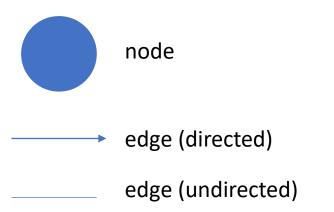
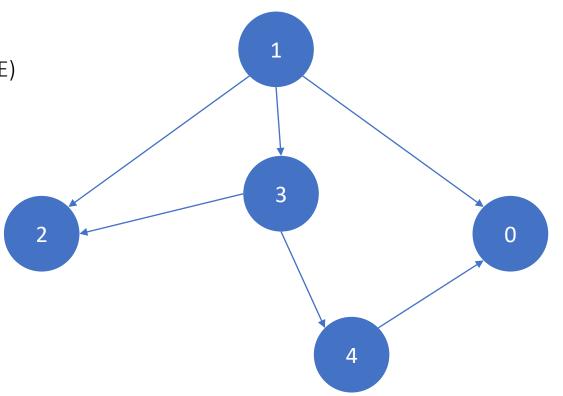
What is a Graph?

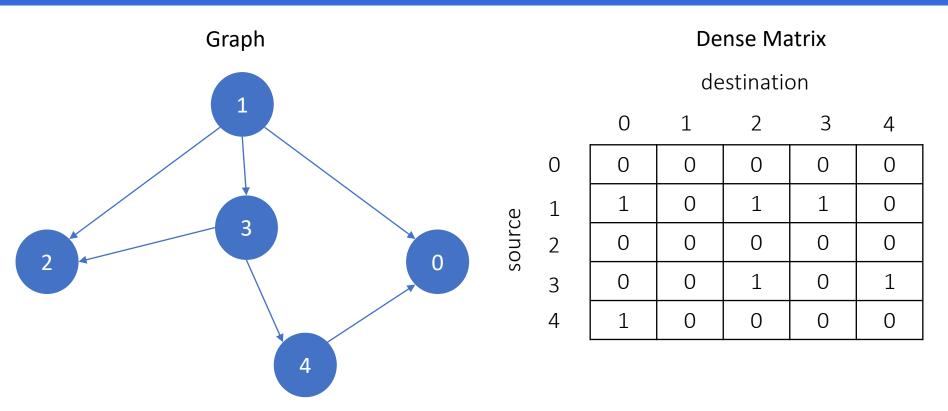
Graph

- data structure
- consists of nodes (N) and edges (E)
- \blacksquare G = (N, E)
- directed vs. undirected Graph

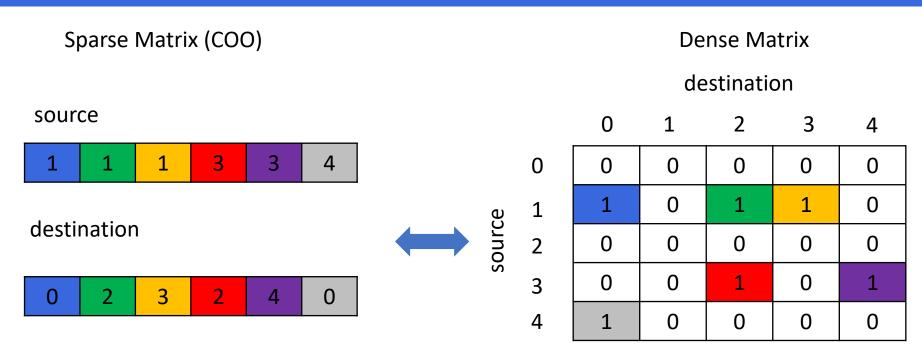




Graph Formats – Dense Matrix



Dense and Sparse Matrix



Dimensions: 2 vectors with # of edges

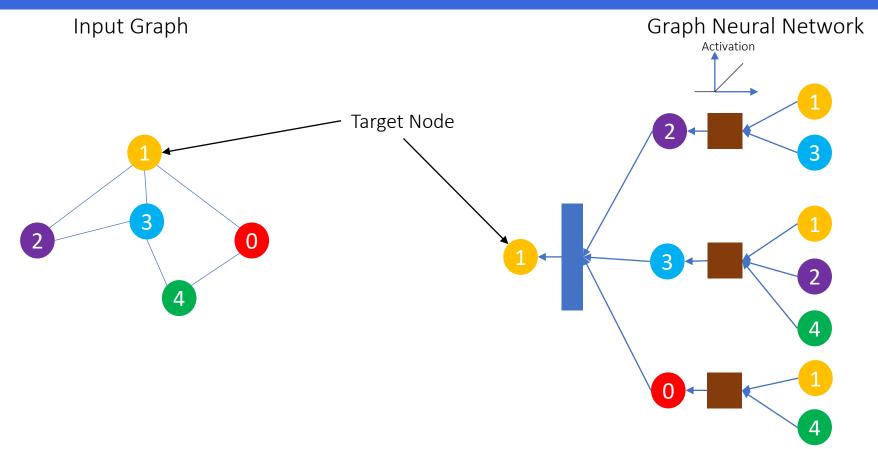
Dimension: #nodes x #nodes

What are GNNs?

Neural Network Architecture

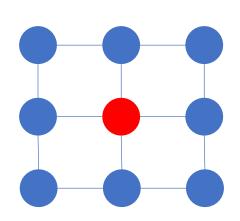
- combine deep learning and graph theory
- suitable for Graphs
- help analyzing graphs
- understand relationships between objects
- create predictions

How do GNNs work?

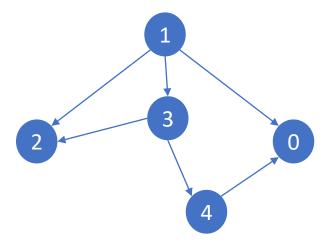


GNNs and CNNs

- lots of similarities with Convolutional Neural Networks (CNN)
- CNNs very useful for computer vision
- CNNs suitable for images (euclidean space), but not for graphs (non-euclidean space)



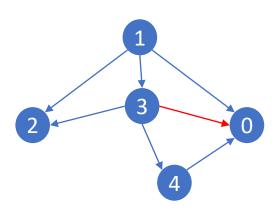
Euclidean Space



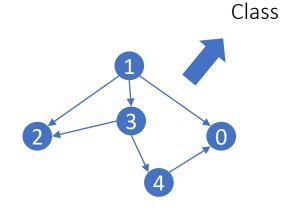
Non-Euclidean Space

Applications

Link Prediction

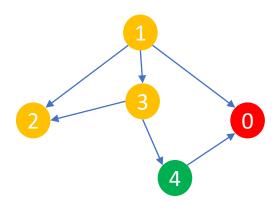


predict link between nodes **Graph Classification**



- predict graph class
- e.g. text classification, social network analysis

Node Classification



predict node class

Advantages / Disadvantages



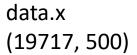
- learn representations of nodes / edges and capture complex relationships
- can be used to predict graphs with varying sizes and structures
- applicable to different tasks like node classification, link prediction, graph classification, and more
- model real-world systems like social networks, recommender systems, or drug discovery

- usually shallow networks and thus not suitable for very large datasets
- changing graph structure might require frequent re-training
- computationally expensive
- require significant training data
- can suffer from overfitting, especially on noisy or very sparse data
- still very new → more standardization required, more architectures, metrics

Coding

- PubMed dataset
- consists of 19.717 scientific publications
- diabetes classified into three classes
- 88.648 edges
- 500 features
- Task: predict node class







data.edge_indices (2, 88648)



data.y (19717)