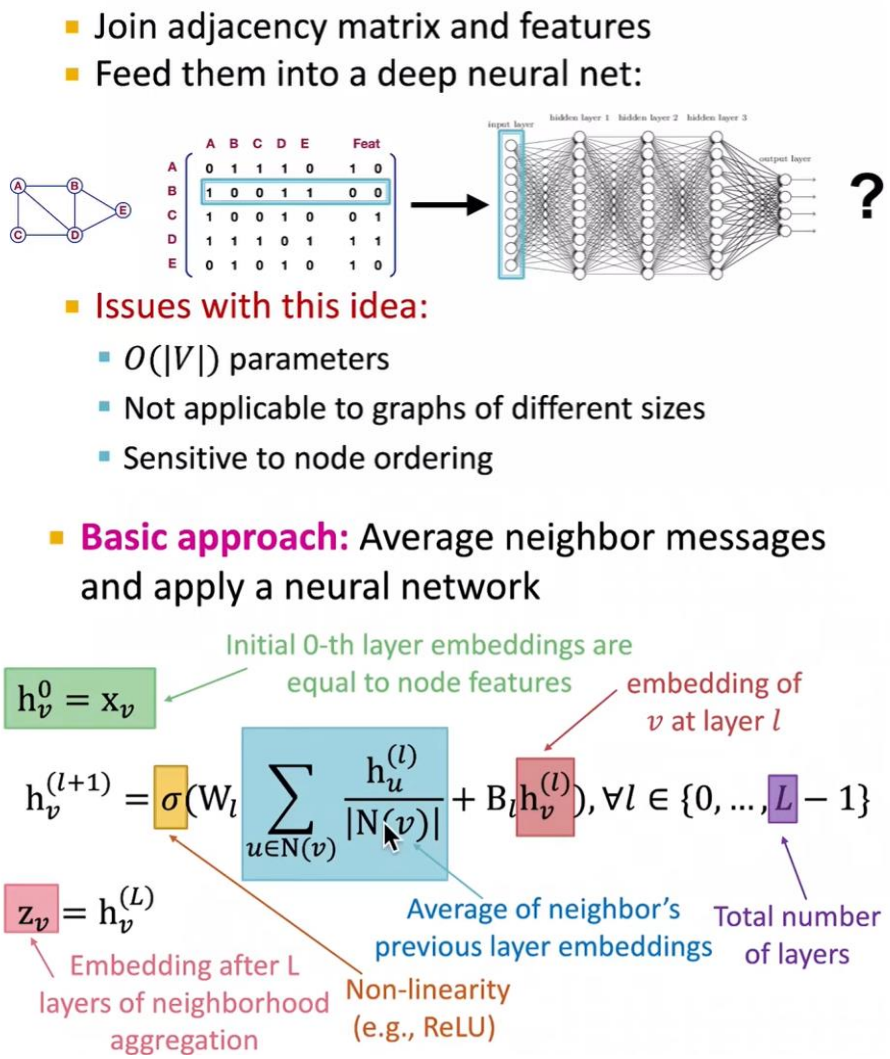
3. Graph Neural Network

- How is node and graph classification done?



The goal of this process is to learn the W and B weights, which are common among different nodes but dedicated to each layer. Note that the initial emmbedings are equal to node features.

- Message passing

The idea behind message passing is to allow nodes to communicate with their neighboring nodes by exchanging information through the edges. This information exchange is often referred to as "messages."

- Each node aggregates messages from its neighbors. The messages are computed by applying a function to the features of the node and its neighbors.
- The aggregated messages are then combined with the current node's features to update the node's representation. This combined information is often referred to as the "hidden state" of the node.
- The updated node representations can then be used for downstream tasks, such as node classification or graph-level predictions.

Message aggregation is a crucial component of the message passing process in GNNs. It involves computing a summary representation of the messages received from neighboring nodes. Different methods can be used for message aggregation, and they can have a significant impact on the GNN's performance and expressive power.

- Sum aggregation: Messages are simply summed up to form the aggregated message.
- Mean aggregation: Messages are averaged to compute the aggregated message.
- Max aggregation: The maximum value among the messages is selected as the aggregated message.
- Graph-specific aggregation functions: More sophisticated aggregation functions can be used, such as attention mechanisms that assign different weights to messages based on their relevance.

- **Graph summarization:**

Graph summarization finds smaller representations of graphs resulting in faster runtime of algorithms, reduced storage needs, and noise reduction. Graph summarization algorithms often produce either summary graphs in the form of supergraphs or sparsified graphs, or a list of independent structures. Supergraphs are the most common product, which consist of supernodes and original nodes and are connected by edges and superedges, which represent aggregate edges between nodes and supernodes.

The primary goal of **graph pooling** is to create a more compact representation of a graph, which can be particularly beneficial when dealing with large graphs that might be computationally intensive to process. Graph pooling methods aim to achieve this reduction in graph size while preserving important graph characteristics, such as connectivity patterns, neighborhood relationships, and node attributes.