

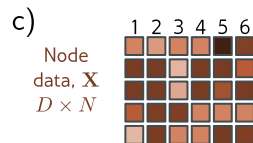
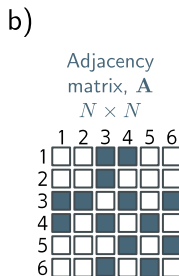
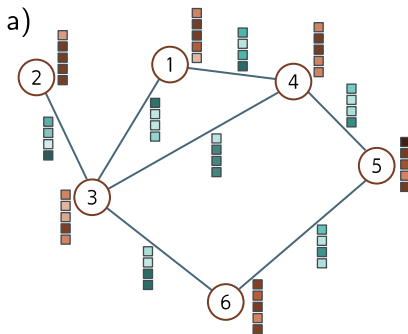
# Graph Neural Networks

Motivation

Dr. Alireza Aghamohammadi

# What are Graph Neural Networks?

- ❖ Graph Neural Networks (GNNs) integrate graph structures with deep learning techniques.
- ❖ They enable learning and representation of information from graph data, including nodes, edges, and their features.
- ❖ GNNs are particularly powerful for handling large-scale graph datasets.



## Permutation Invariance in Graphs

- ❖ In graphs, node indexing is arbitrary, meaning the structure of the graph remains unchanged under reordering.
- ❖ Permuting node indices modifies the node feature matrix  $X$  and the adjacency matrix  $A$ :
  - ❑ Columns of  $X$  are rearranged.
  - ❑ Both rows and columns of  $A$  are permuted.
- ❖ This reordering can be expressed using a *permutation matrix*  $P$ , where each row and column has exactly one entry equal to 1, and all other entries are 0.
- ❖ Mathematically, a permutation can be applied as follows:

$$X' = XP,$$

$$A' = P^T AP,$$

where post-multiplying by  $P$  permutes the columns, and pre-multiplying by  $P^T$  permutes the rows.

# Applications of Graph Neural Networks

- ❖ Recommendation Systems
- ❖ Drug Discovery and Molecular Analysis
- ❖ Mechanical Reasoning
- ❖ Code Completion