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

Part 5. Applications


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Part 5. Applications

Part 1. Introduction | Part 2. Inputs | Part 3. Message Passing | Part 4. Training Strategies | **Part 5. Applications** | Part 6. Discussions

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

SCAN ME

Presenter

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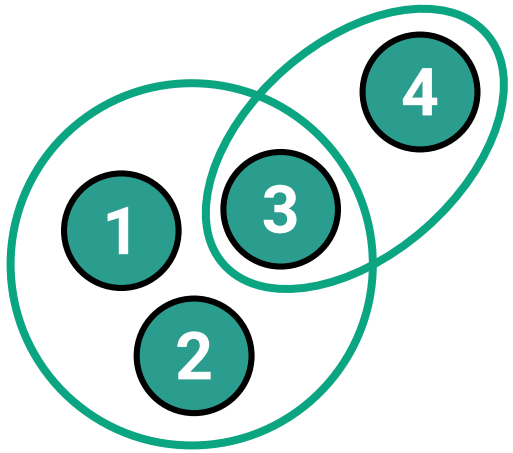
KAIST

What are Some Issues in Applying HNNs?

- Two major issues include:
  - Q1) How to **express the raw data** as hypergraphs?
  - Q2) How to **formulate the learning task** for an HNN?

Raw data



Hypergraph

Node Prediction
or
Hyperedge Prediction

Learning task formulation

What are Notable Applications of HNNs?

- In the following domains, we will cover how the issues have been addressed:

Recommender system

Bioinformatics & Medical science

Time series analysis

Computer vision

What are Notable Applications of HNNs? (cont.)

- In the following domains, we will cover how the issues have been addressed:

Recommender system

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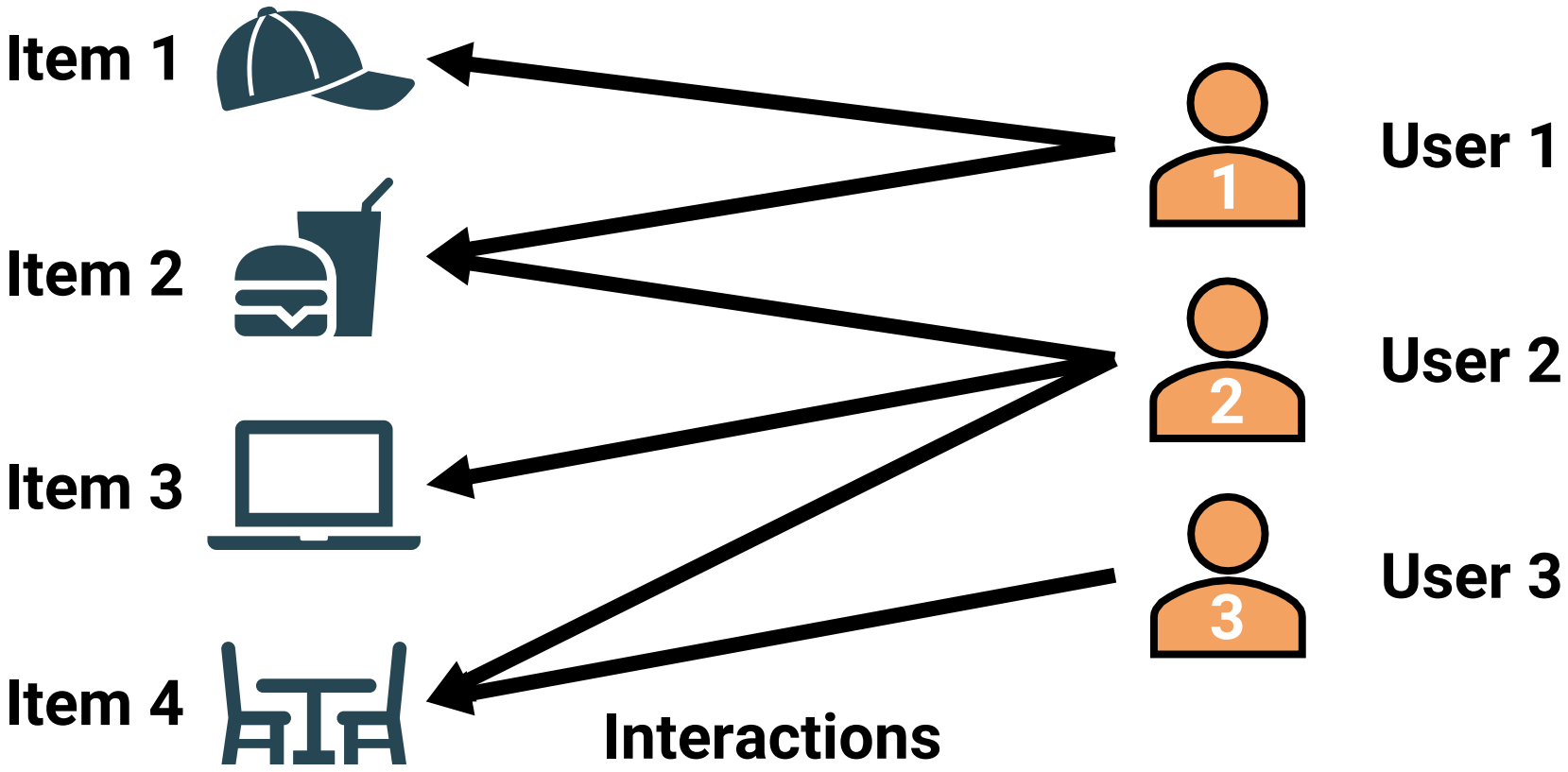
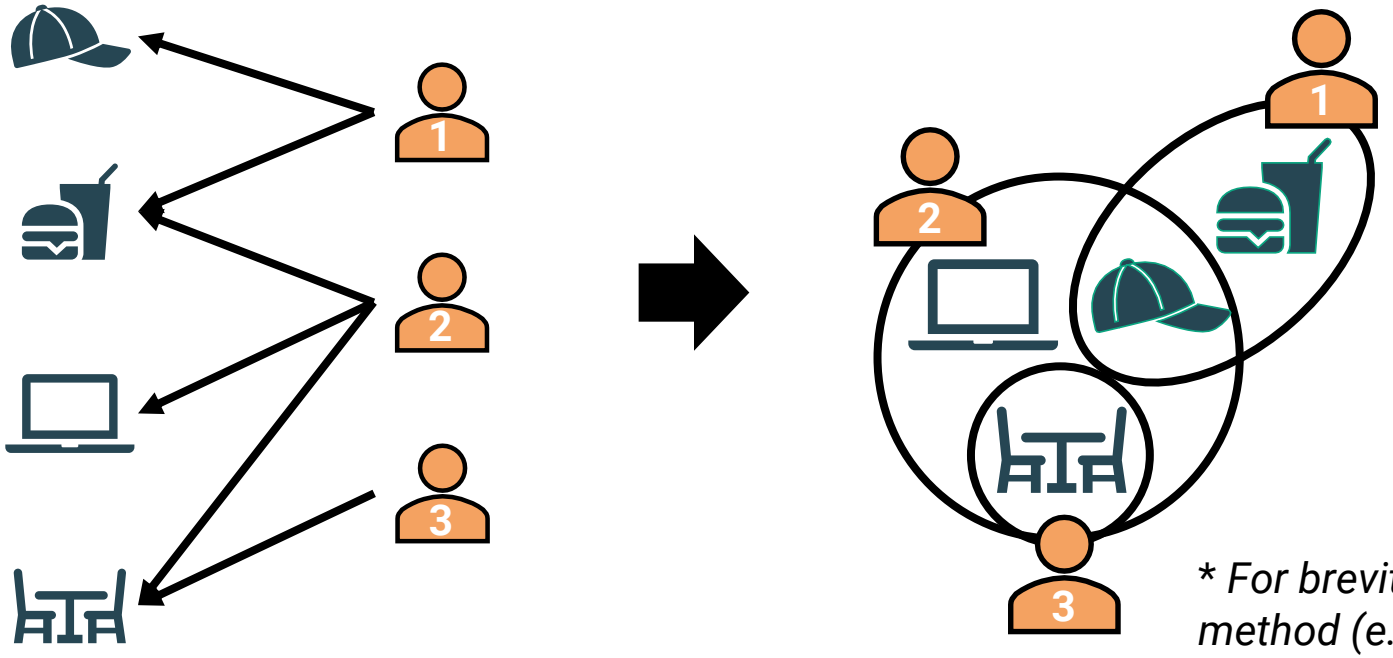
Recommendation: Hypergraph Construction

- **Raw data** typically include users & items and their interactions.



Recommendation: Hypergraph Construction (cont.)

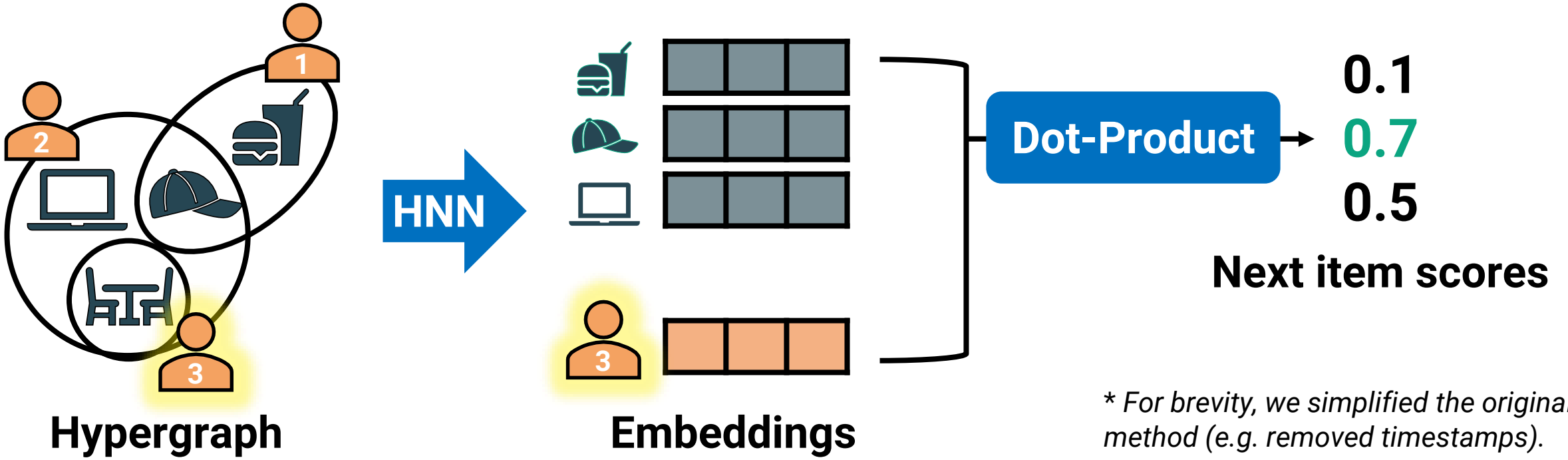
- Wang et al. (2020) converted the **interactions** into a hypergraph
  - A node is an item; a hyperedge is a user.
  - A user hyperedge connects all item nodes that it interacted with.



** For brevity, we simplified the original method (e.g. removed timestamps).*

Recommendation: Task Formulation

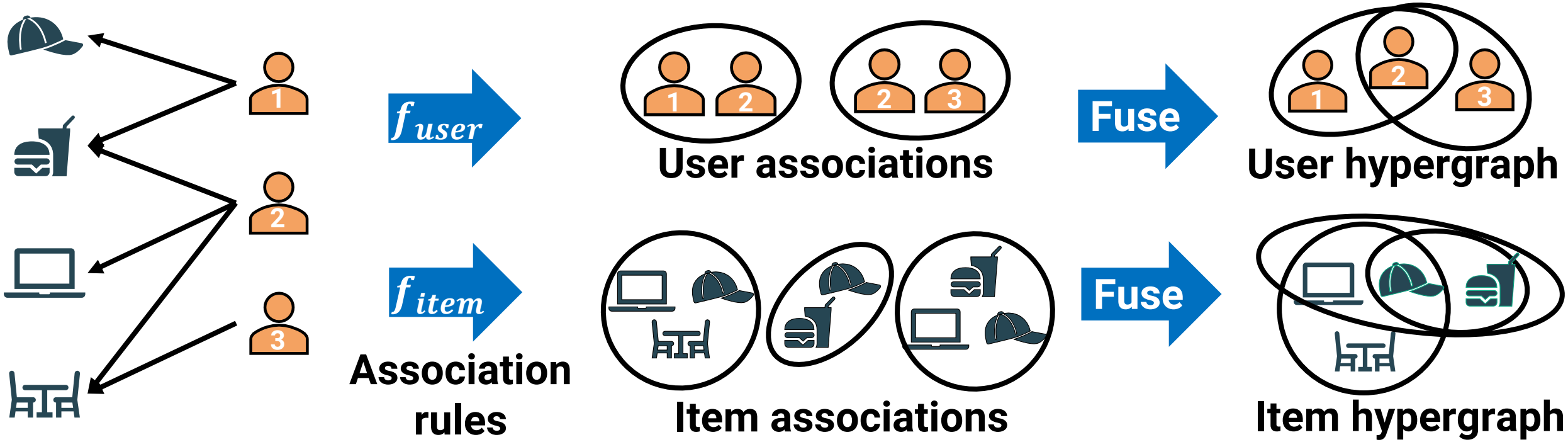
- Wang et al. (2020) used an HNN for **next-item recommendation.**
  - An HNN encodes nodes and hyperedges.
  - The embeddings are used to predict items that users will interact next.



** For brevity, we simplified the original method (e.g. removed timestamps).*

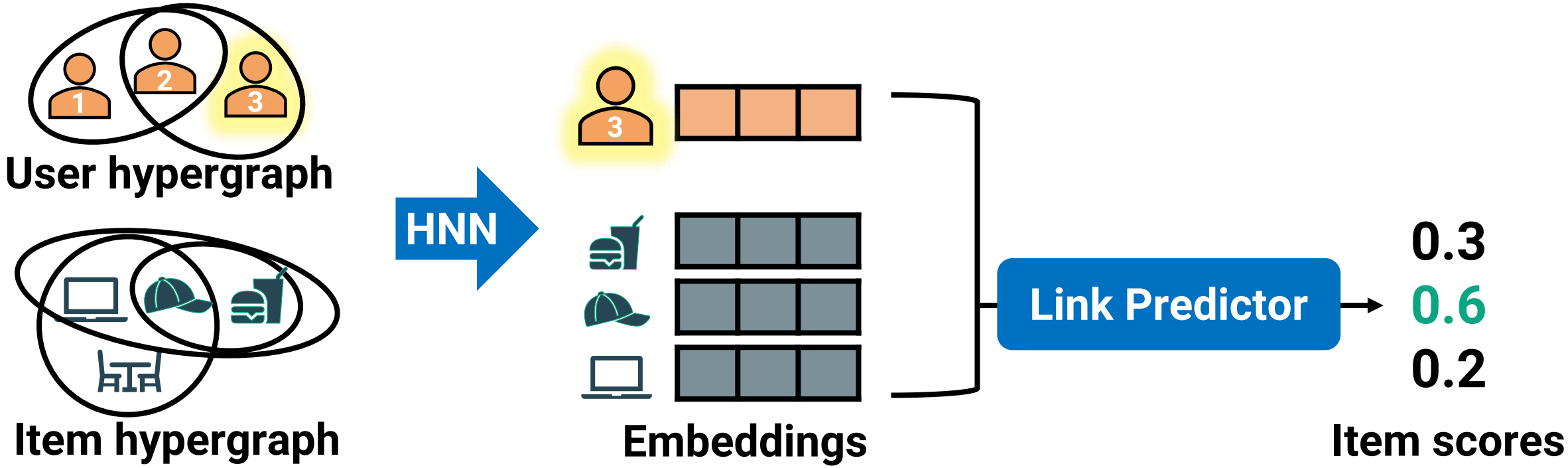
Recommendation: Hypergraph Construction (cont.)

- Ji et al. (2020) used **association rules** to construct two hypergraphs.
  - The pre-determined association rules aim to capture high-order information among users and among items, returning two hypergraphs.



Recommendation: Task Formulation (cont.)

- Ji et al. (2020) used an HNN for **collaborative filtering**.
  - An HNN encodes user nodes and item nodes.
  - The embeddings are used to recommend items for users.



What are Notable Applications of HNNs? (cont.)

- In the following domains, we will cover how the issues have been addressed:

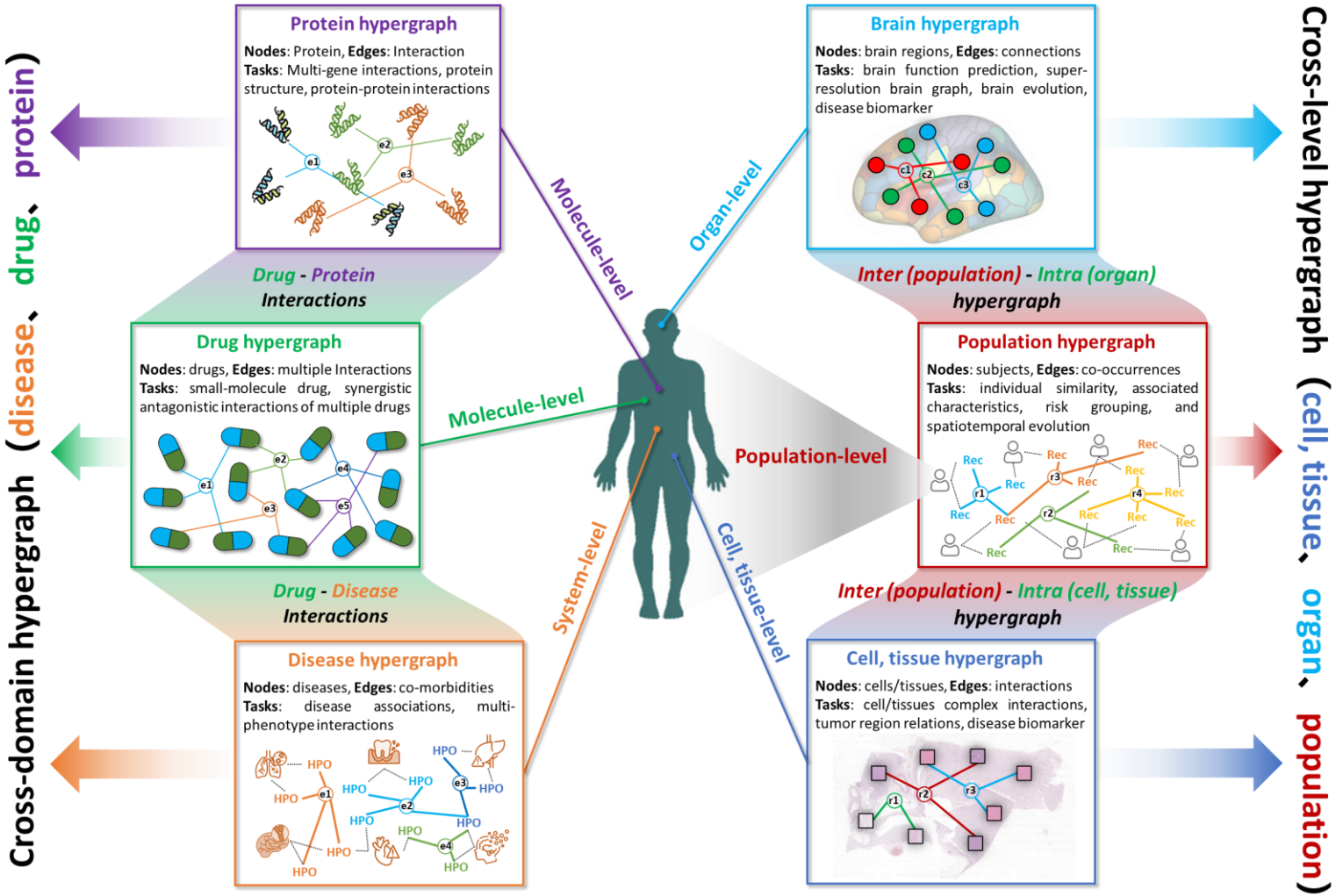
Recommender system

Bioinformatics & Medical science

Time series analysis

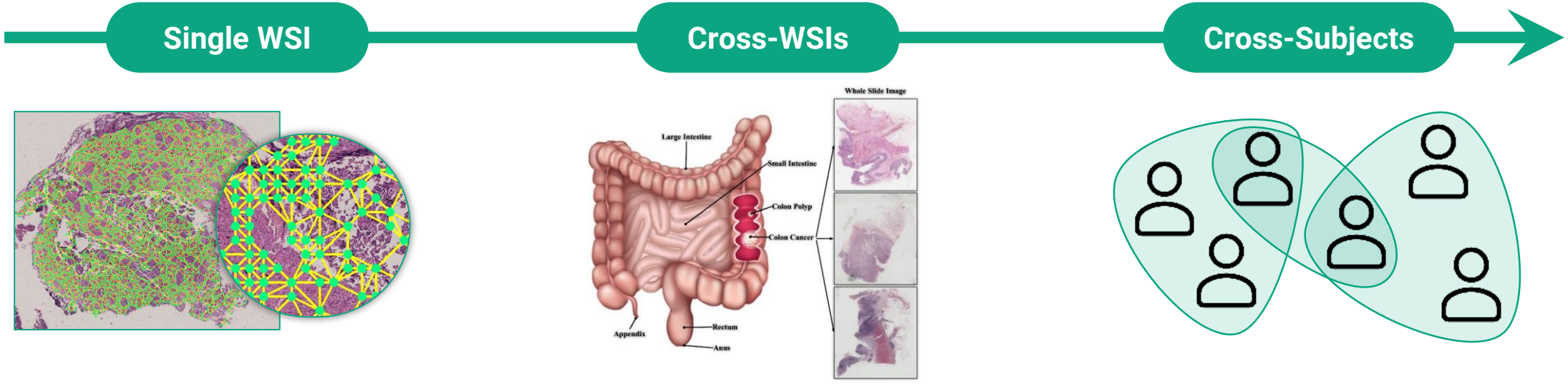
Computer vision

Hypergraph in Bioinformatics and Medical Science



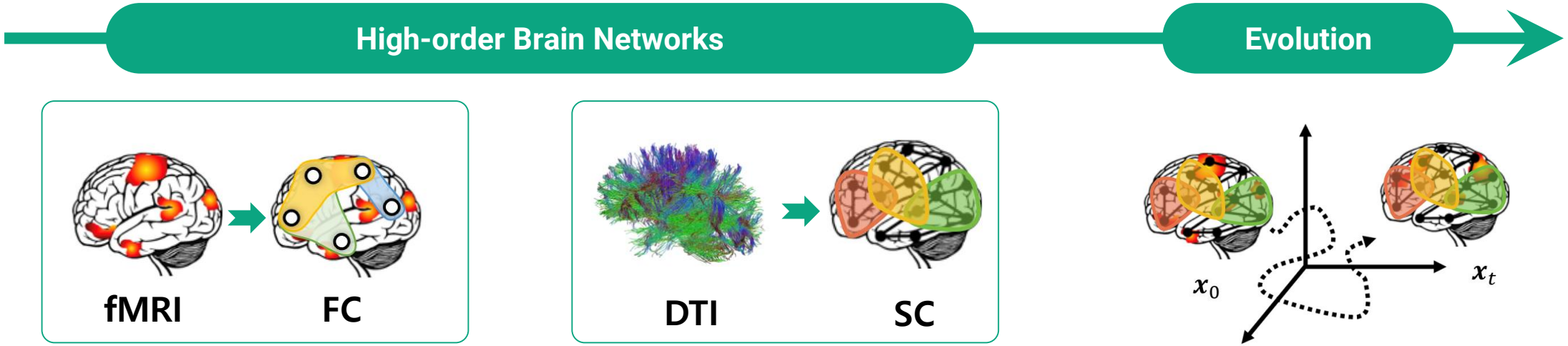
Pathology Analysis

- Gigapixel WSIs contains multiple high-order correlations
  - Within a single WSI
  - Cross-WSIs for a single subject
  - Cross-subjects



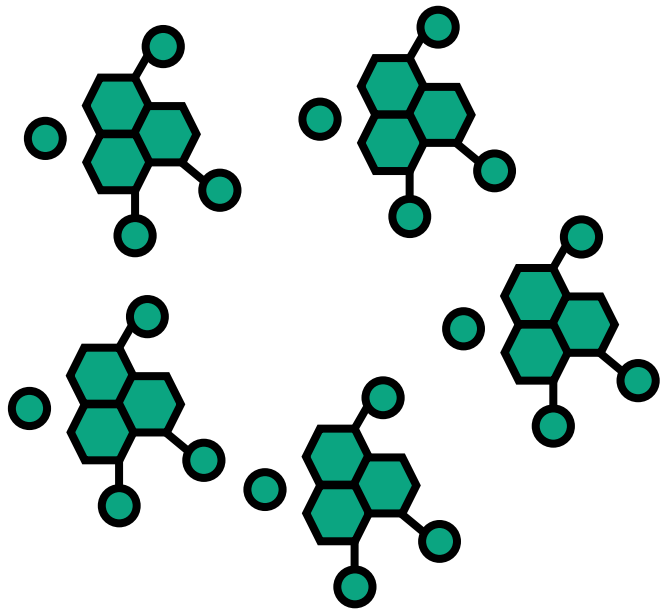
Brain Network

- Functional and Structural Brain Network contains high-order correlations
  - Within individual functional network or structural network
  - Functional and structural network coupling
  - Brain network evolution

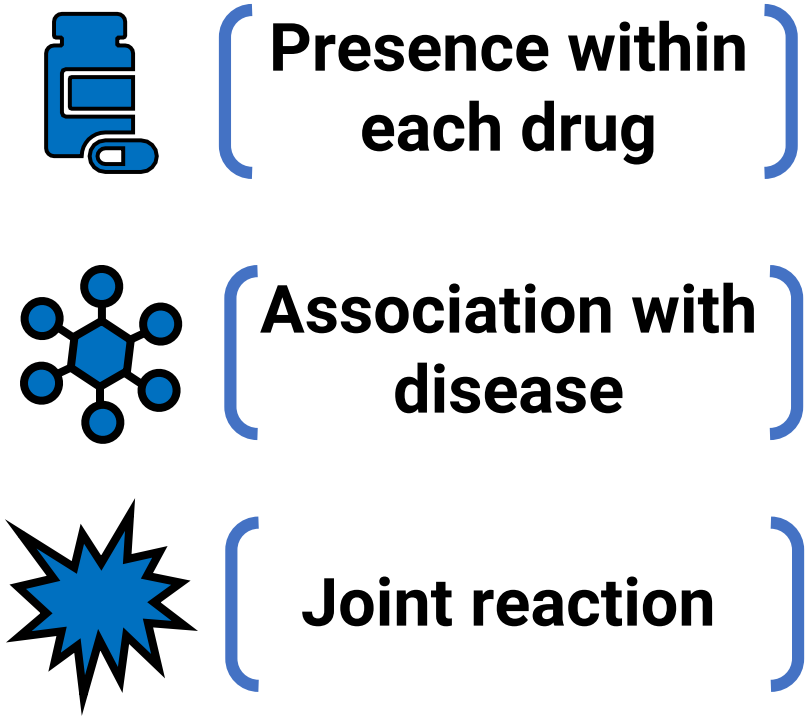


Bioinformatics: Hypergraph Construction

- **Raw data** typically include molecular-level structures and their relations.



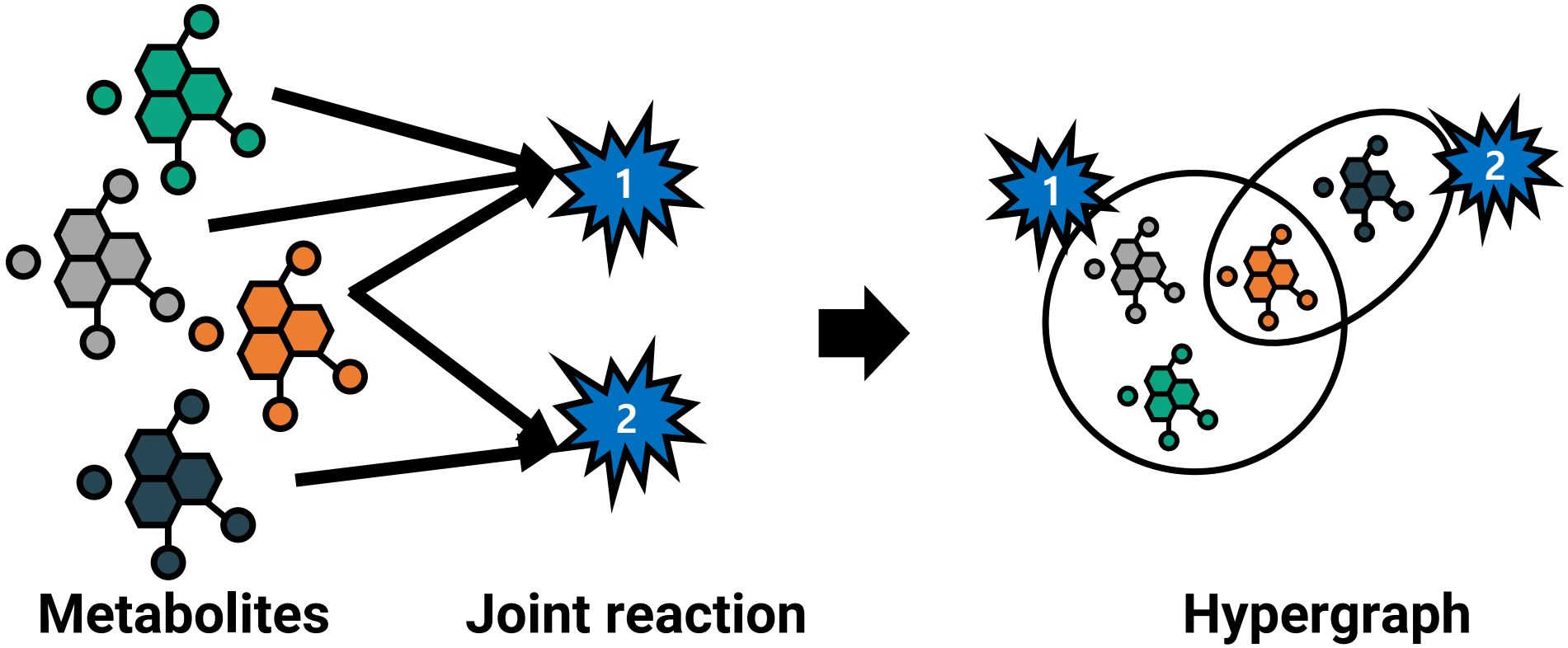
Molecular-level structures



Joint relations examples

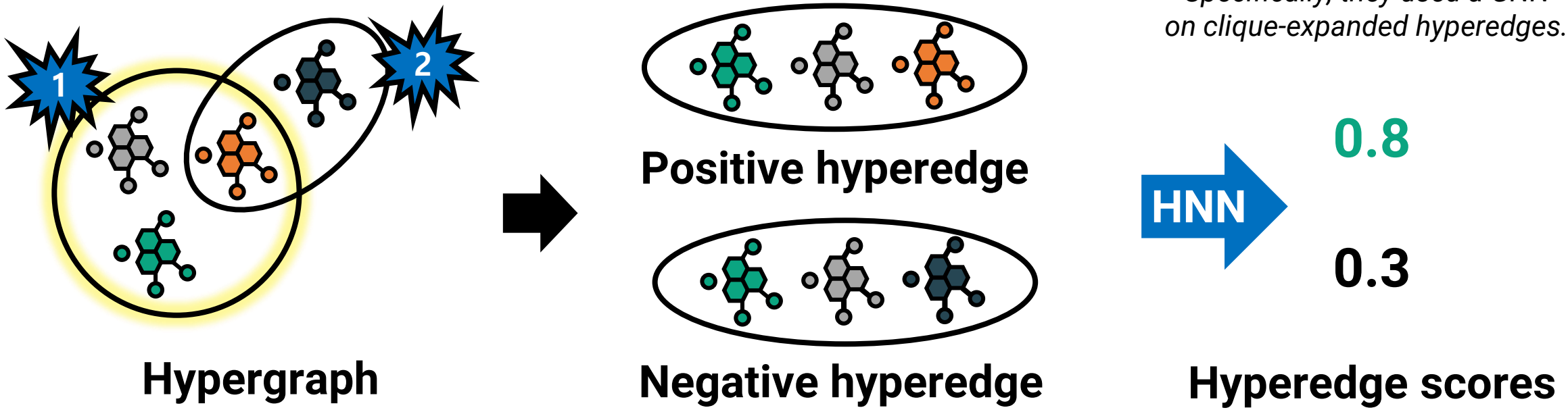
Bioinformatics: Hypergraph Construction (cont.)

- Chen et al. (2023) transforms a **metabolic network** into a hypergraph.
  - A node is metabolite; a hyperedge connects those with joint reaction.



Bioinformatics: Task Formulation

- Chen et al. (2023) used an HNN to **predict missing metabolic reaction**.
  - An HNN learns to classify negative and positive hyperedges, where negative hyperedges represent false joint reactions.



** Specifically, they used a GNN on clique-expanded hyperedges.*

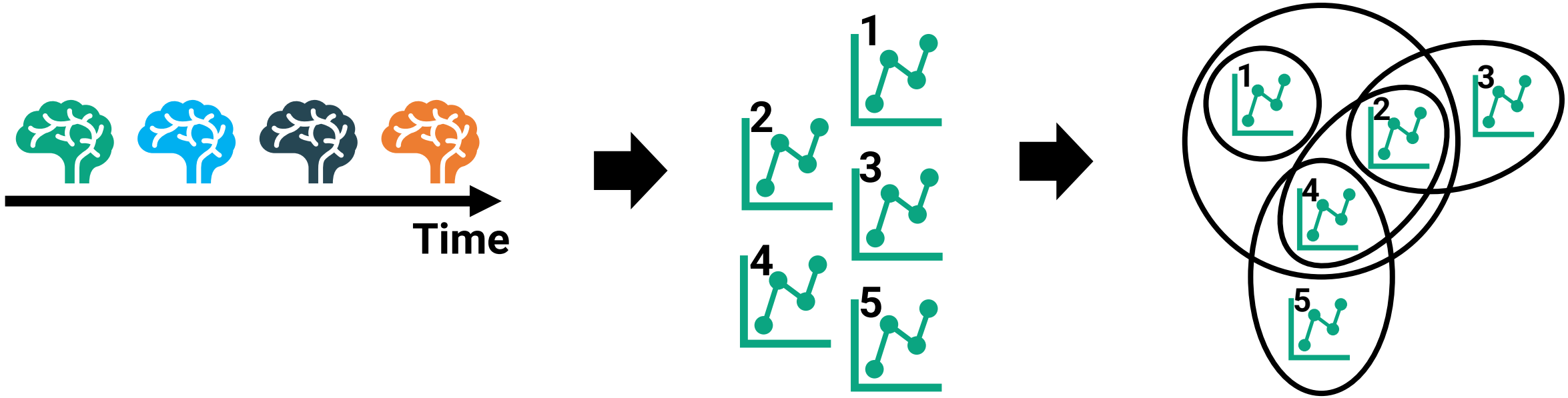
fMRI Data: Hypergraph Construction

- **Raw data** typically is series of brain images with brain signals.
  - The images can be parcellated into signals from region-of-interests (ROIs).

3D brain images in time series

fMRI Data: Hypergraph Construction (cont.)

- Wang et al. (2023) converted **fMRI** data into a hypergraph.
  - A node is a ROI; for each ROI, its hyperedge connects the most similar ROIs (estimated by a learning algorithm).

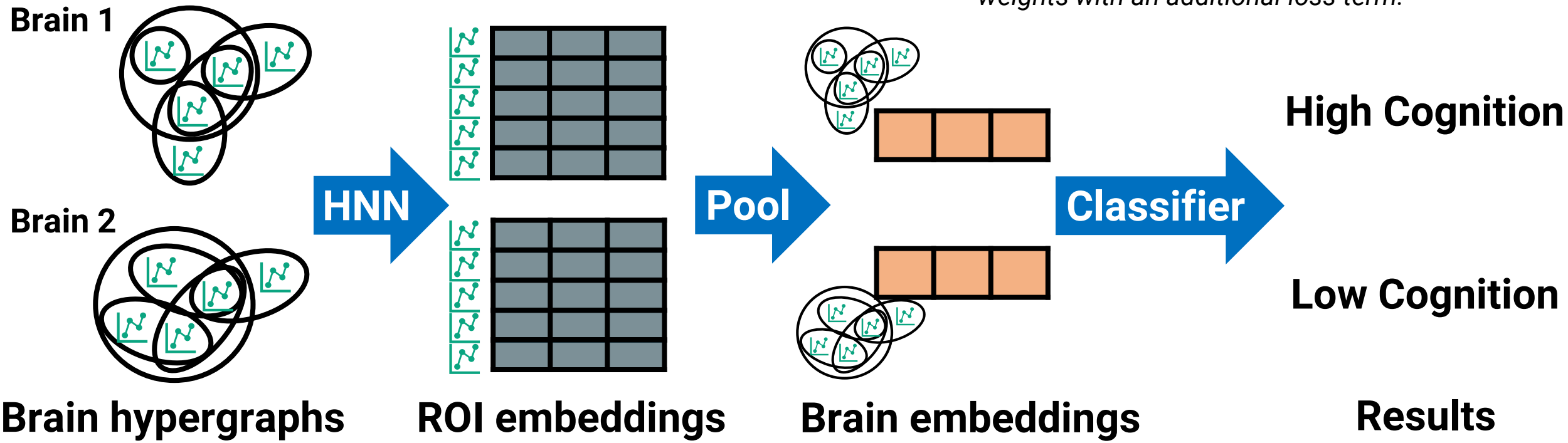


3D brain images **Signal series from ROIs** **Hypergraph**

fMRI Data: Task Formulation

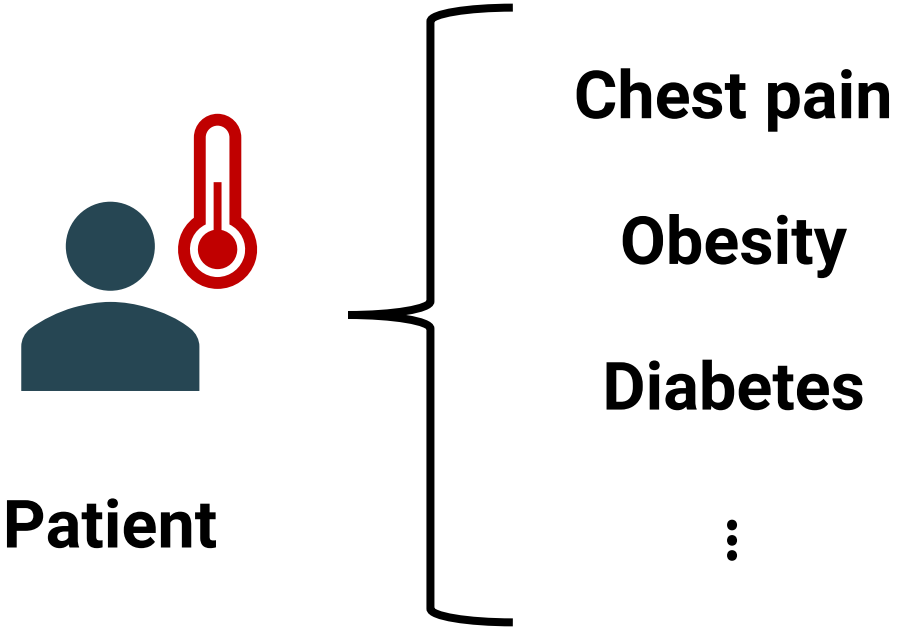
- Wang et al. (2023) used an HNN to **predict ages & cognitive functions.**
  - An HNN encodes brain hypergraphs for classification.

** Specifically, they also estimated hyperedge weights with an additional loss term.*



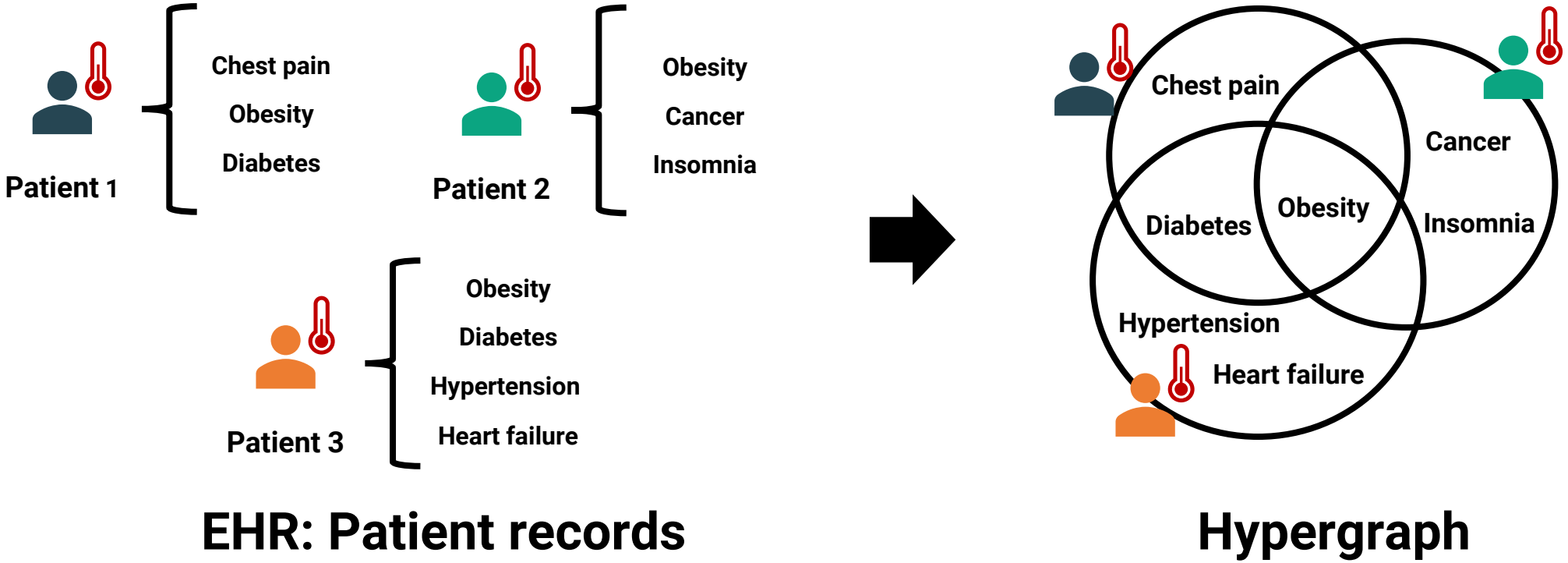
EHR: Hypergraph Construction

- **Raw data** typically include medical codes and records of each patient.



EHR: Hypergraph Construction (cont.)

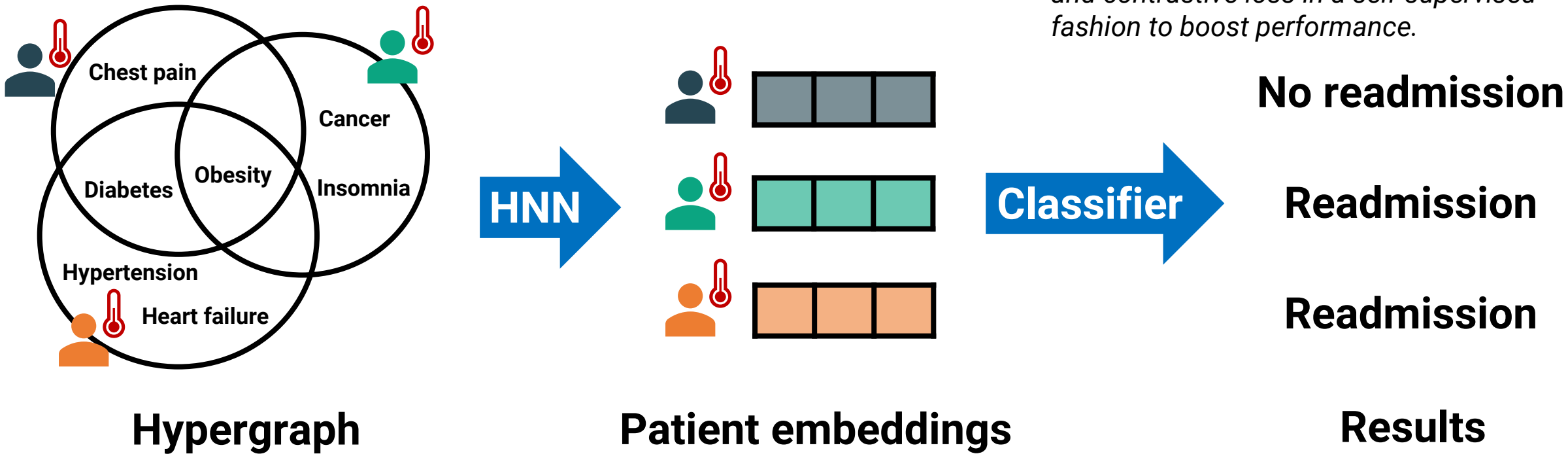
- Cai et al. (2022) converted **patient records** into a hypergraph.
  - A node is a medical code; a hyperedge is each patient visit.



EHR: Task Formulation

- Cai et al. (2022) used an HNN to **predict mortality & readmission**.
  - The HNN encodes hyperedges for their classification.

** Specifically, they leveraged multiple views and contrastive loss in a self-supervised fashion to boost performance.*



What are Notable Applications of HNNs? (cont.)

- In the following domains, we will cover how the issues have been addressed:

Recommender system

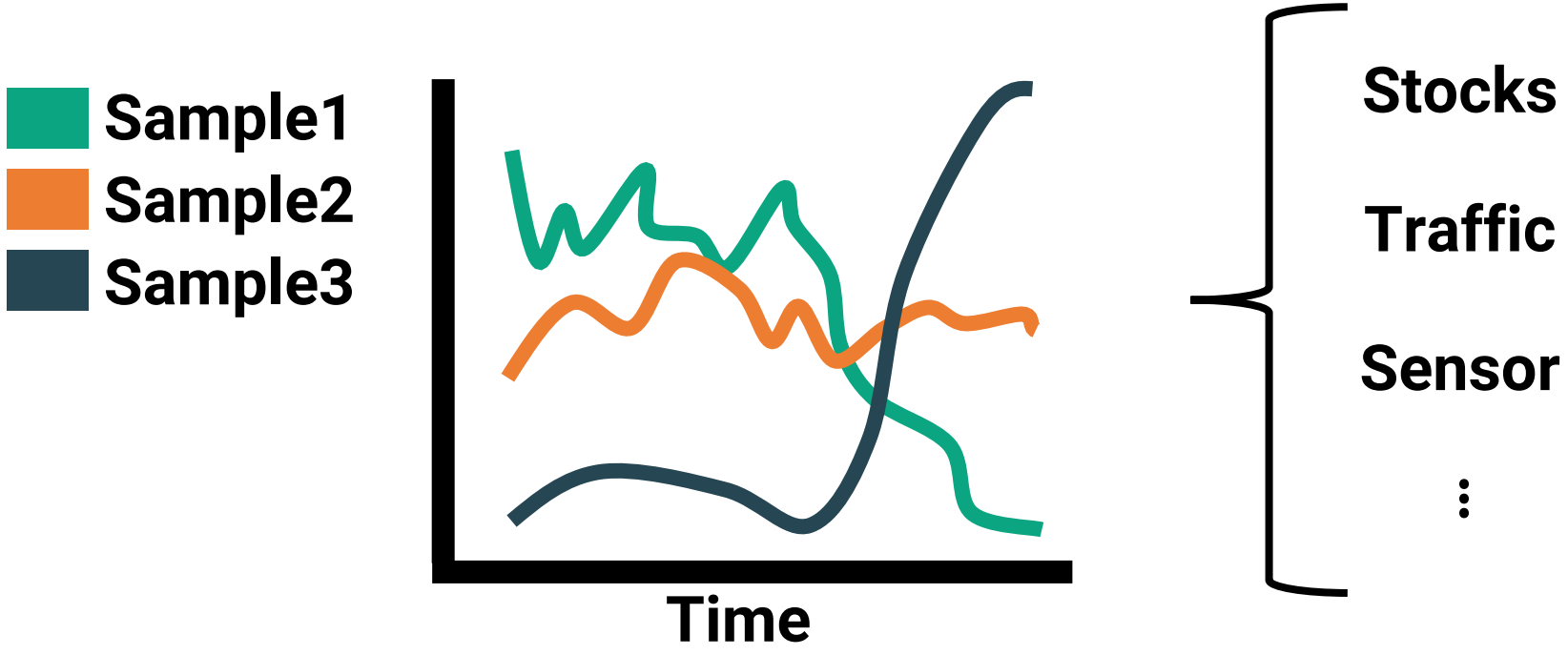
Bioinformatics & Medical science

Time series analysis

Computer vision

Time Series: Hypergraph Construction

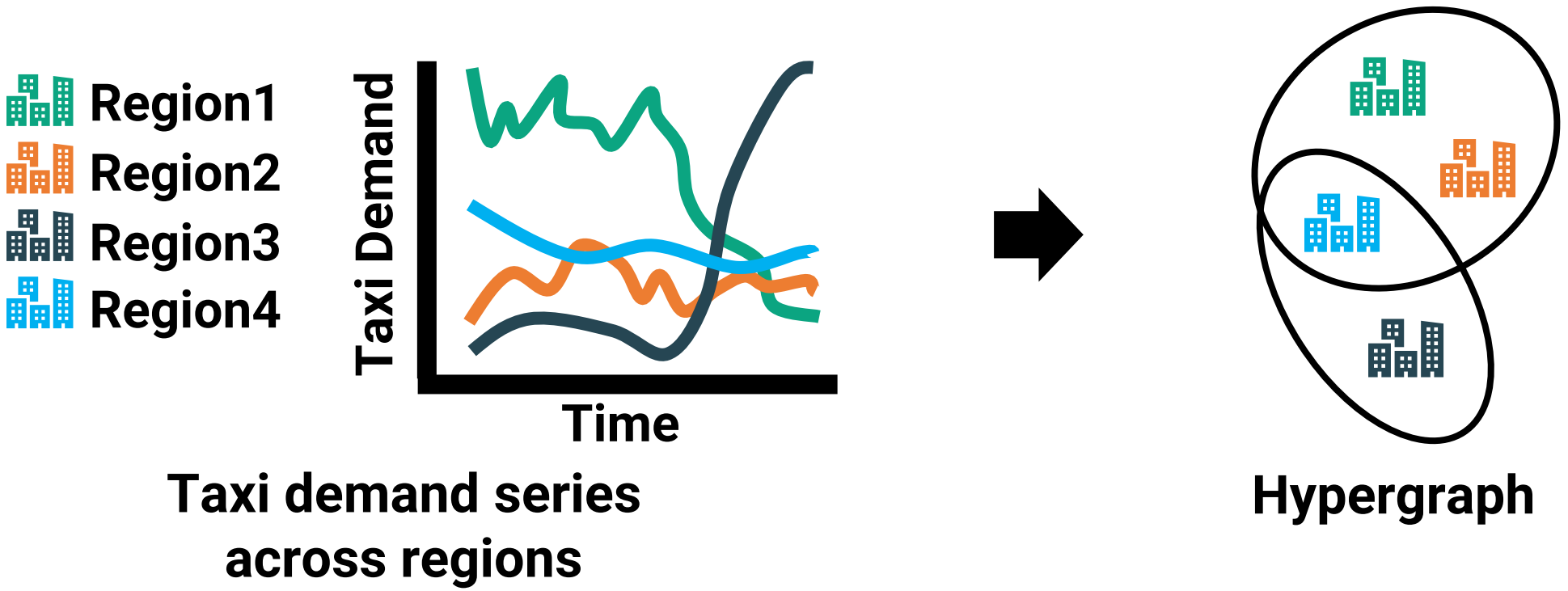
- **Raw data** typically are periodically recorded data over time.



Time series data **Examples**

Time Series: Hypergraph Construction (cont.)

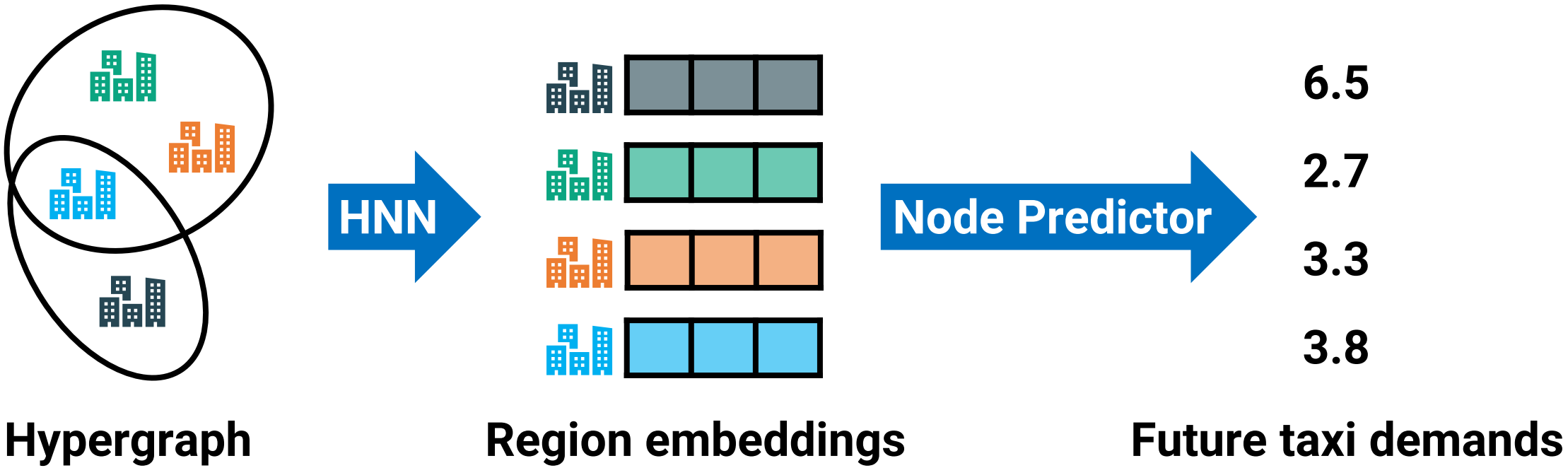
- Yi et al. (2020) converted **taxi demand** data into a hypergraph.
  - A node is a region; a hyperedge connects regions with similar taxi demand patterns (found by an algorithm).



Time Series: Task Formulation

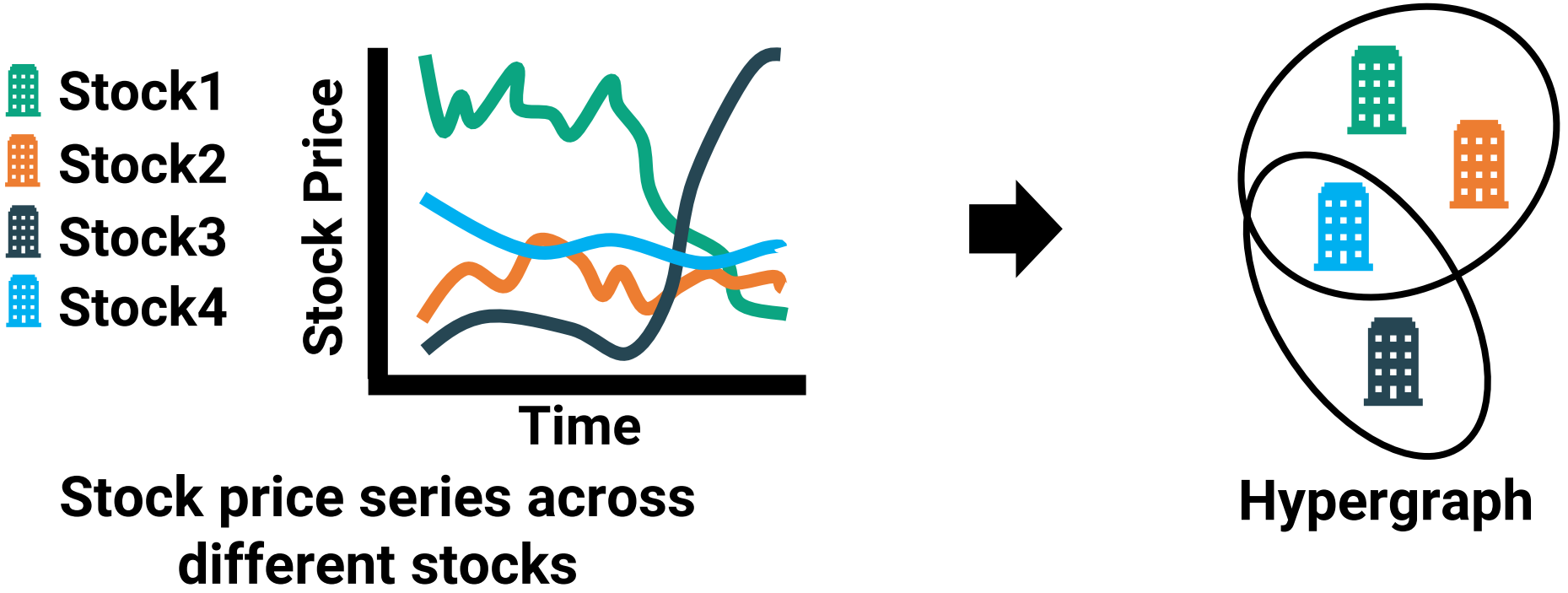
- Yi et al. (2020) used an HNN to predict **future taxi demands** in each region.
  - The HNN encodes each city to predict its future taxi demand.

** Specifically, they further used an RNN to model the temporal aspects of the series.*



Time Series: Hypergraph Construction (cont.)

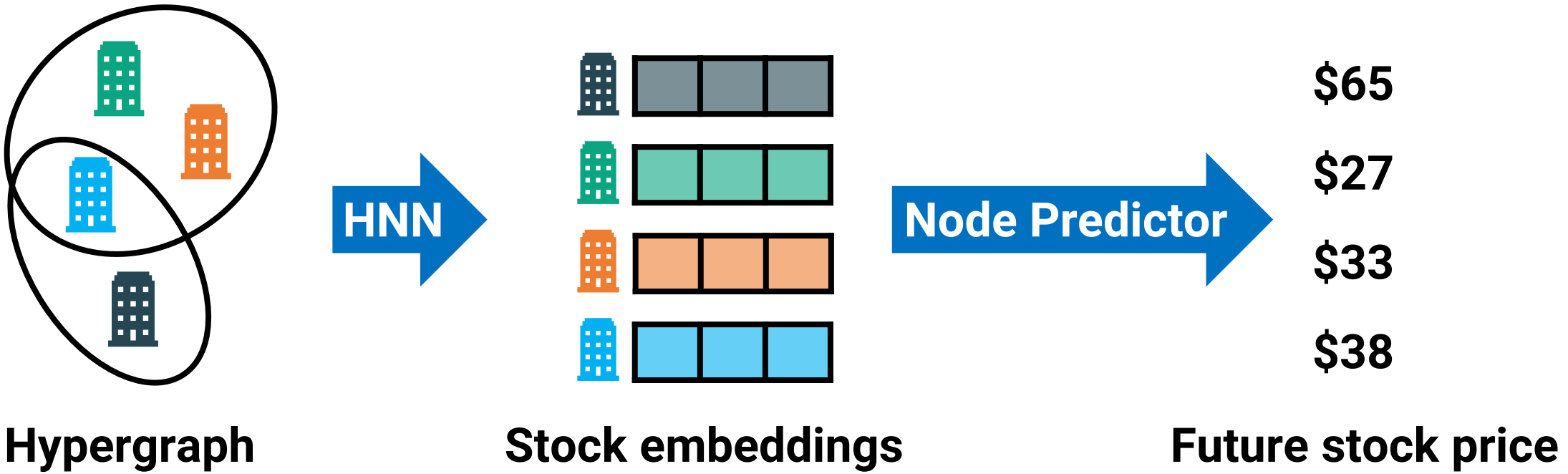
- Sawhney et al. (2021) converted **stock price** data into a hypergraph.
  - A node is a stock; a hyperedge connects stocks (i.e., companies) in the same industry or with 1st or 2nd order relations (heuristically determined).



Time Series: Task Formulation (cont.)

- Sawhney et al. (2021) used an HNN to **predict future stock price**.
  - The HNN encodes each stock to predict its future price.

** Specifically, they further used an RNN and attention to model the temporal aspects of the series.*



What are Notable Applications of HNNs? (cont.)

- In the following domains, we will cover how the issues have been addressed:

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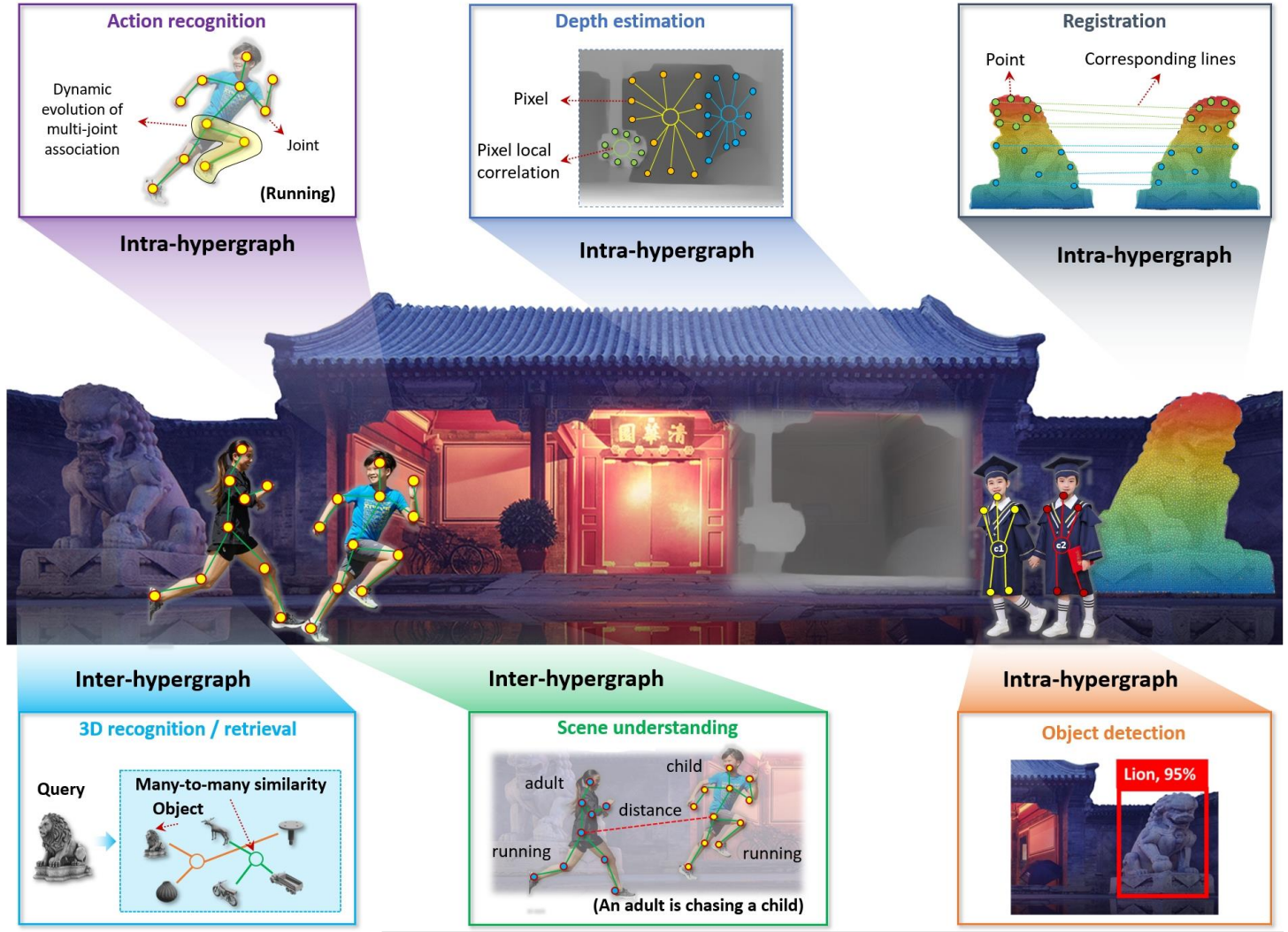
Hypergraph in Computer Vision

- Action Recognition
- Depth Estimation
- Registration
- 3D Recognition/Retrieval
- Scene Understanding
- Object Detection



Vision: Hypergraph Construction

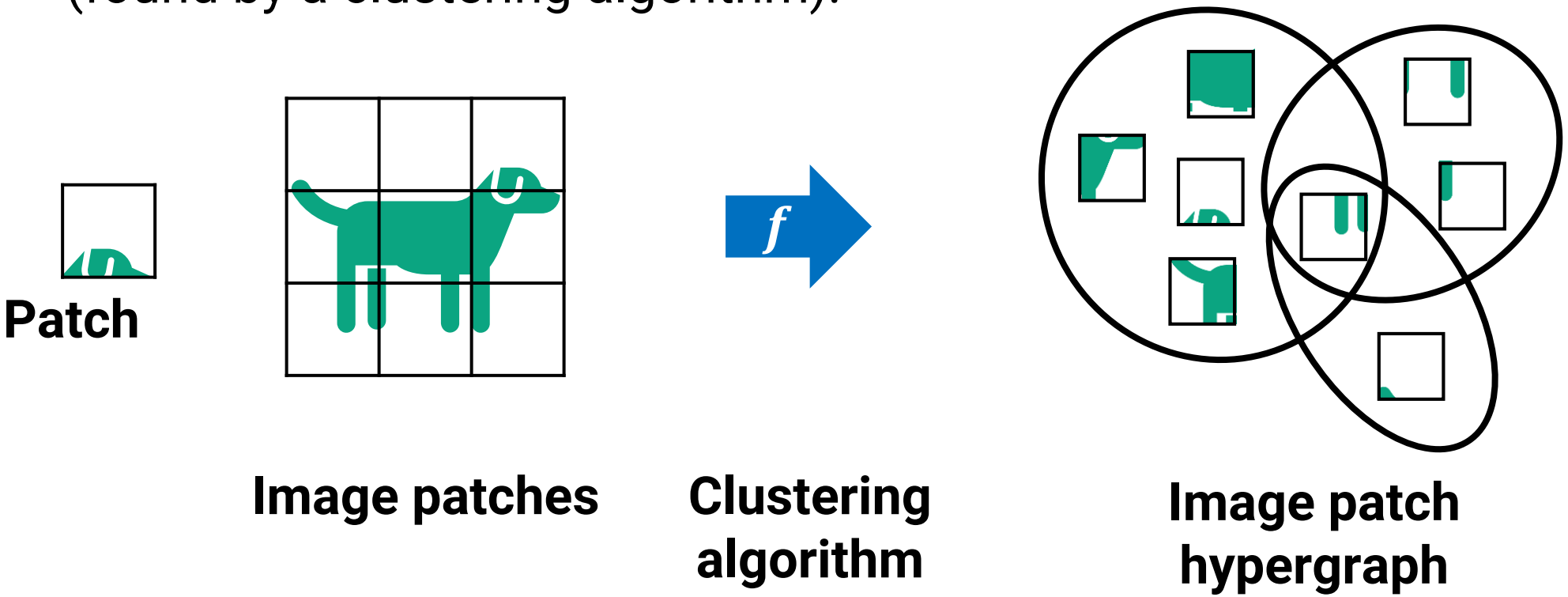
- **Raw data** typically are images in pixels or voxels.

Pixel images

Voxel images

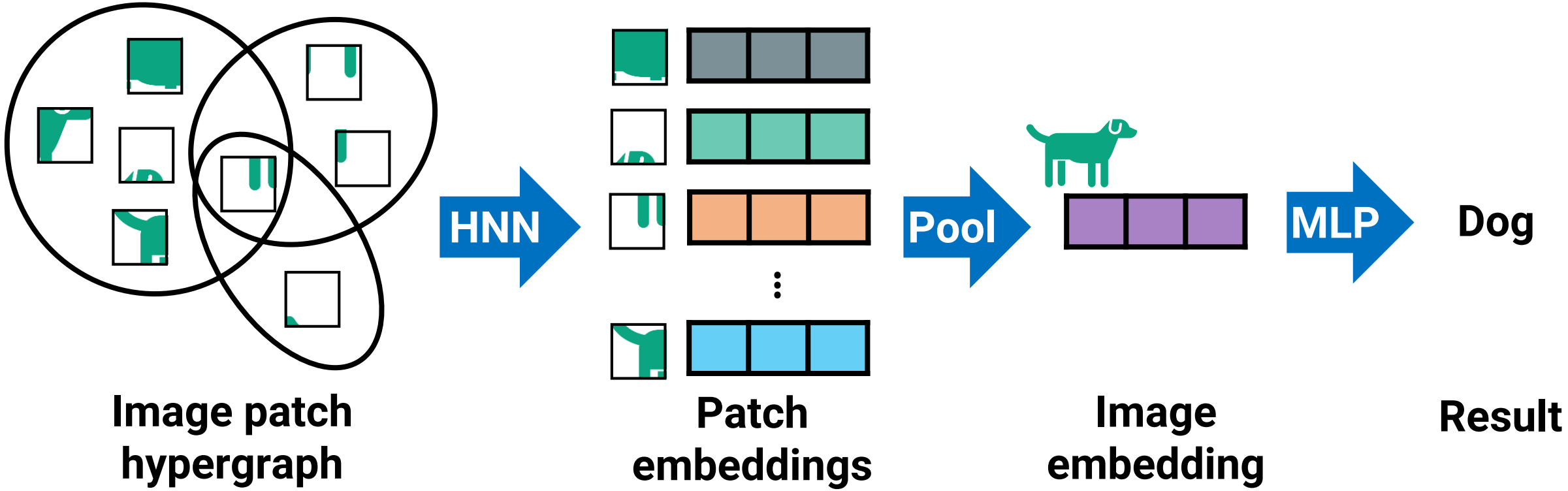
Vision: Hypergraph Construction (cont.)

- Han et al. (2023) converted **pixel image** data into a hypergraph.
  - A node is a image patch; a hyperedge connects similar patches (found by a clustering algorithm).



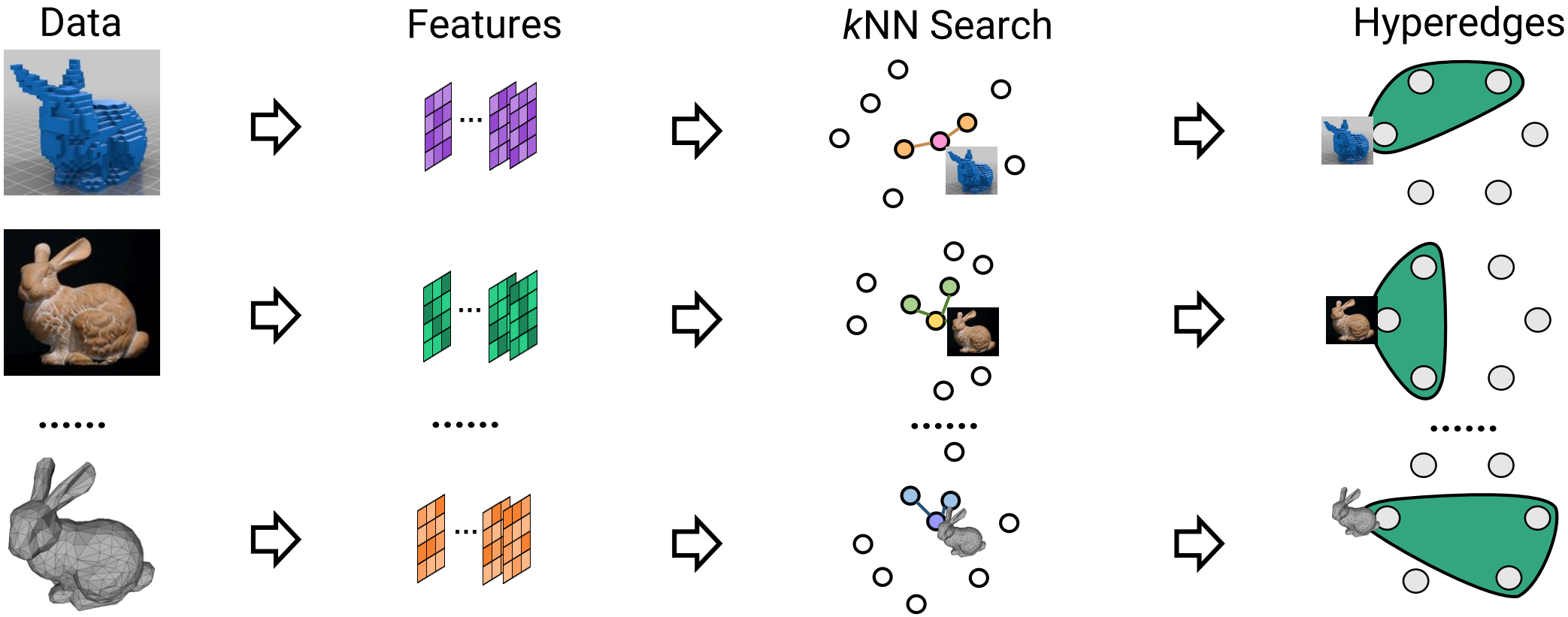
Vision: Task Formulation (cont.)

- Han et al. (2023) used an HNN to **classify** or **detect images**.
  - The HNN encodes each patch and pools them to make predictions.



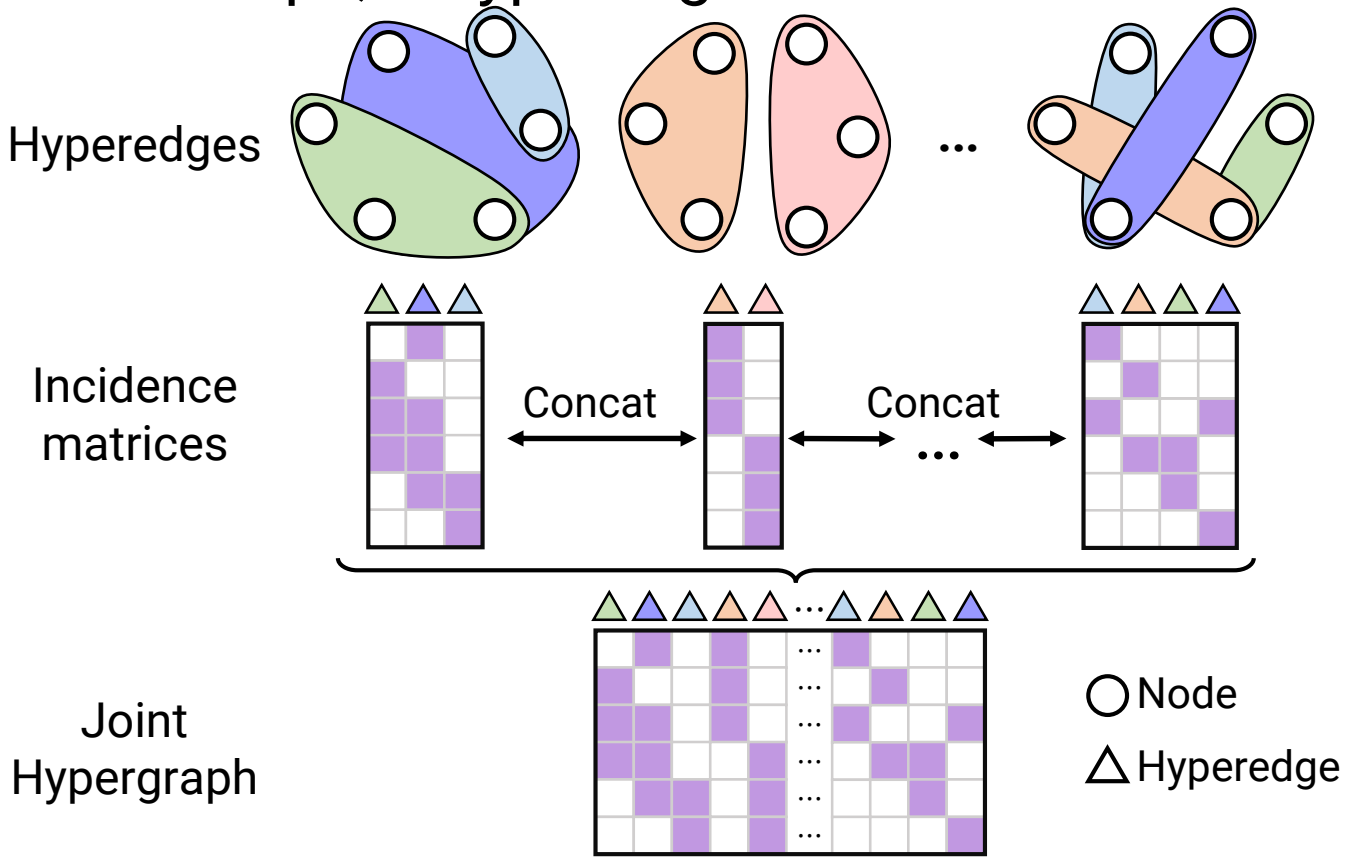
Vision: Hypergraph Construction (cont.)

- Bai et al. (2021) converted **multi-modal 3D object** into a hypergraph.
  - A node is a 3D object; a hyperedge connects the similar objects.



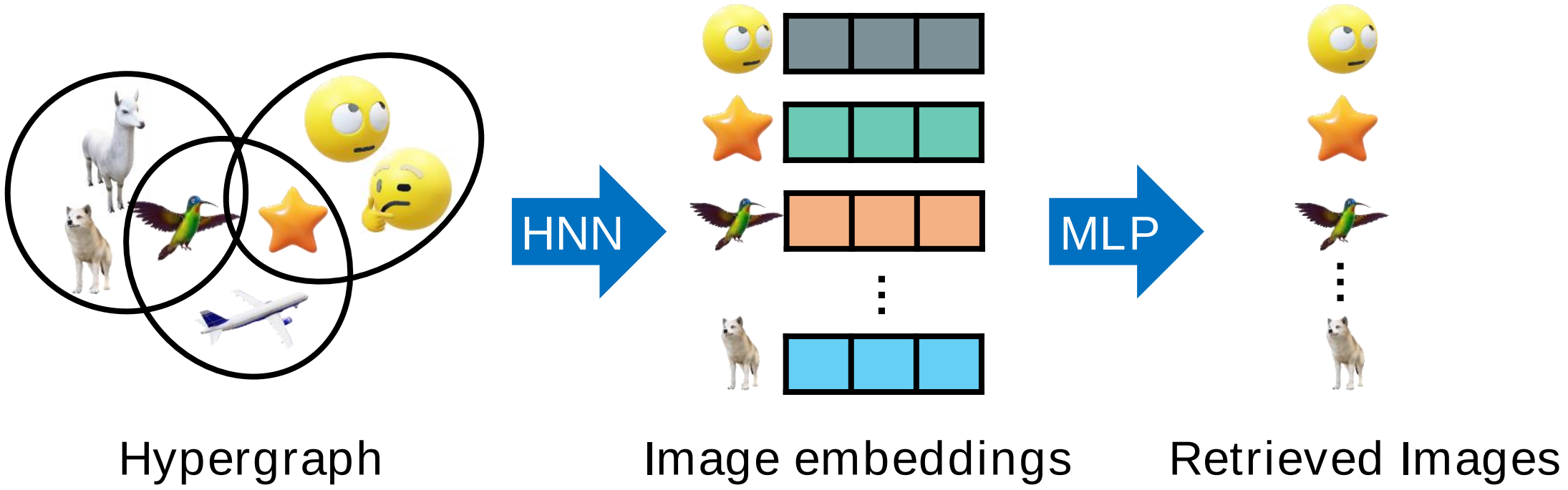
Vision: Hypergraph Construction (cont.)

- Bai et al. (2021) joined multi-scale hyperedges to the hypergraph
  - A node is a 3D shape; a hyperedge connects the similar shapes



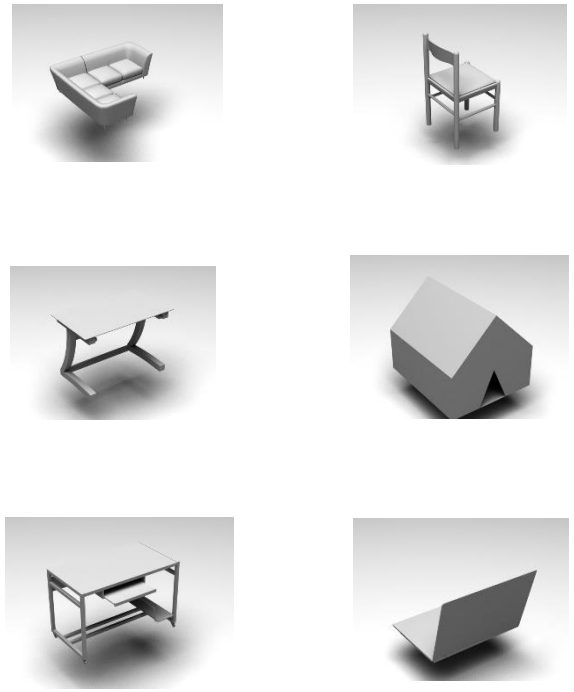
Vision: Task Formulation

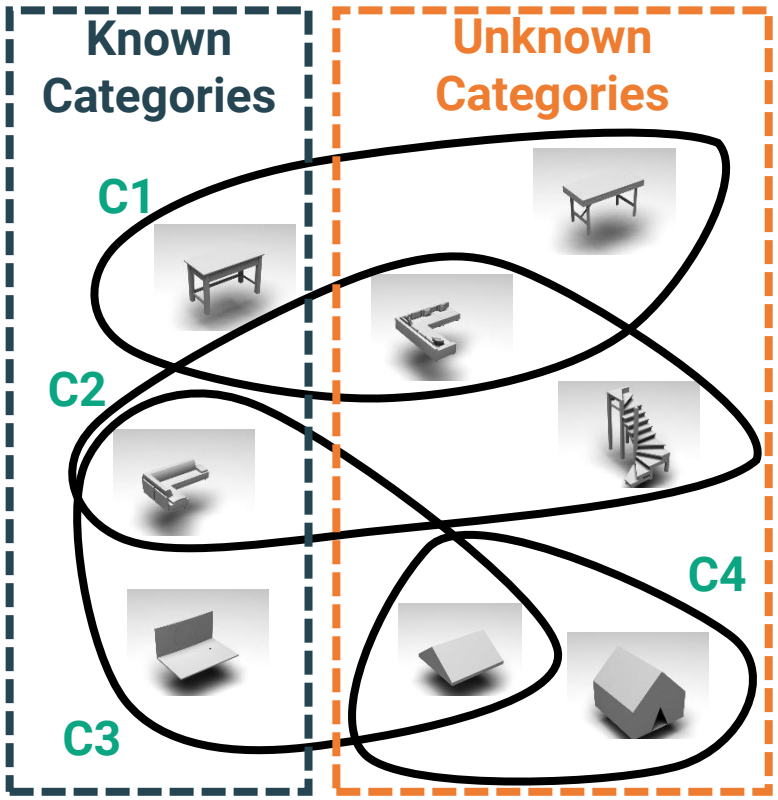
- Bai et al. (2021) used an HNN for **3D object retrieval and recognition**.
  - The HNN captures relationships among 3D objects in **multi-scale.**



Vision: Hypergraph Construction (cont.)

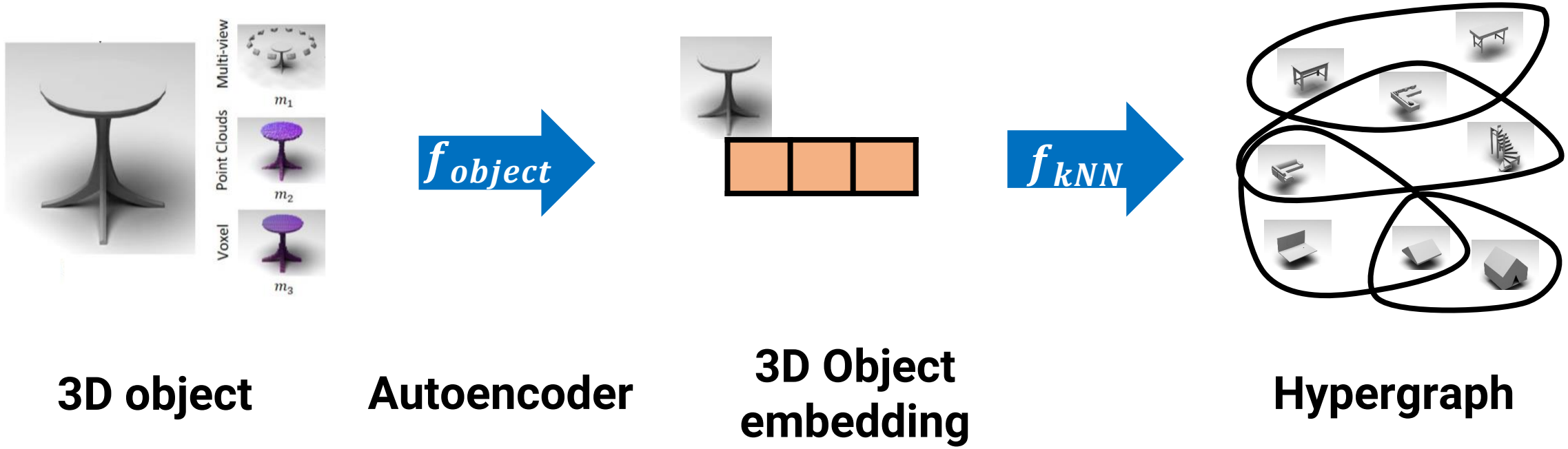
- Feng et al. (2023) converted **3D objects** into a hypergraph.
  - A node is a 3D object; a hyperedge represents a category.





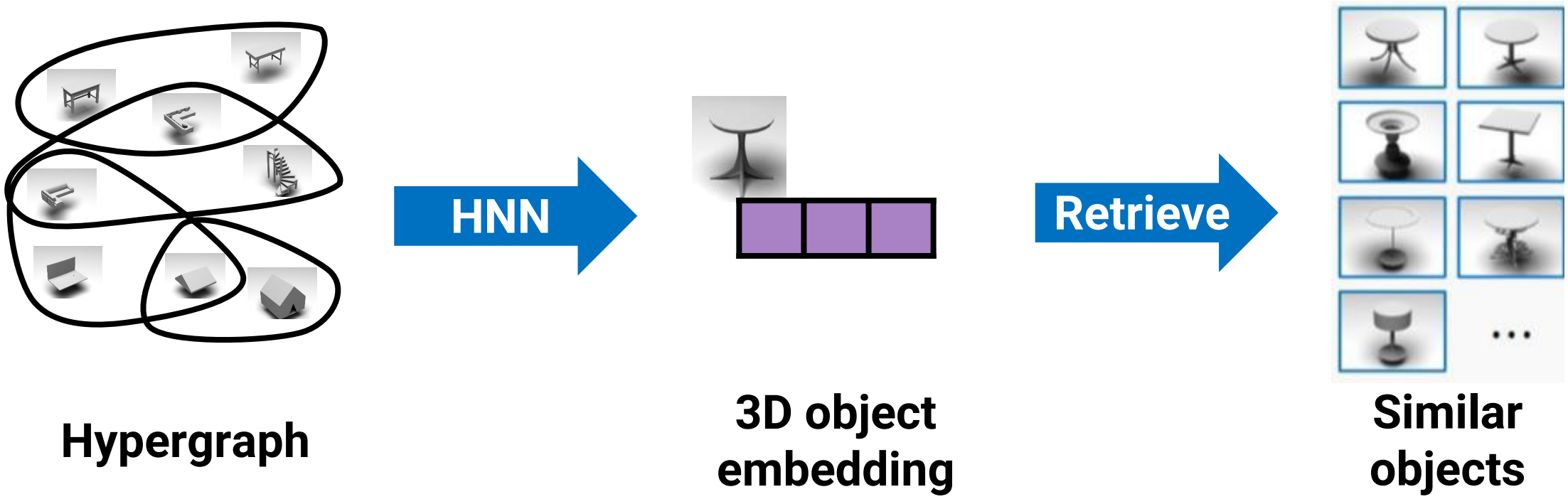
Vision: Hypergraph Construction (cont.)

- To find object categories (i.e., hyperedges), Feng et al. (2023) used **autoencoder**-based embedding and **kNN**-based similarity search.



Vision: Task Formulation (cont.)

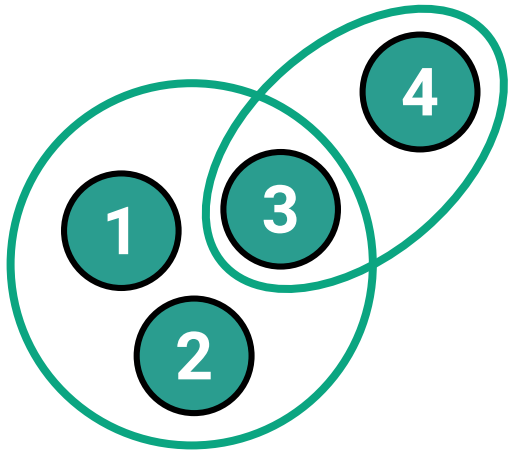
- Feng et al. (2023) used an HNN for **3D object retrieval**.
  - The HNN exploits the connections in multimodal data.



Part 5 Summary

- Two key issues include:
  - Q1) How to **express the raw data** as hypergraphs?
  - Q2) How to **formulate the learning task** for an HNN?

Raw Data



Hypergraph

Node Prediction
or
Hyperedge Prediction

Learning Task Formulation

Part 5 Summary (cont.)

- We covered how the issues have been addressed in:

Recommender system

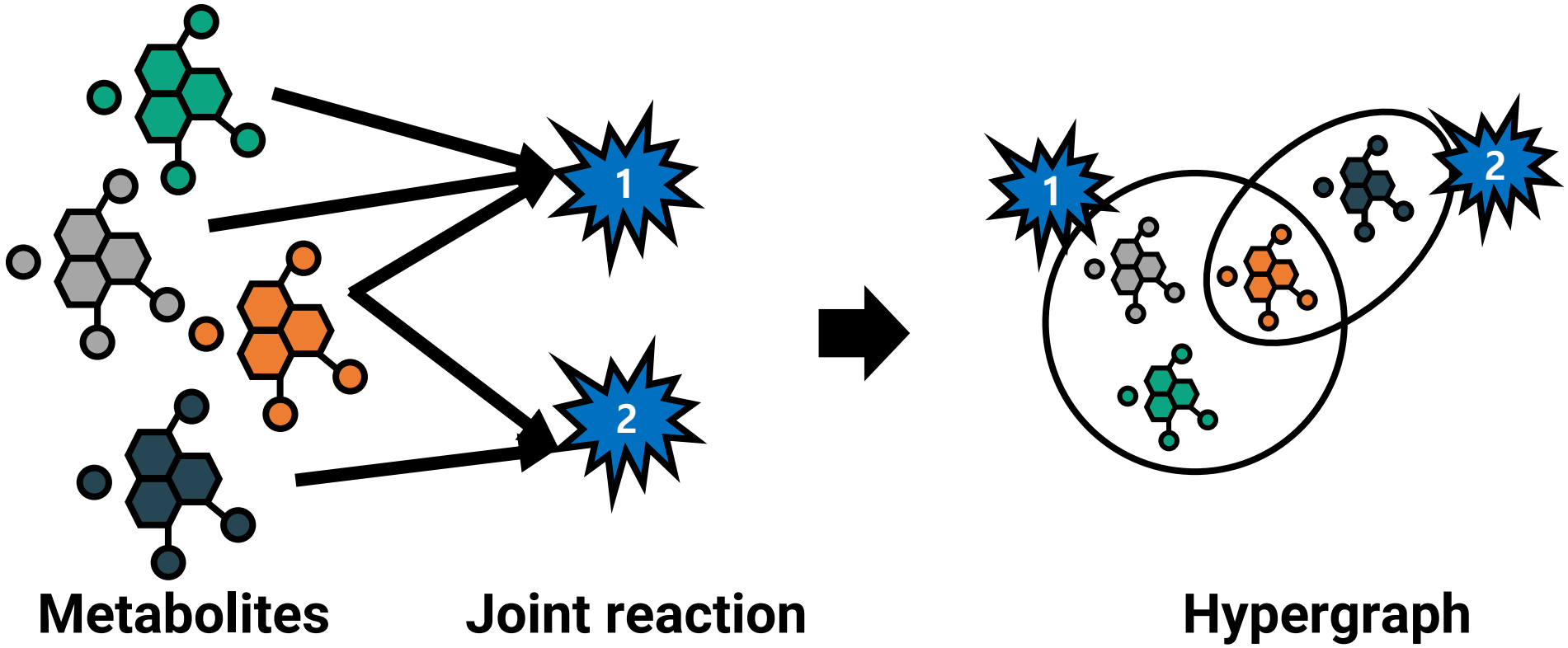
Bioinformatics & Medical science

Time series analysis

Computer vision

Part 5 Summary (cont.)

- After determining the nodes, hyperedges were constructed often by
  - 1) **Domain knowledge** or 2) similarity search



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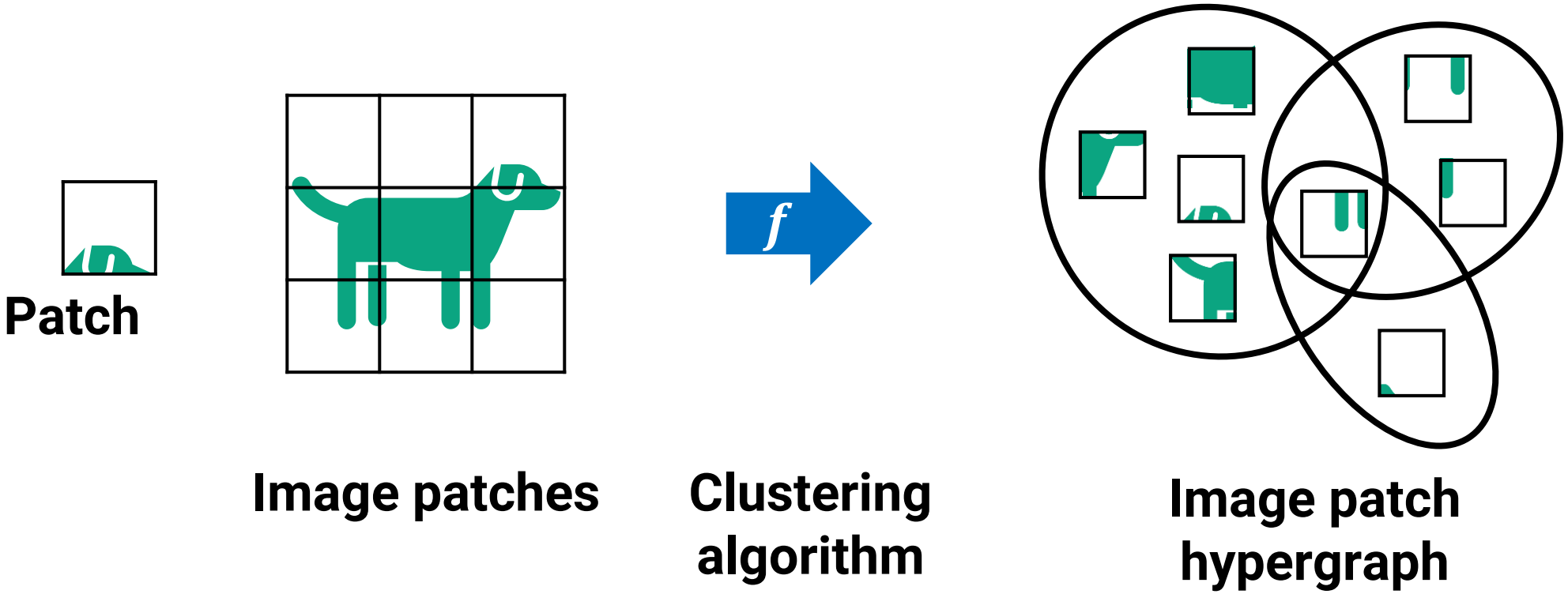
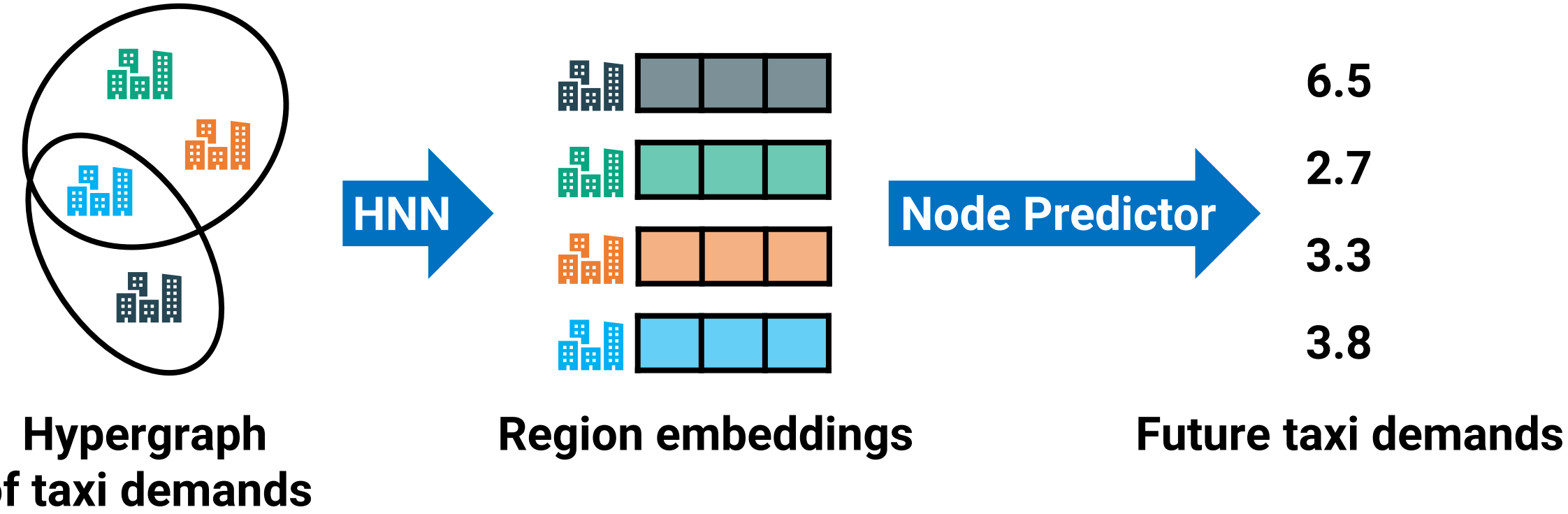


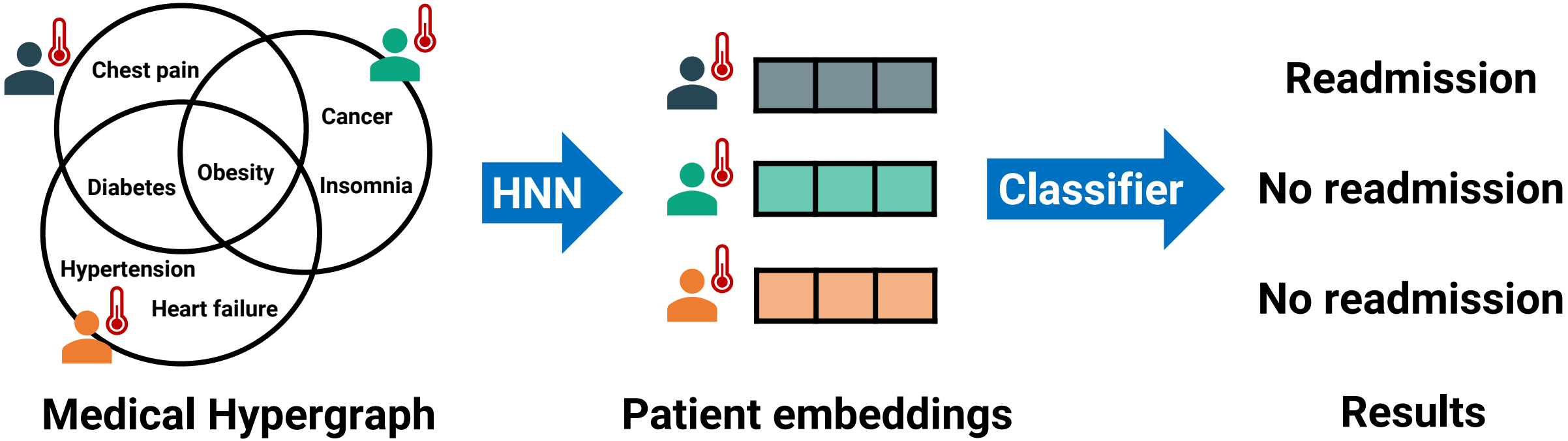
Part 5 Summary (cont.)

- After constructing the hypergraphs, HNNs often were used to predict
  - 1) **nodes**, 2) hyperedges, or 3) hypergraphs



Part 5 Summary (cont.)

- After constructing the hypergraphs, HNNs often were used to predict
  - 1) nodes, 2) **hyperedges**, or 3) hypergraphs



Part 5 Summary (cont.)

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  - 1) nodes, 2) hyperedges, or 3) **hypergraphs**