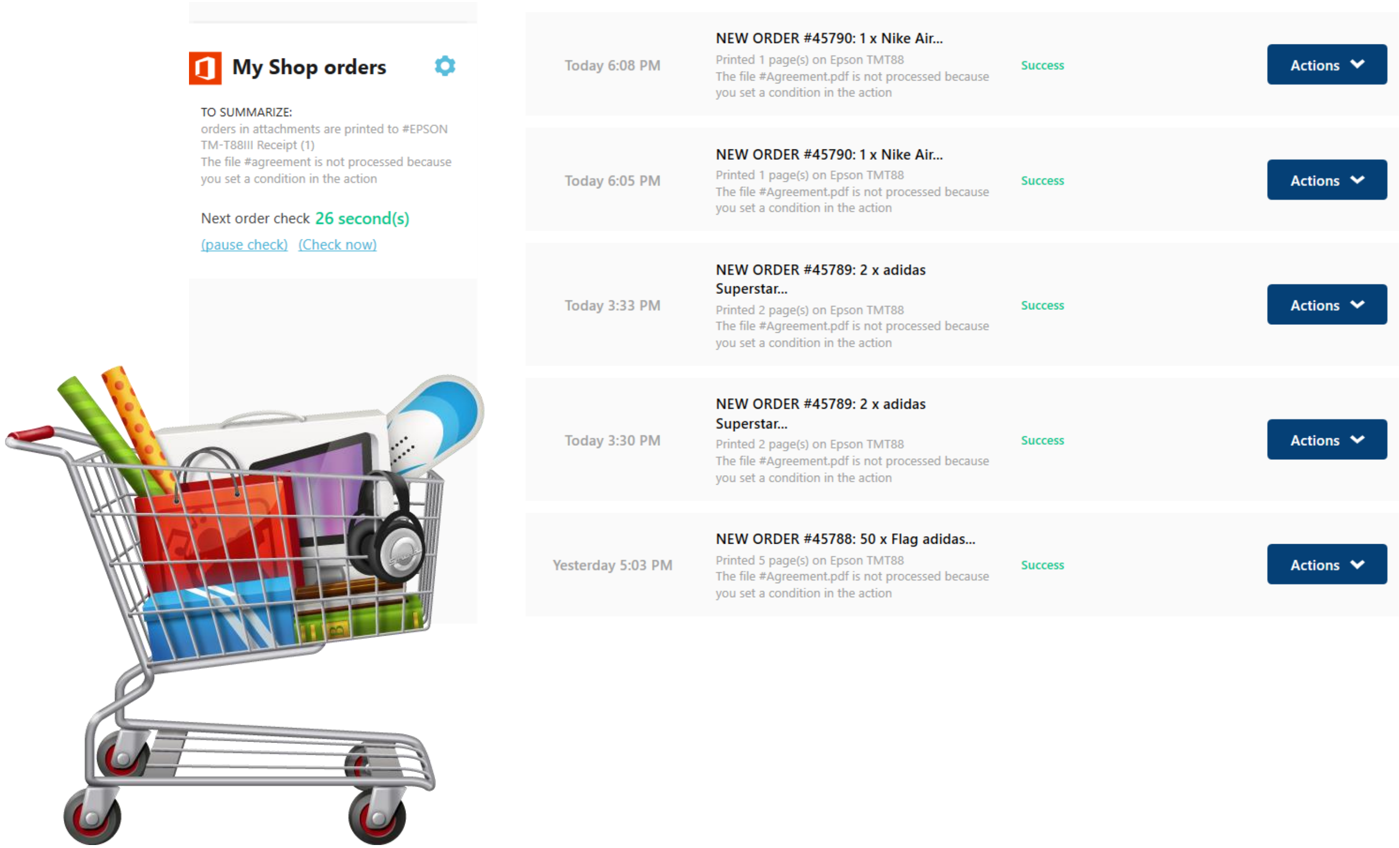
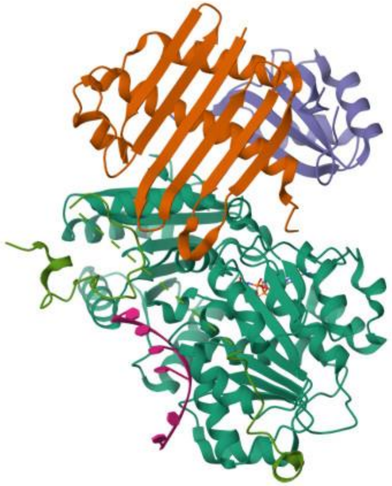
Higher-Order Interactions are Everywhere (cont.)

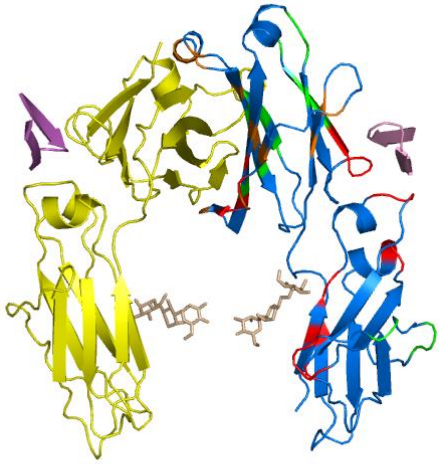
- **[Example 3]** Co-purchasing of items



Higher-Order Interactions are Everywhere (cont.)

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





Hypergraphs Model Higher-Order Interactions (cont.)

- Higher-order interactions are widely modeled using **hypergraphs**.
  - A hypergraph consists of a **node** set and a **hyperedge** set.

Co-Authorship

Hypergraphs Model Higher-Order Interactions (cont.)

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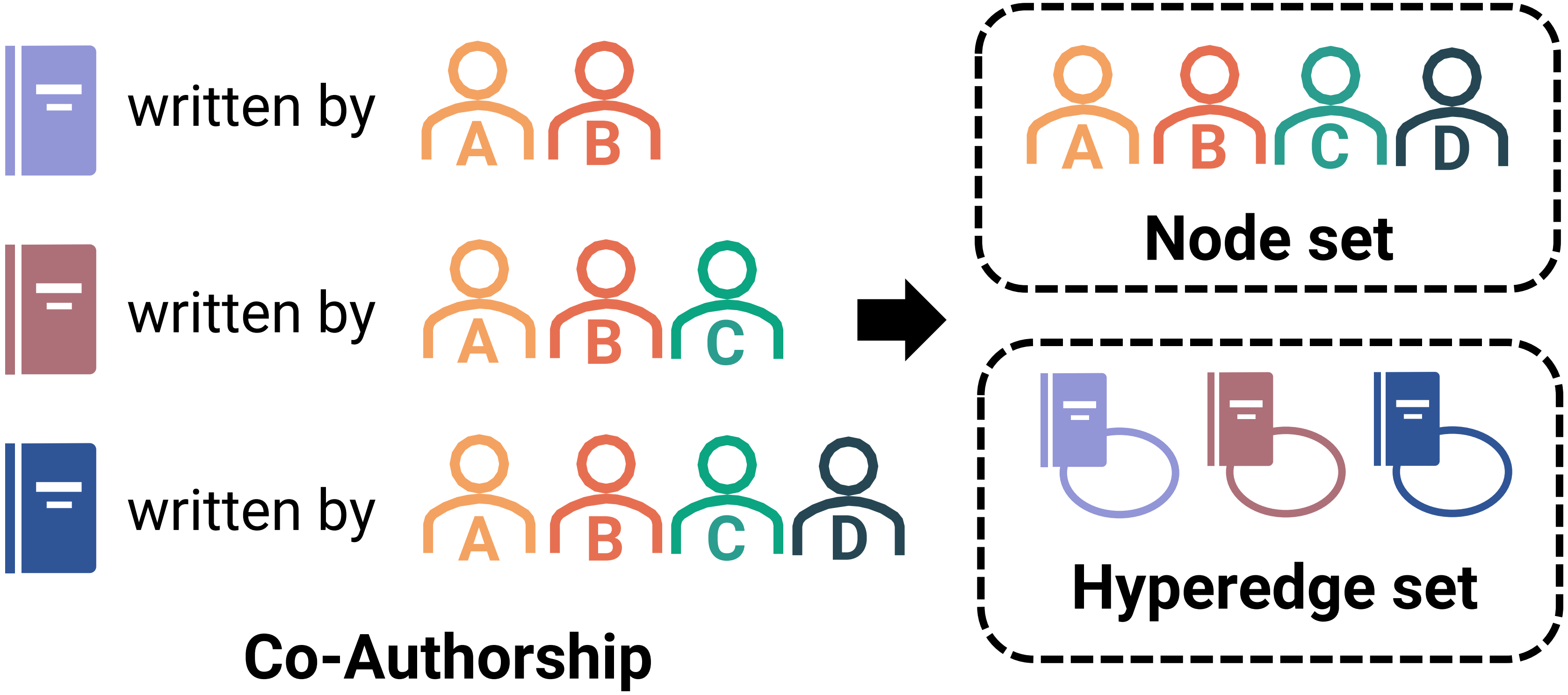
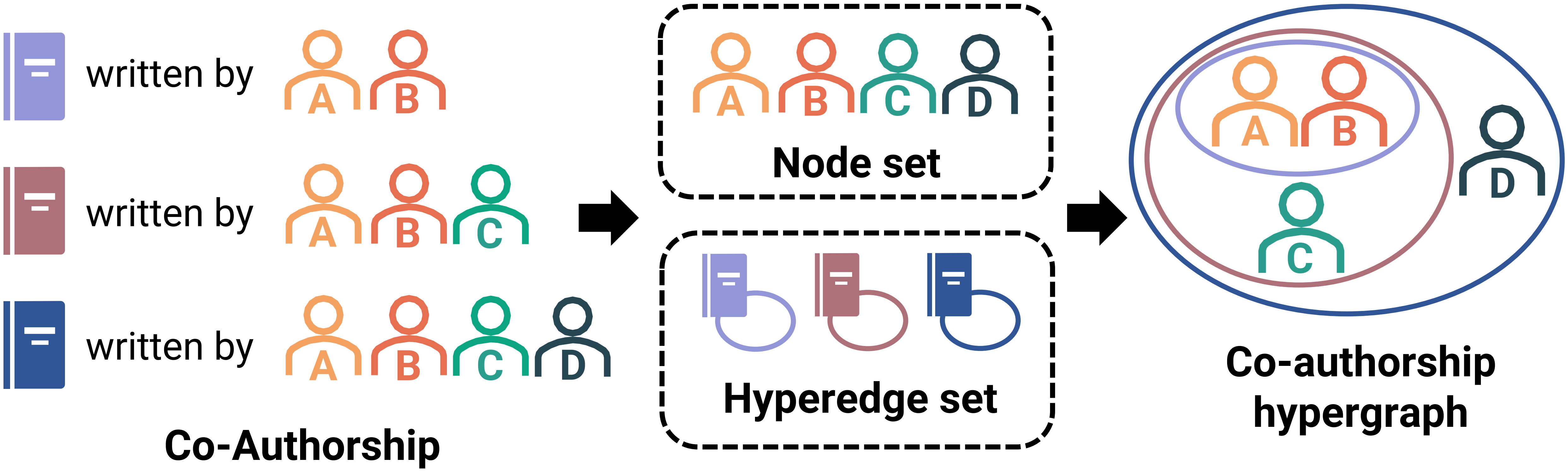


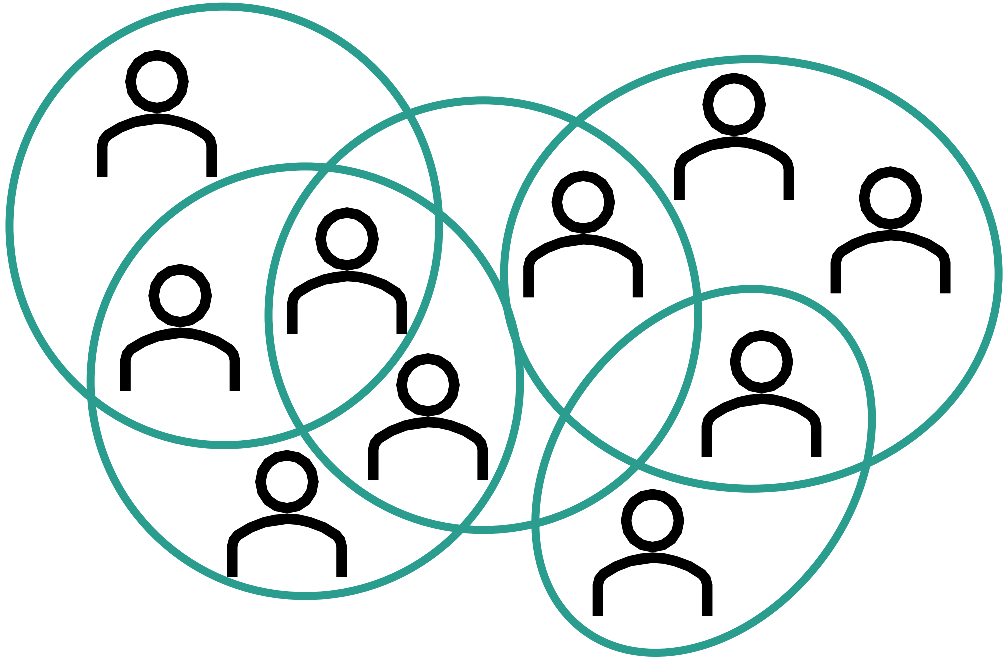
Hypergraphs Model Higher-Order Interactions (cont.)

- Higher-order interactions are widely modeled using **hypergraphs**.
  - A hypergraph consists of a **node** set and a **hyperedge** set.



Machine Learning Tasks on Hypergraphs

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



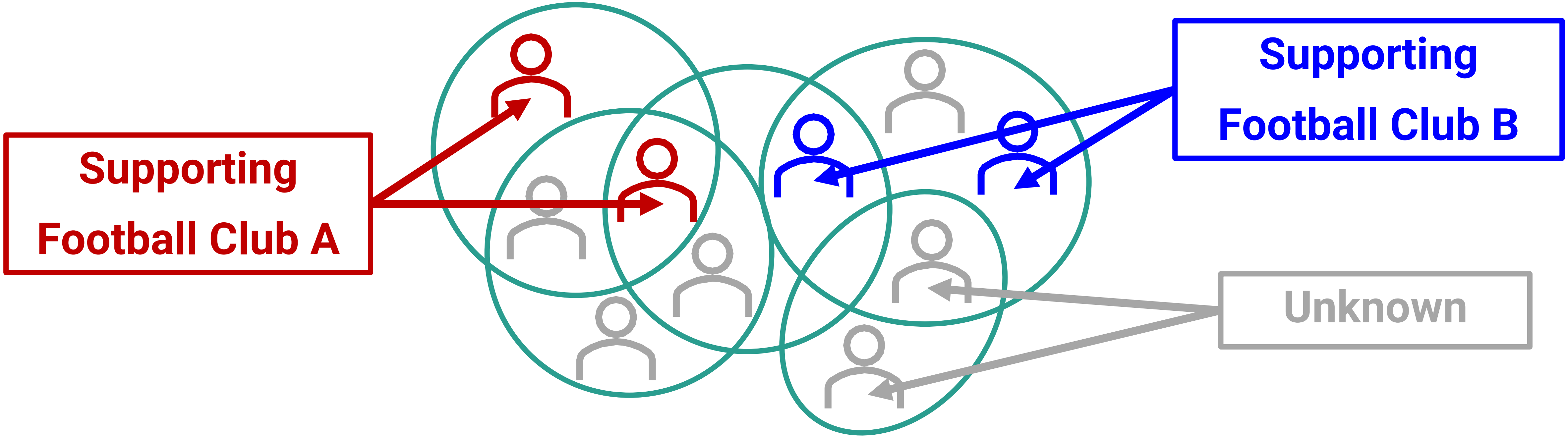
Social media hypergraph

[Nodes] Social media users

[Hyperedge] A set of users involved in the same group chatting

Machine Learning Tasks on Hypergraphs (cont.)

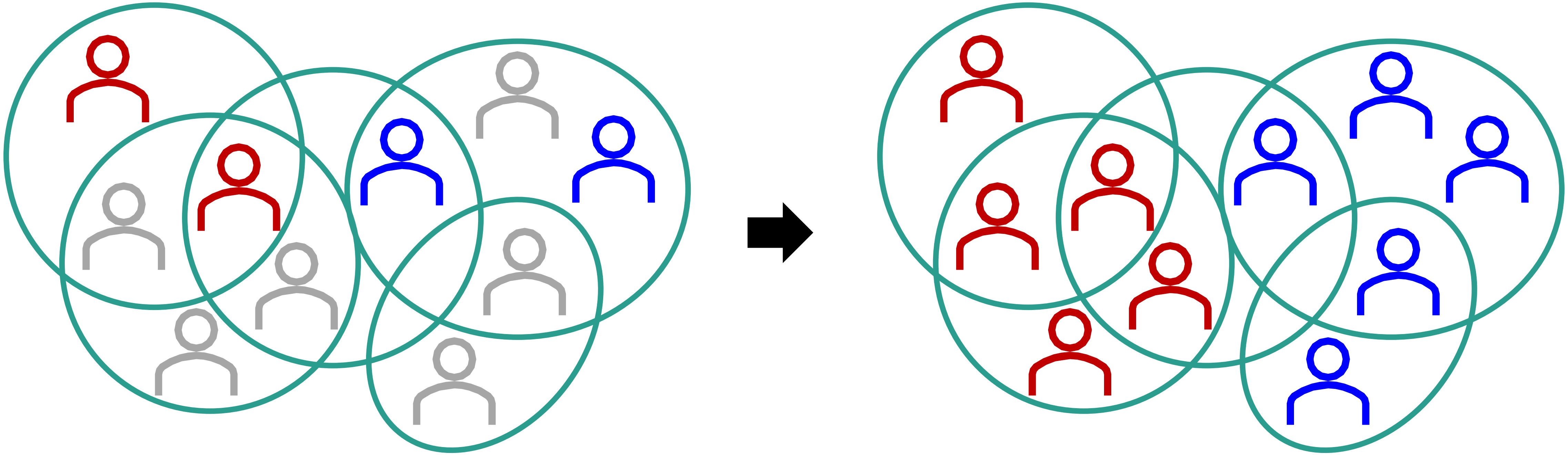
- There are various machine learning tasks on hypergraphs.
  - The first example is a **node classification** task.



Which club does each user support?

Machine Learning Tasks on Hypergraphs (cont.)

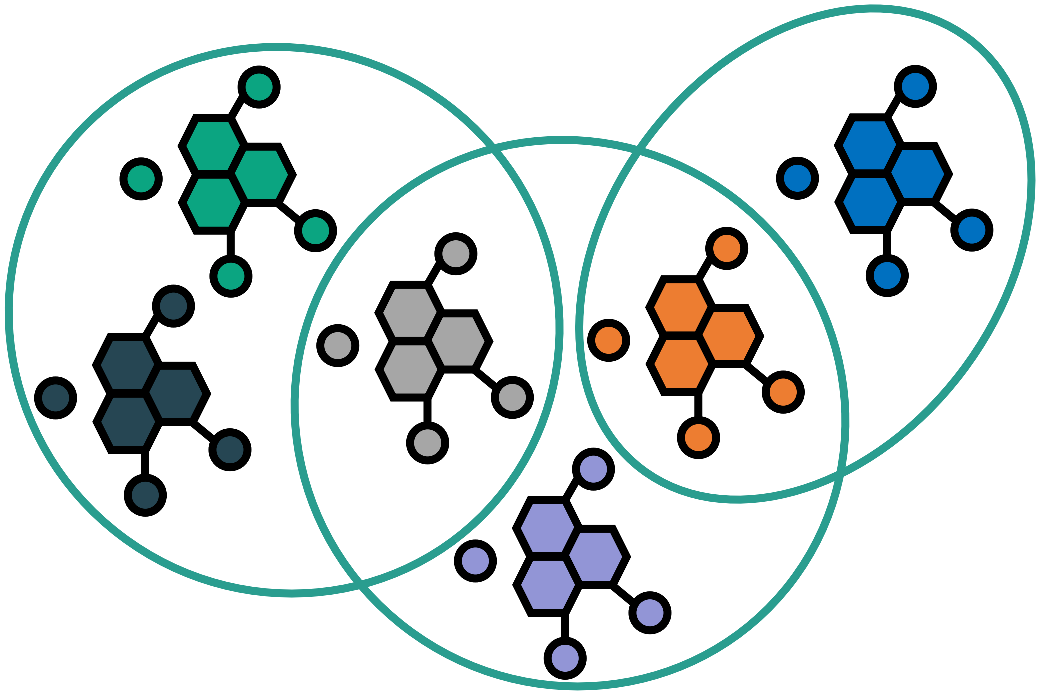
- There are various machine learning tasks on hypergraphs.
  - The first example is a **node classification** task.



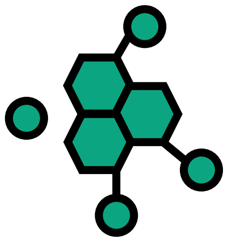
The node classification task formalizes this user profiling.

Machine Learning Tasks on Hypergraphs (cont.)

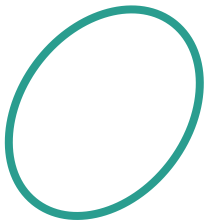
- There are various machine learning tasks on hypergraphs.
  - The second example is a **hyperedge prediction** task.



Metabolic reaction hypergraph



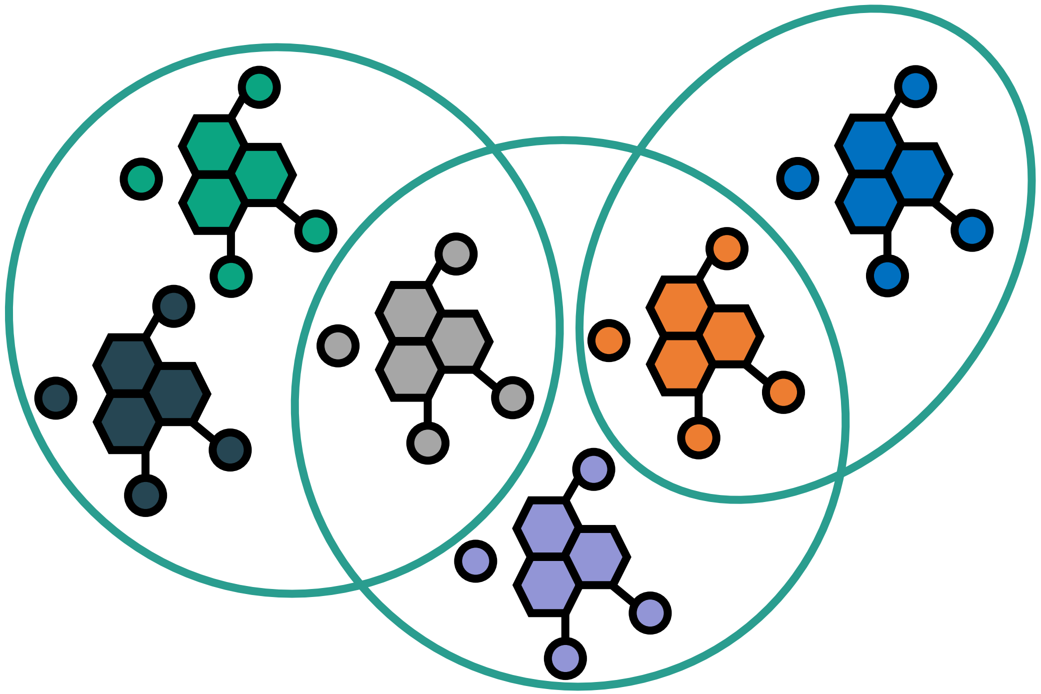
[Nodes] Metabolites



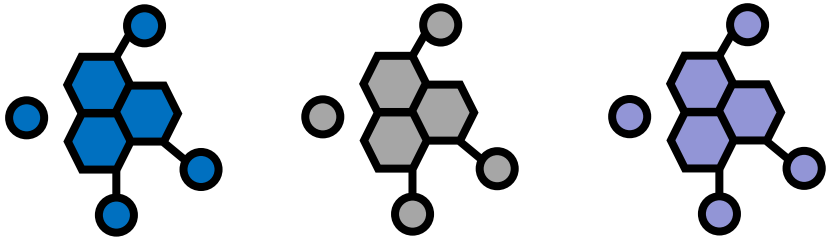
[Hyperedge] A set of metabolites involved in the same chemical reaction.

Machine Learning Tasks on Hypergraphs (cont.)

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



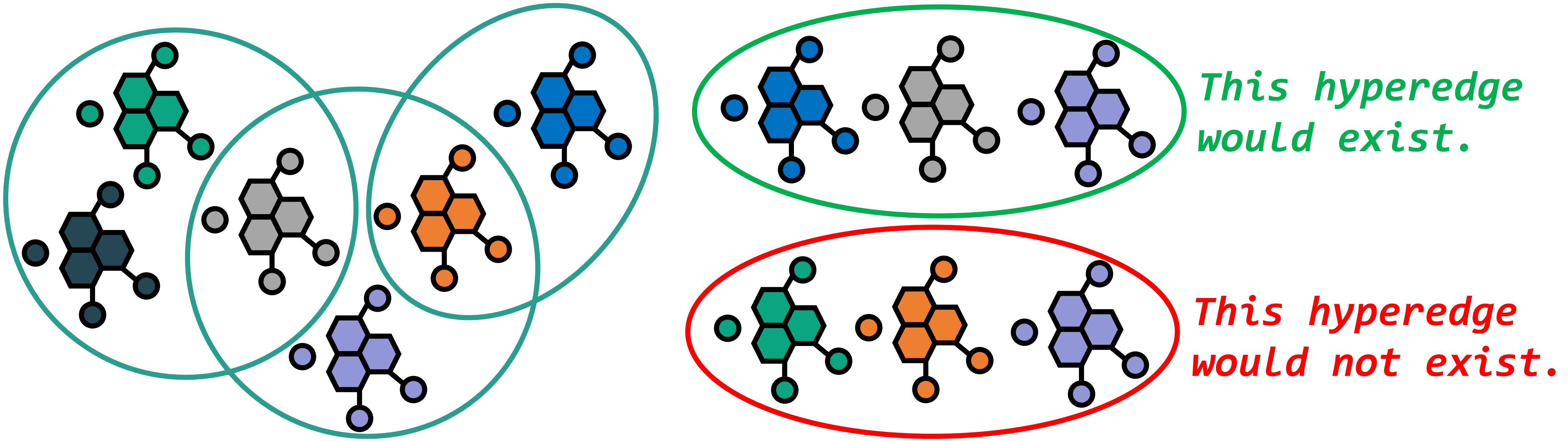
Metabolic reaction hypergraph



Would these three metabolites react together?

Machine Learning Tasks on Hypergraphs (cont.)

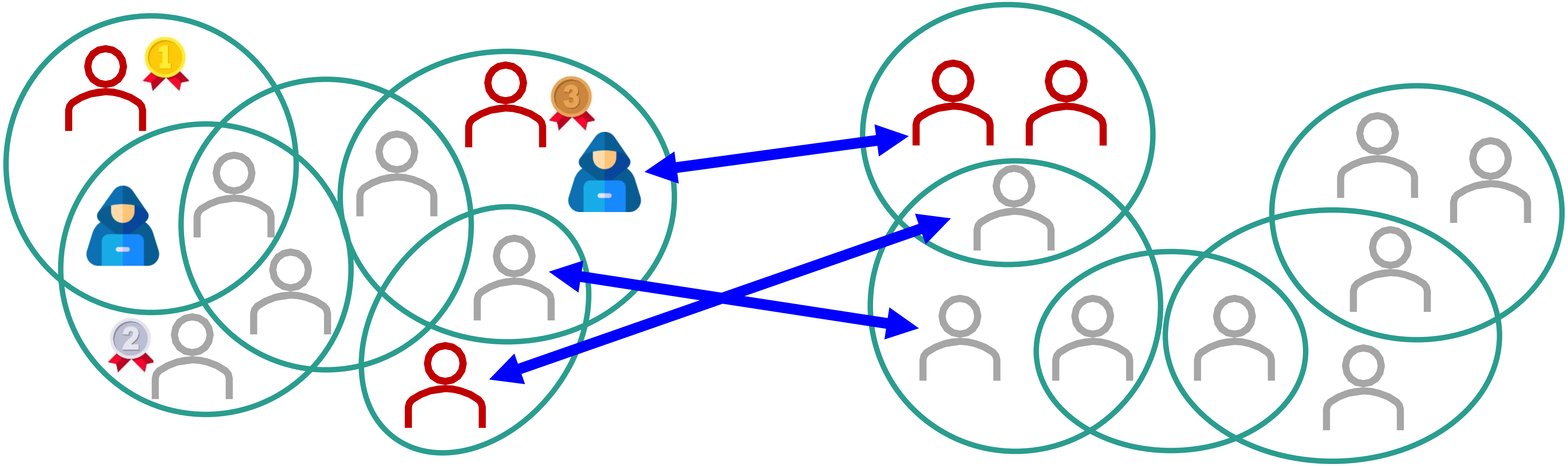
- There are various machine learning tasks on hypergraphs.
  - The second example is a **hyperedge prediction** task.



The hyperedge prediction task formalizes this reaction prediction.

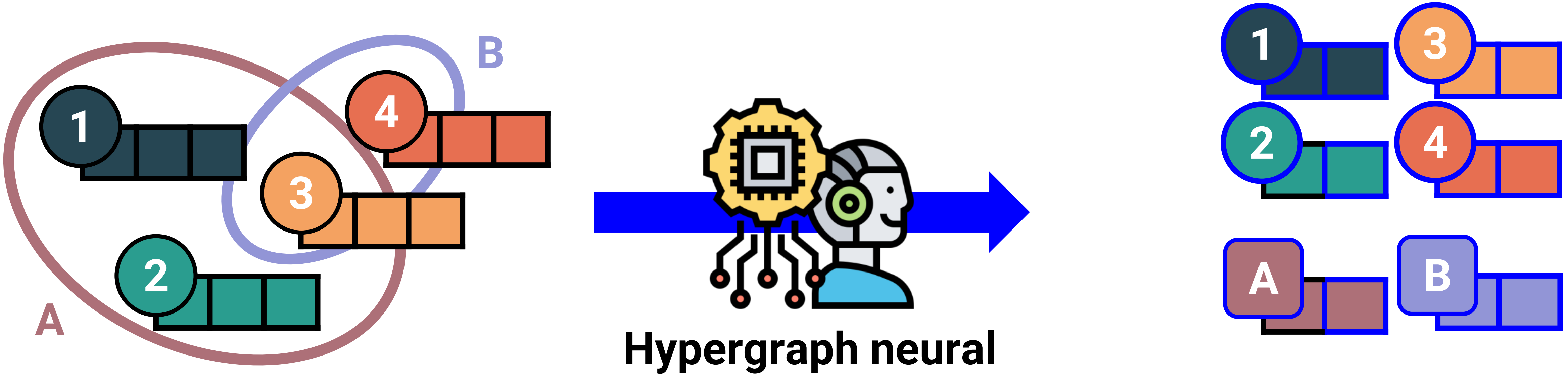
Machine Learning Tasks on Hypergraphs (cont.)

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



Hypergraph Neural Network (HNN)

- **Hypergraph neural networks (HNNs)** are family of neural networks for learning hypergraphs to solve diverse downstream tasks.



Hypergraph and node features

Hypergraph neural network (HNN)

Node (and hyperedge) embeddings

** Note: Hyperedge features can also given as the input.*

Hypergraph Neural Network (cont.)

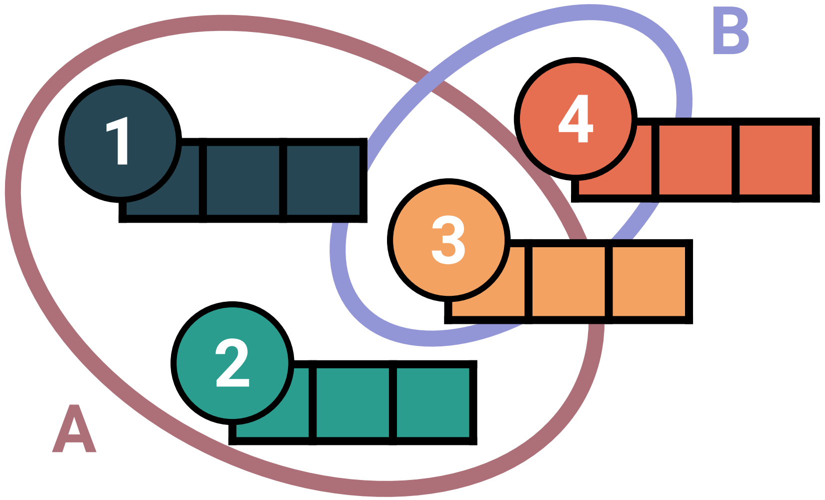
- **Hypergraph neural networks (HNNs)** are state-of-the-art models for many hypergraph downstream tasks.

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?

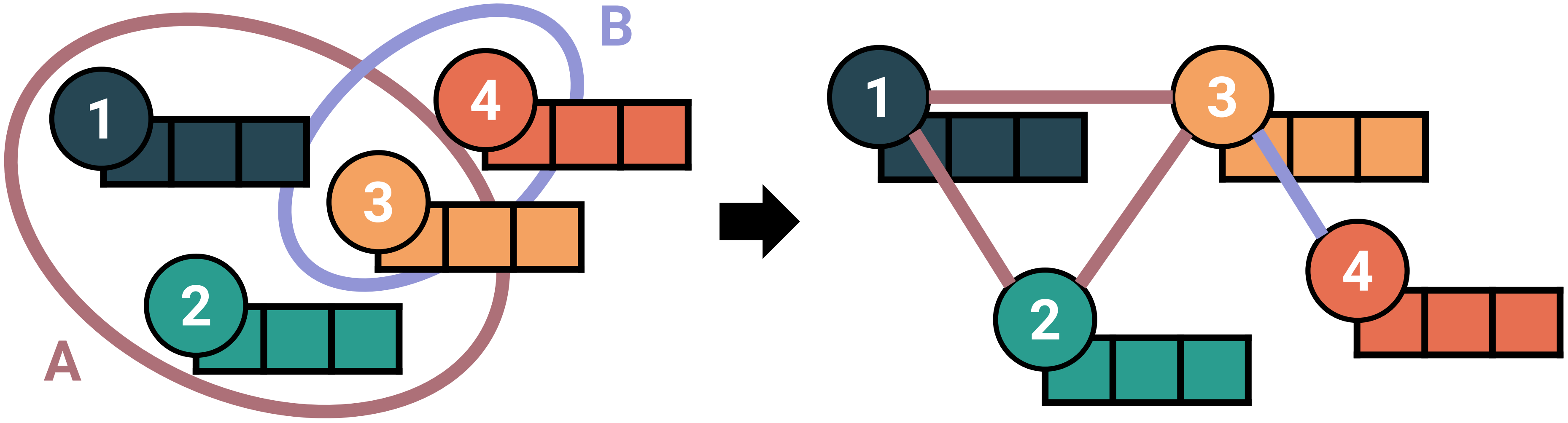
- For hypergraph learning, we can also use **graph neural networks**:
  - [Step 1] Express higher-order interactions with a pairwise graph.
  - [Step 2] Utilize graph neural networks (GNN) on the pairwise graph.



Hypergraph

Why Hypergraph Neural Networks? (cont.)

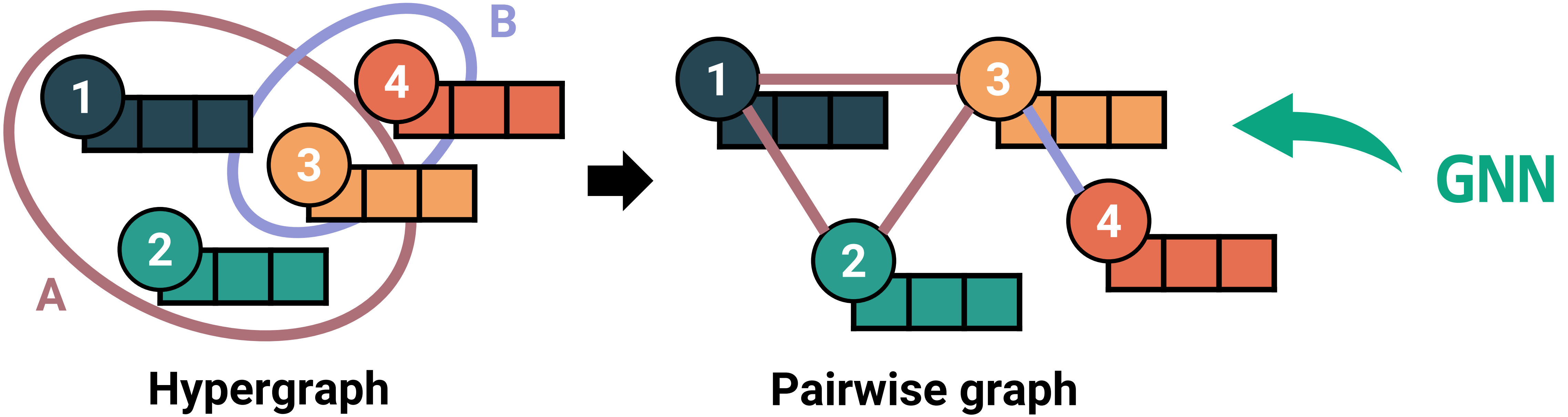
- For hypergraph learning, we can also use **graph neural networks**:
  - **[Step 1]** Express higher-order interactions with a pairwise graph.
  - **[Step 2]** Utilize graph neural networks (GNN) on the pairwise graph.



Hypergraph **Pairwise graph**

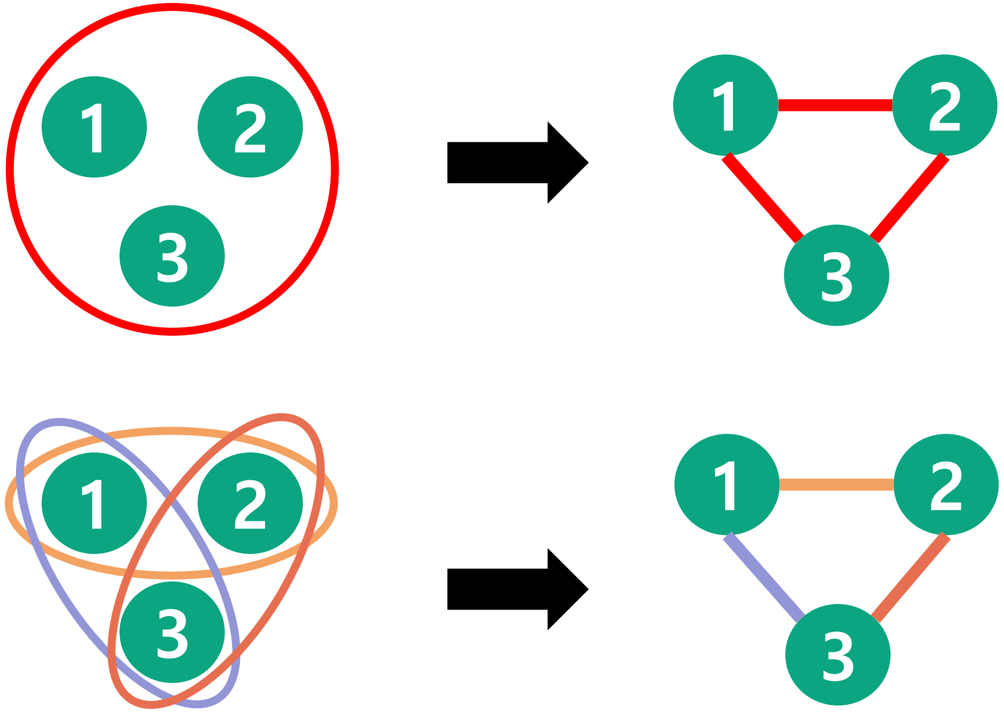
Why Hypergraph Neural Networks? (cont.)

- For hypergraph learning, we can also use **graph neural networks**:
  - **[Step 1]** Express higher-order interactions with a pairwise graph.
  - **[Step 2]** Utilize graph neural networks (GNN) on the pairwise graph.



Why Hypergraph Neural Networks? (cont.)

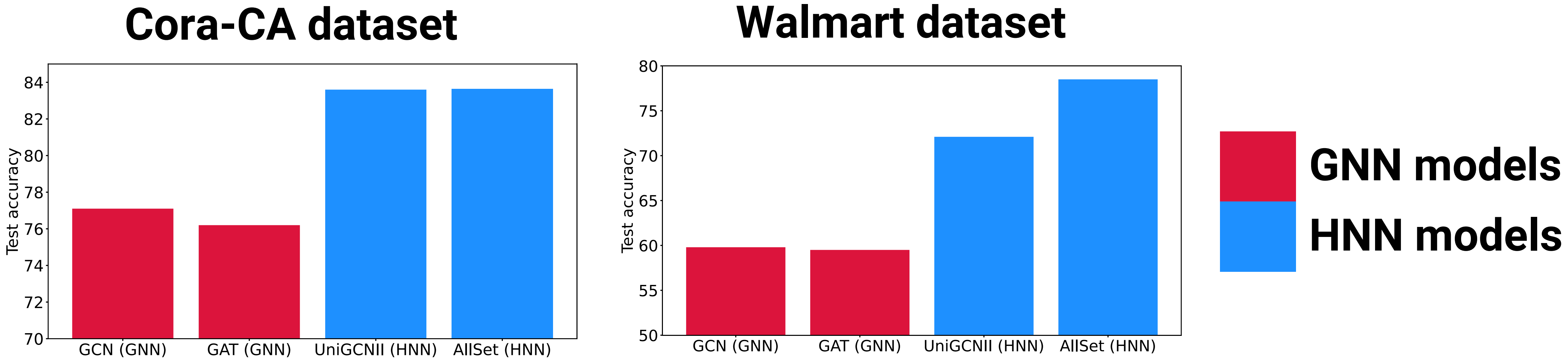
- However, expressing higher-order interactions with a pairwise graph may cause an **information loss** [Zhou et al., 2006].



Resulting in the same structure.

Why Hypergraph Neural Networks? (cont.)

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

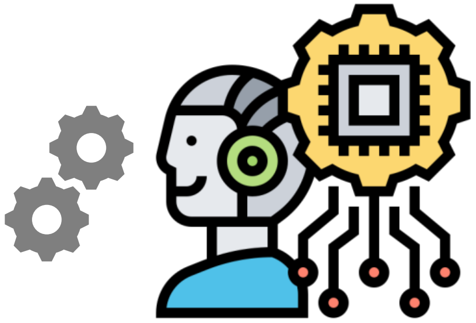


Node classification performance on hypergraph benchmark datasets

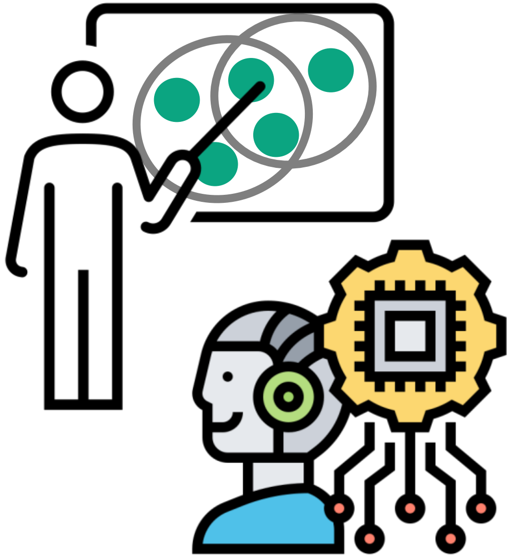
** Results are from [Chien et al., 2022].*

Tutorial Overview

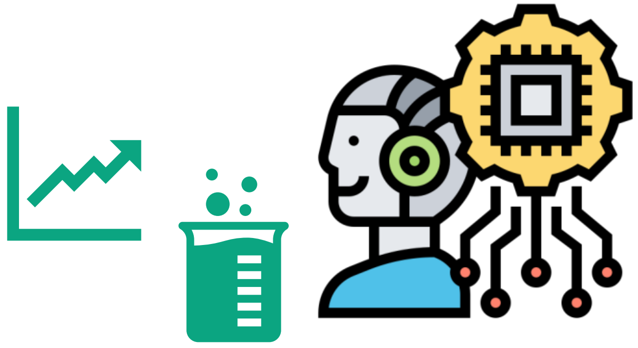
- In this tutorial, we provide an overview of how hypergraph neural networks are **designed, trained, and practically utilized**.



Design choice



Training strategy

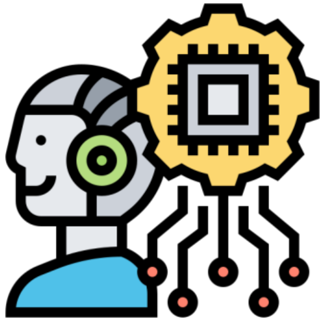


Application

Tutorial Overview (cont.)

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

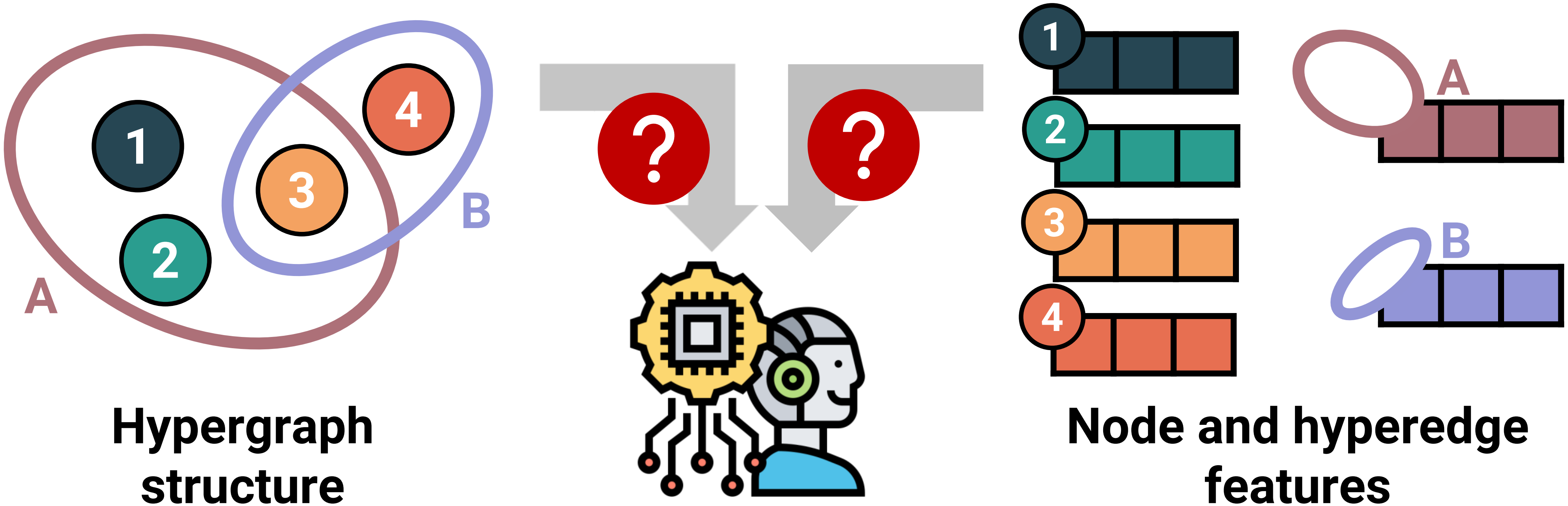
We are now here!



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 are hypergraph structures expressed?
  - **2.2.** What input node and hyperedge features are typically used?

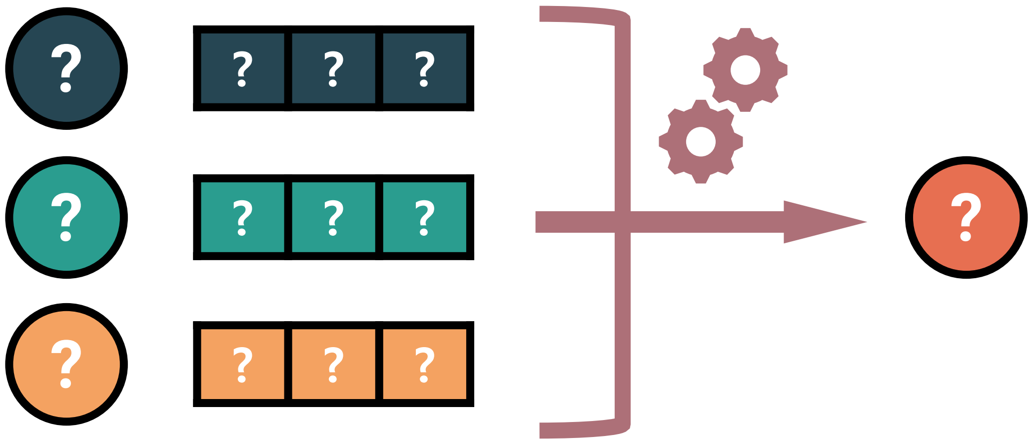


Hypergraph structure

Node and hyperedge features

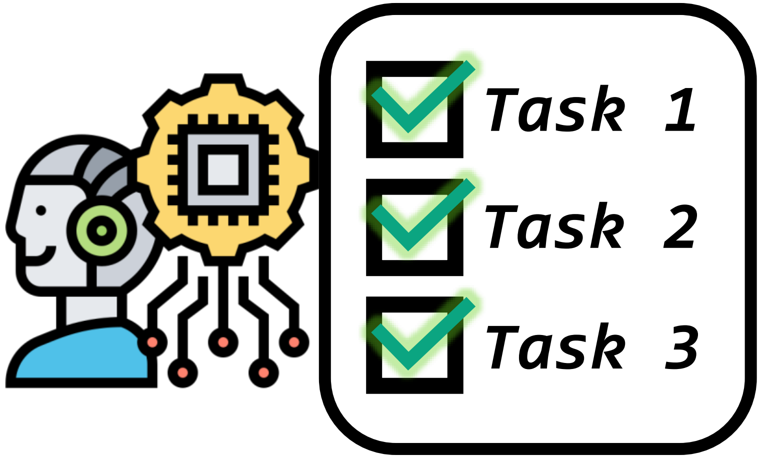
Tutorial Overview (cont.)

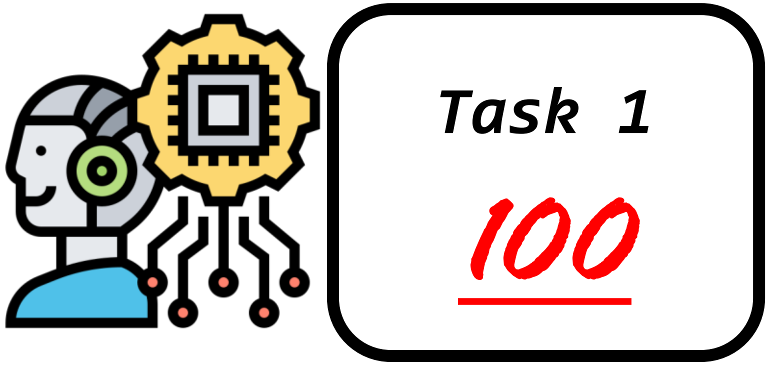
- **[Part 3]** We cover message passing of hypergraph neural networks.
  - **3.1.** Whose messages to aggregate
  - **3.2.** What messages to aggregate
  - **3.3.** How to aggregate messages



Tutorial Overview (cont.)

- **[Part 4]** We cover training strategies of 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 system
  - **5.2.** Bioinformatics and medical science
  - **5.3.** Time series analysis
  - **5.4.** Computer vision

Tutorial Overview (cont.)

- **[Part 6]** We cover discussions regarding hypergraph neural networks.
  - **6.1.** Hypergraph neural network theory
  - **6.2.** Advantages of hypergraph neural networks
  - **6.3.** Hypergraph neural networks for complex hypergraphs