Graph Neural Network

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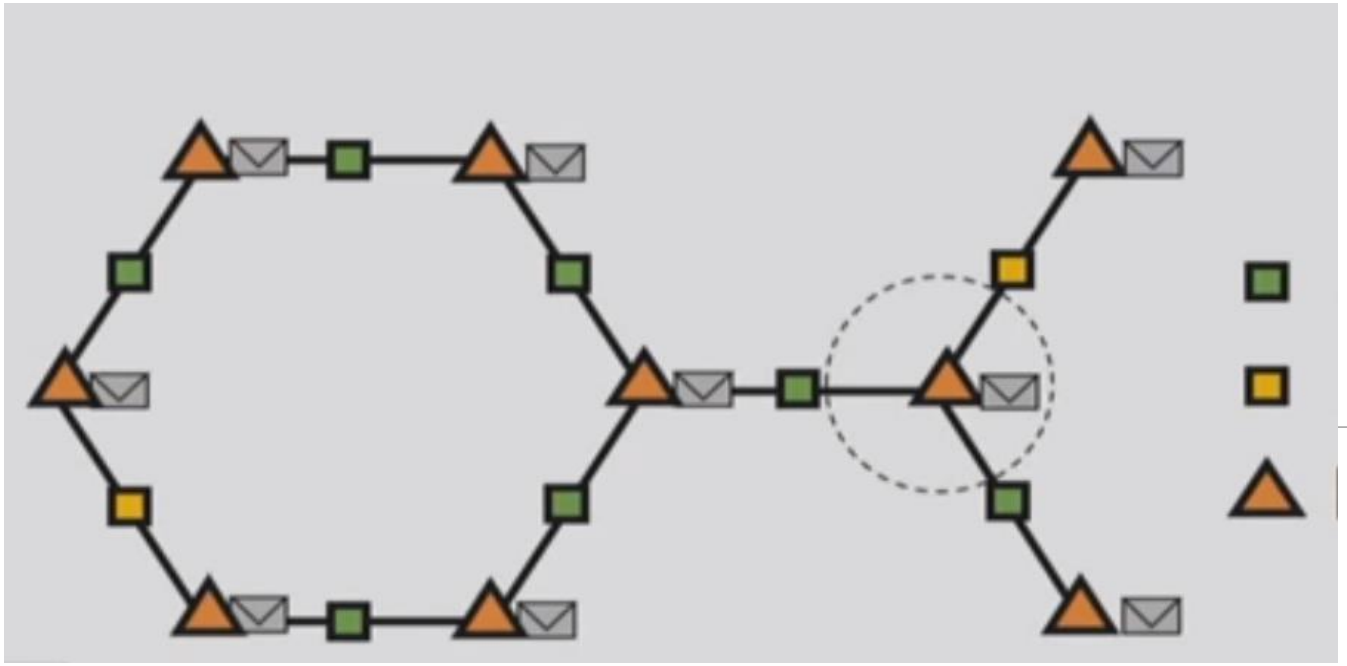
Agenda

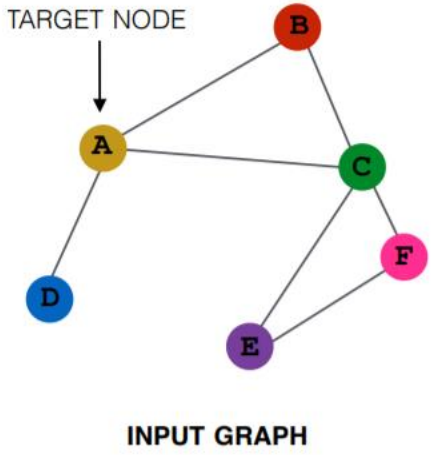
- ✓ Idea of GNN
- ✓ Overview of the model
- ✓ The Math behind GNN
- ✓ Advantages
- ✓ Applications
- ✓ How to start ?
- ✓ References

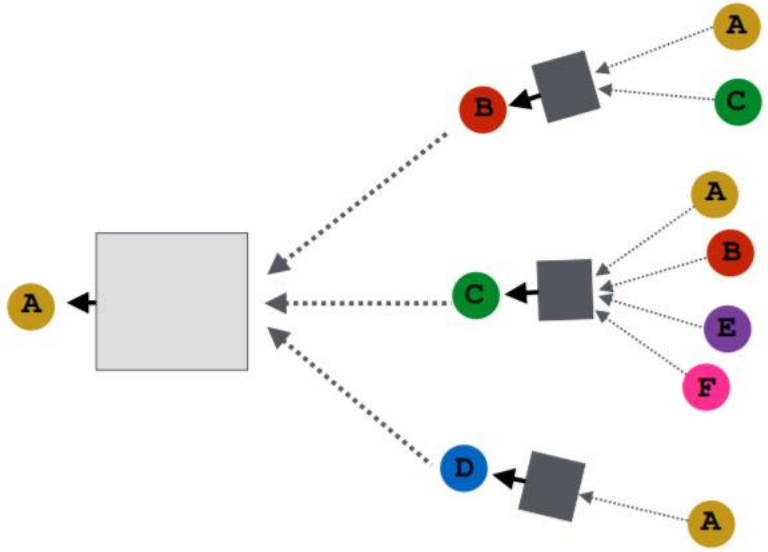


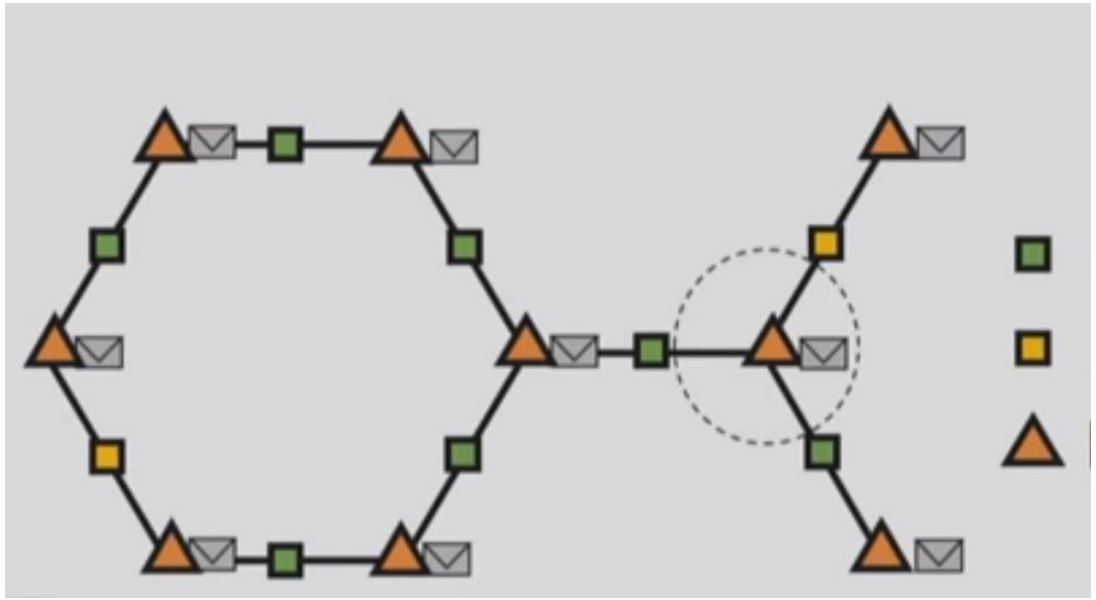
Idea of GNN

GNNs propagate information from all nodes to all neighboring nodes at each timestep.

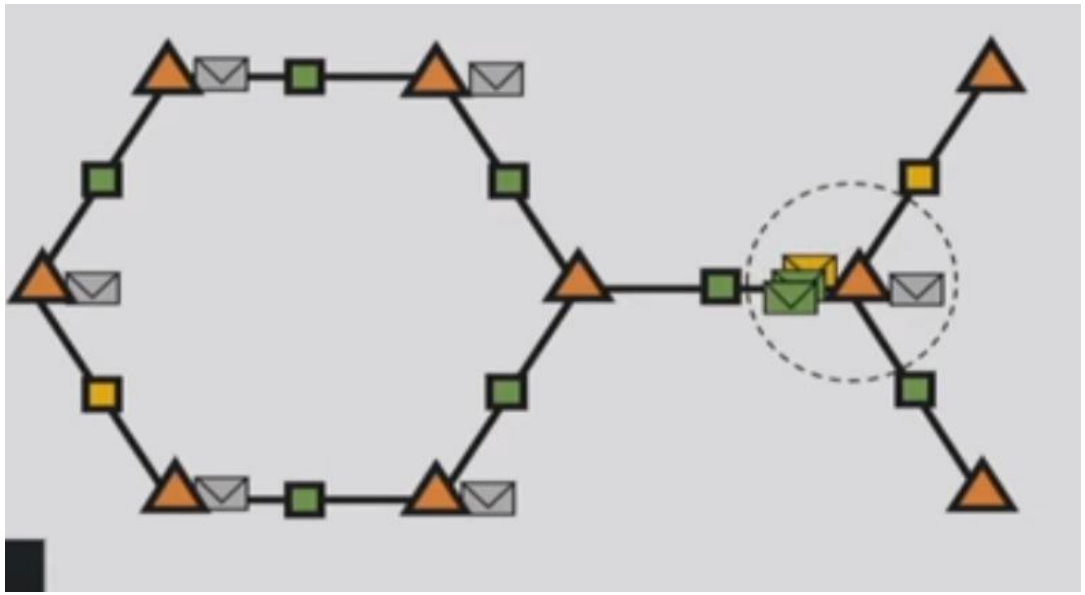
Nodes aggregate information from their neighbors using neural networks.



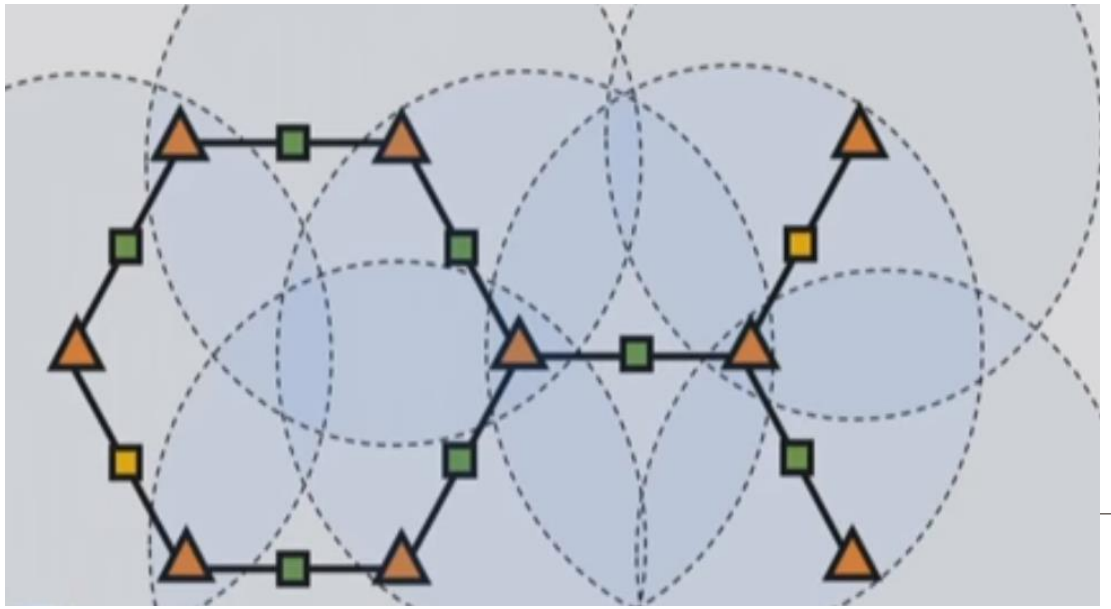




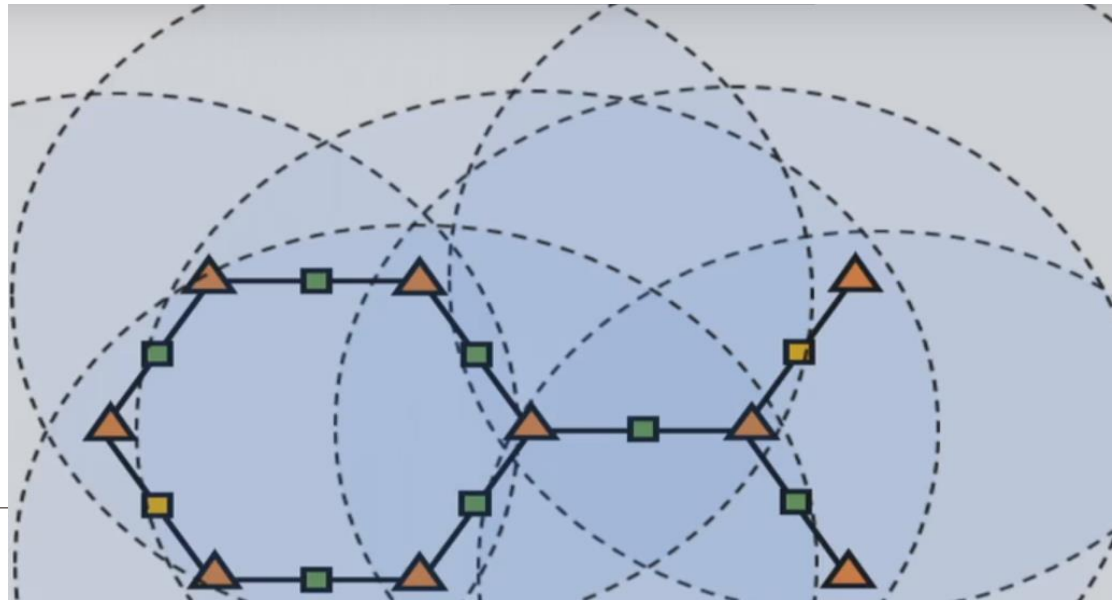
Node n in time T



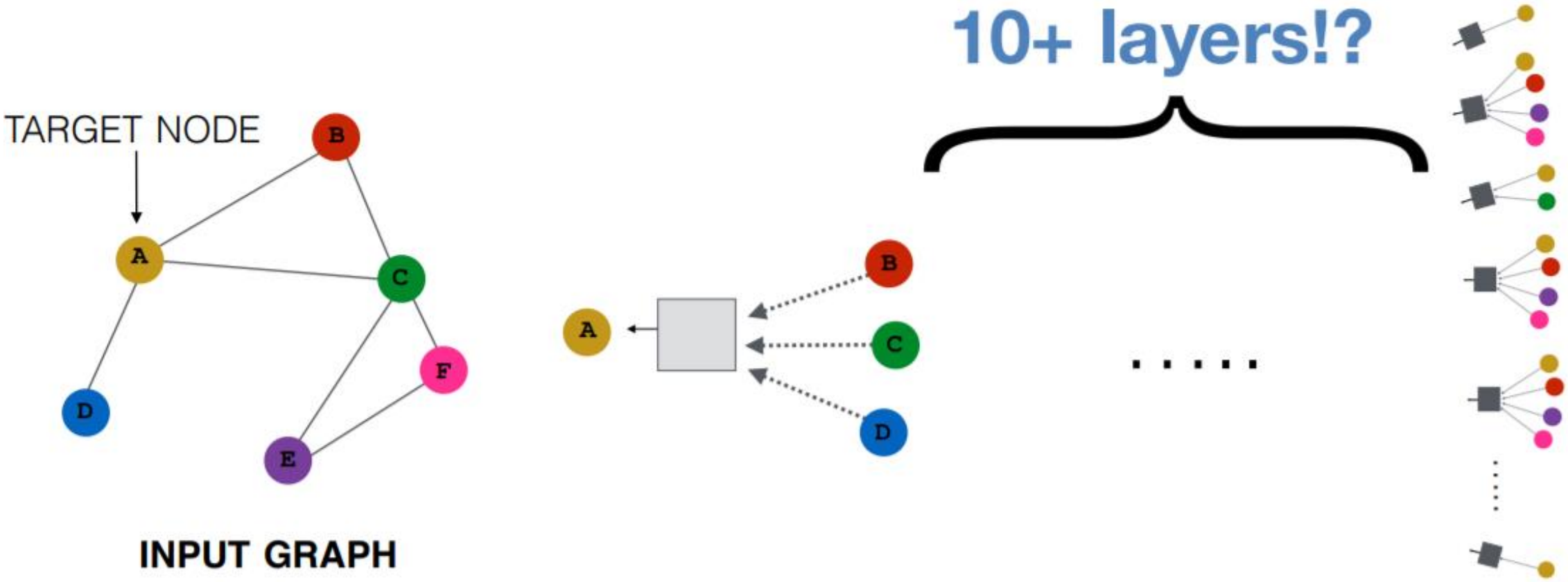
Node n is receiving msgs of T-1 from its neighbors



Information the Node n have in T



Information the Node n have in T+1


TARGET NODE
B
A
C
F
D
E
INPUT GRAPH
A
B
C
D
10+ layers!?
. . . . .

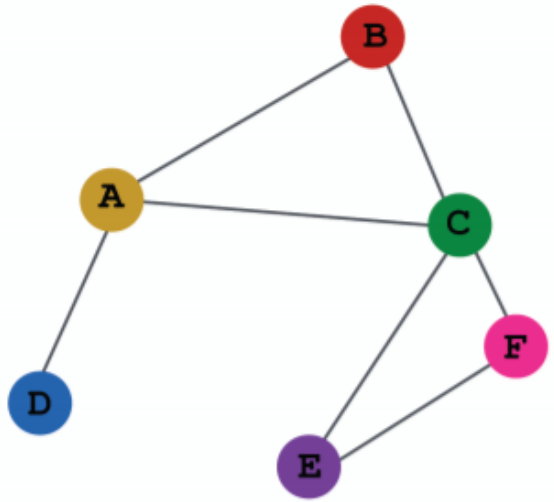
Each node in the graph take an envelop contains the feature of their neighbor

The edges represent the relationship between the connected nodes like the knowledge base.

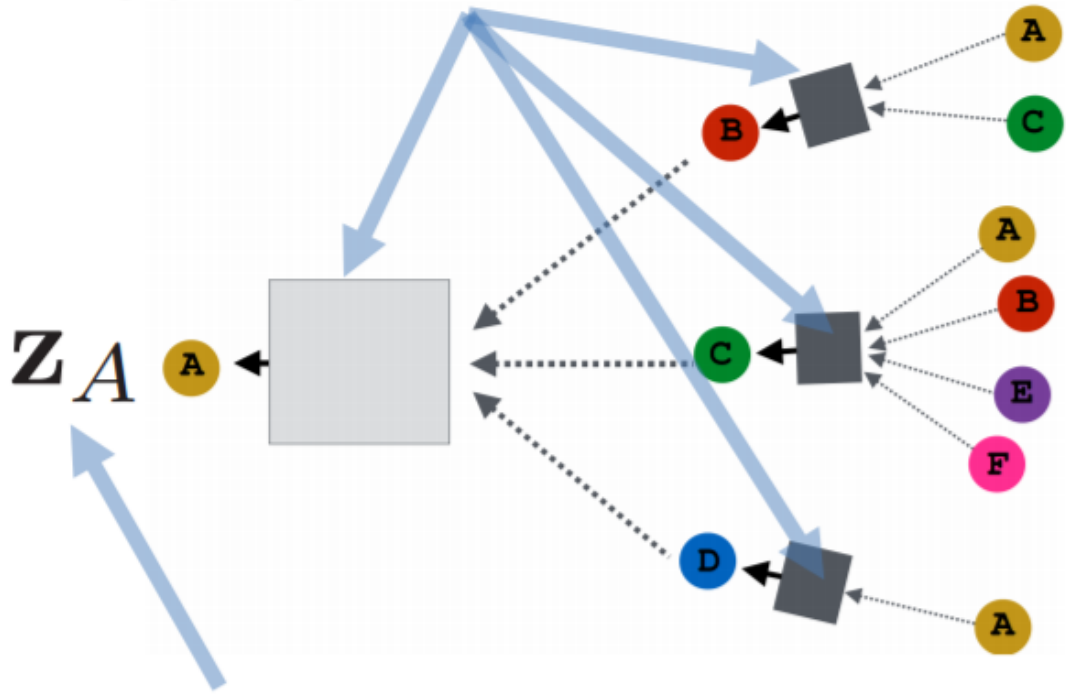
All nodes at time T get messages from their neighbors then aggregate them

Overview of the GNN

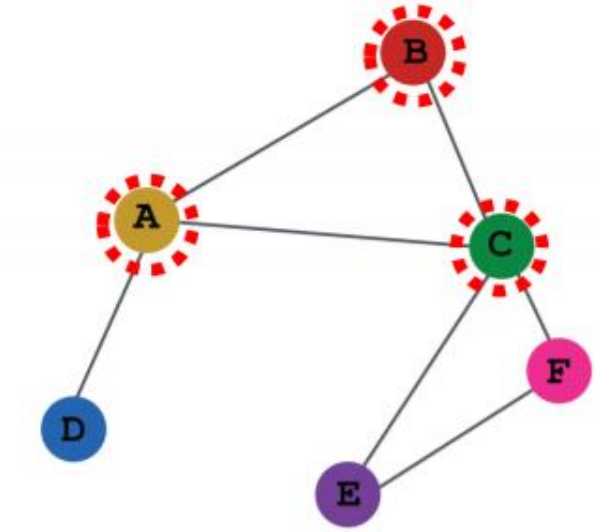
1) Define a neighborhood aggregation function.



INPUT GRAPH

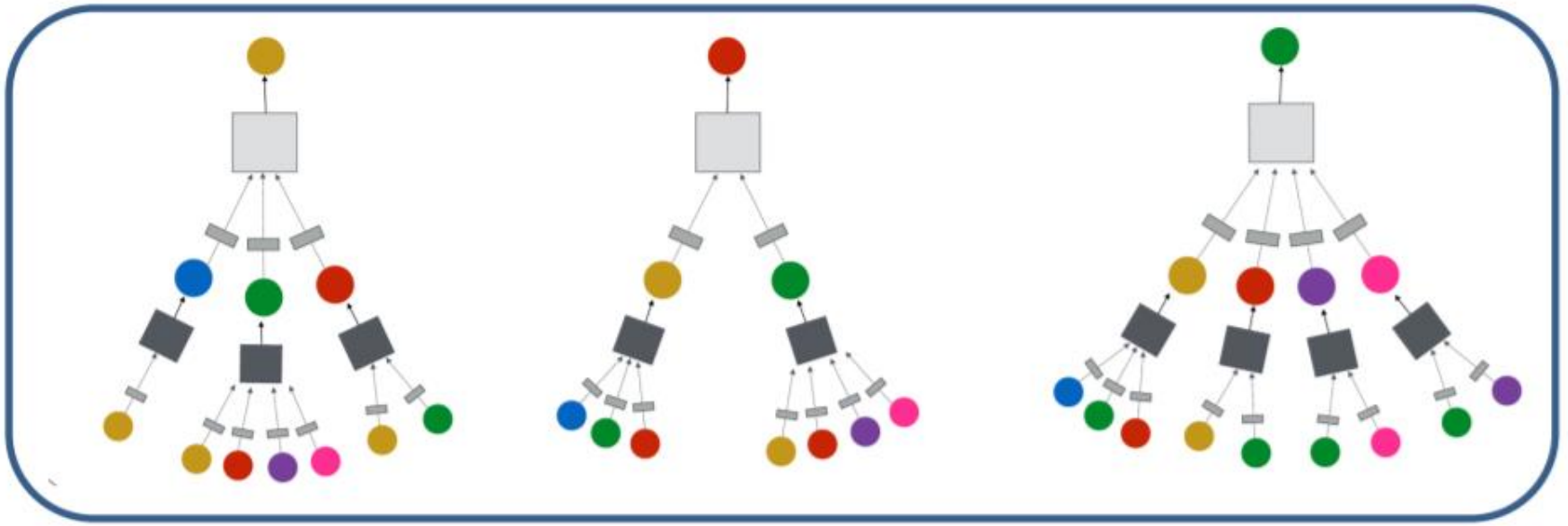


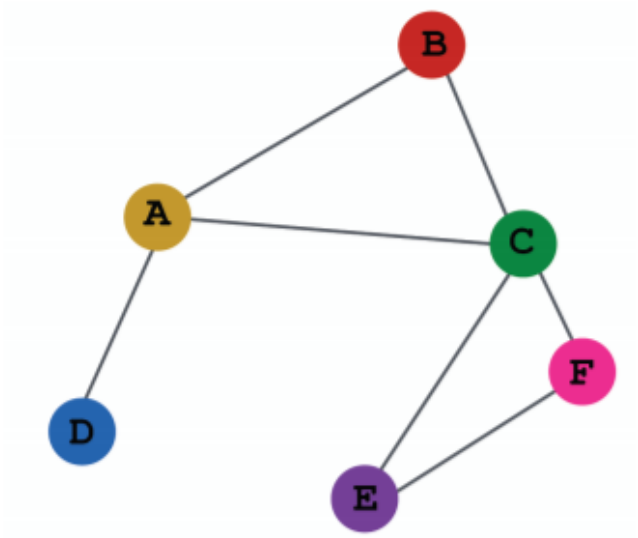
2) Define a loss function on the embeddings, $\mathcal{L}(z_u)$



INPUT GRAPH

3) Train on a set of nodes, i.e., a batch of compute graphs

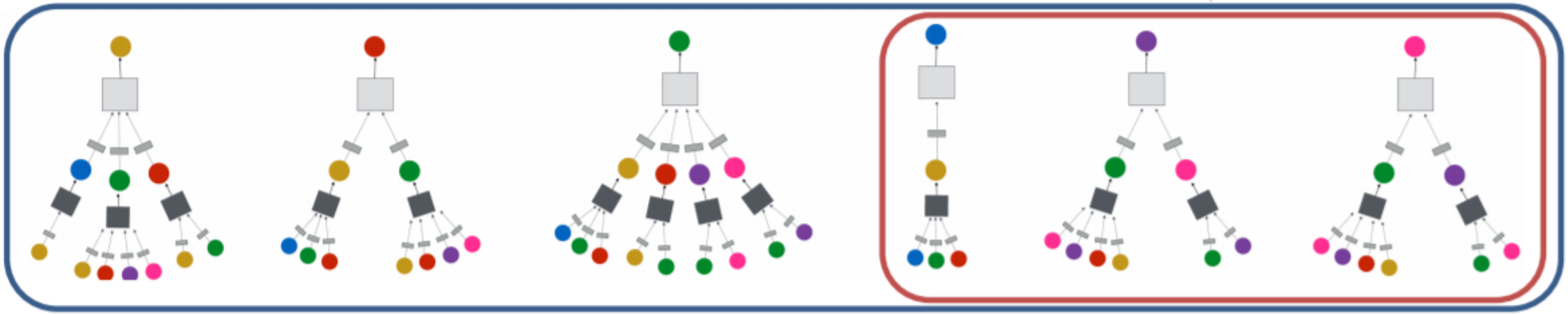




INPUT GRAPH

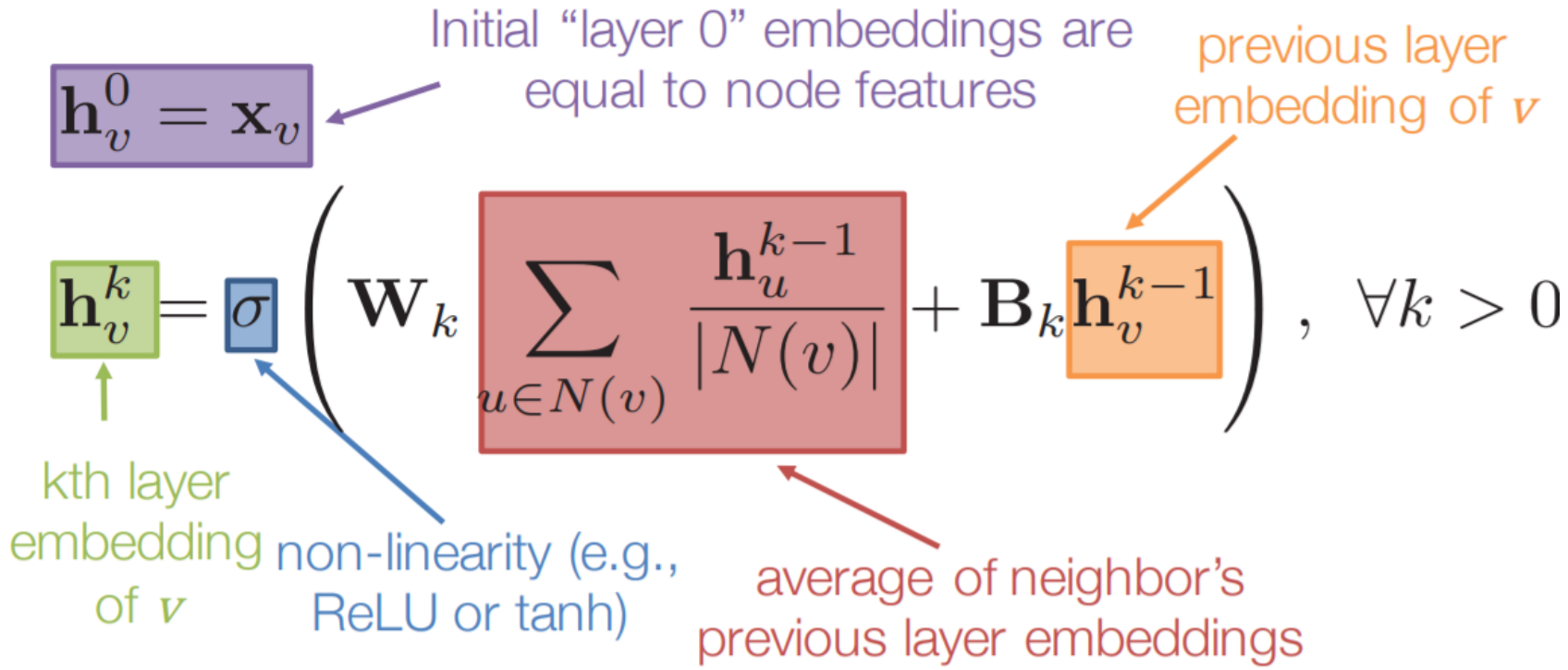
4) Generate embeddings for nodes as needed

Even for nodes we never trained on!!!!



Mathematical Approach

- **Basic approach:** Average neighbor messages and apply a neural network.



Advantages of GNN

- Could be represented in **adjacency matrix**.
- Graphs could be drawn in **many different ways & shapes**.
- Trees and sequence are a sub-sequent of graph.
- Graph networks can generalize and extend various types of neural networks to perform calculations on the graph.
- GNNs can directly work on graph structure to extract hidden features.
- It can extract hidden features that are **invariant under variable renaming**. Logical formulas have a property that **renaming of the propositional variables does not change their semantics**.
- The graph networks framework is based on **graph-to-graph modules**.
- Generate **embedding for new nodes without re-training the models.**

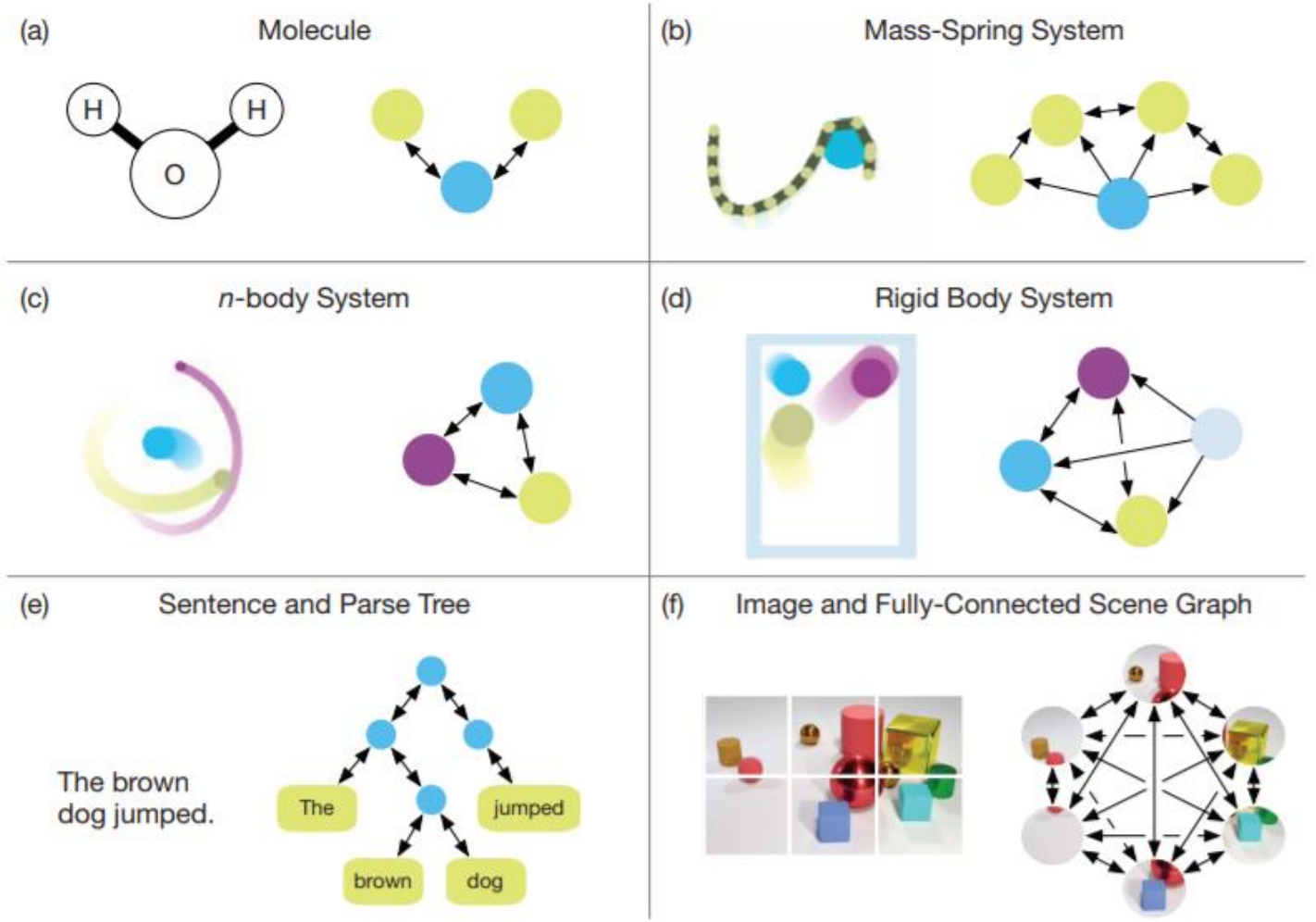
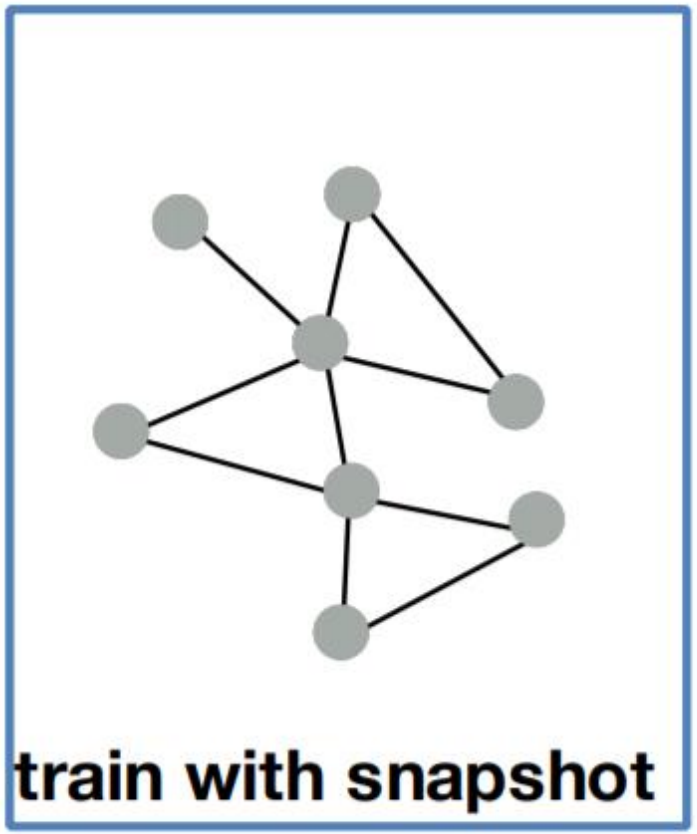
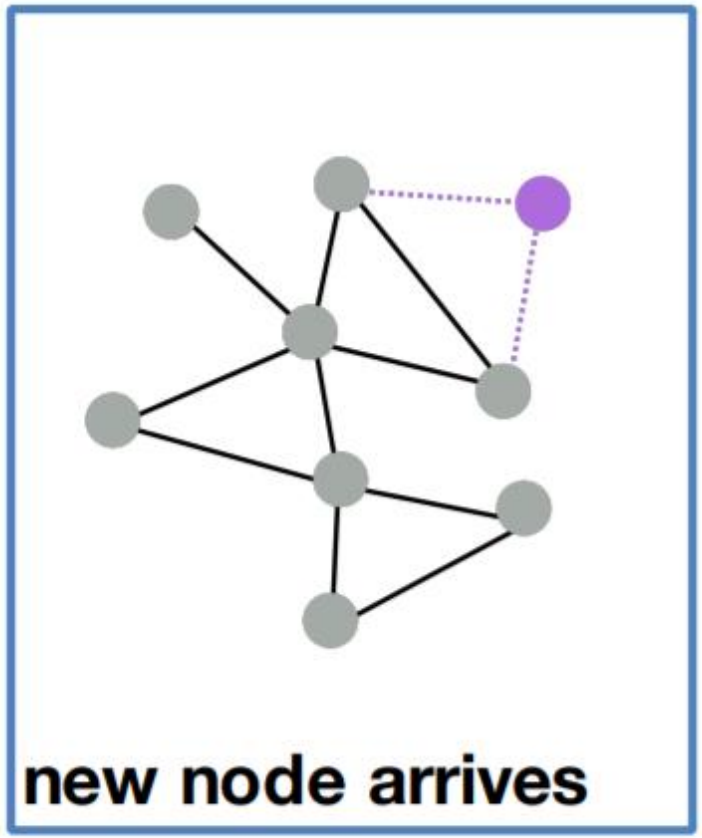
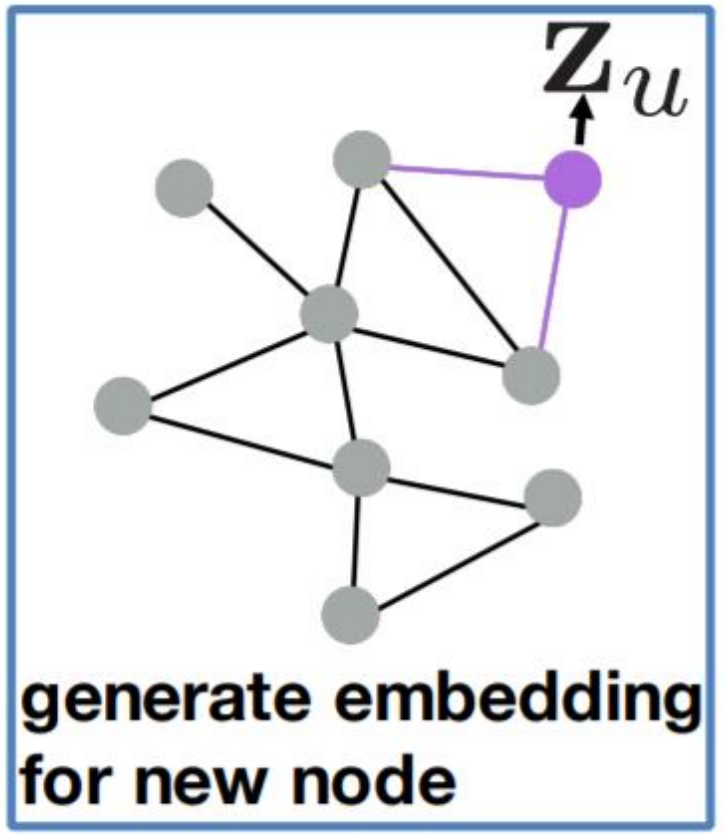


Figure 2: Different graph representations. (a) A molecule, in which each atom is represented as a node and edges correspond to bonds (e.g. Duvenaud et al., 2015). (b) A mass-spring system, in which the rope is defined by a sequence of masses which are represented as nodes in the graph (e.g. Battaglia et al., 2016; Chang et al., 2017). (c) A n-body system, in which the bodies are nodes and the underlying graph is fully connected (e.g. Battaglia et al., 2016; Chang et al., 2017). (d) A rigid body system, in which the balls and walls are nodes, and the underlying graph defines interactions between the balls and between the balls and the walls (e.g. Battaglia et al., 2016; Chang et al., 2017).







Many application settings constantly encounter previously unseen nodes.
e.g., Reddit, YouTube, GoogleScholar, ….

Need to generate new embeddings "on the fly"

Applications

- **Relational reasoning**: Drawing logical conclusions of how different objects and things relate to one another
- **Combinatorial Generalization**: Constructing new inferences, behaviors, and predictions from known building blocks
- **Chemistry and Drugs industry**
- **Program (code) understanding.**
- **Deep reinforcement learning:** network to evaluate RL agents.
- **Social networking profiling**.
- **Computer vision:** doing many vision recognition such as action recognition, and describing image situation.

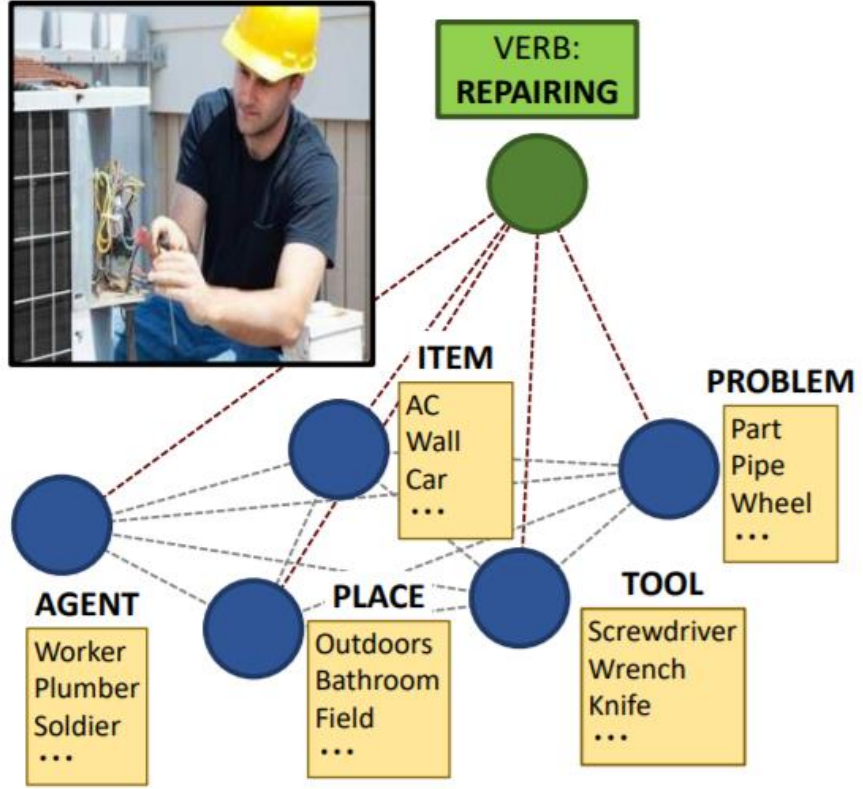


Figure 1. Understanding an image involves more than just predicting the most salient action. We need to know who is performing this action, what tools (s)he may be using, *etc*. Situation recognition is a structured prediction task that aims to predict the verb and its *frame* that consists of multiple role-noun pairs. The figure shows a glimpse of our model that uses a graph to model dependencies between the verb and its roles.

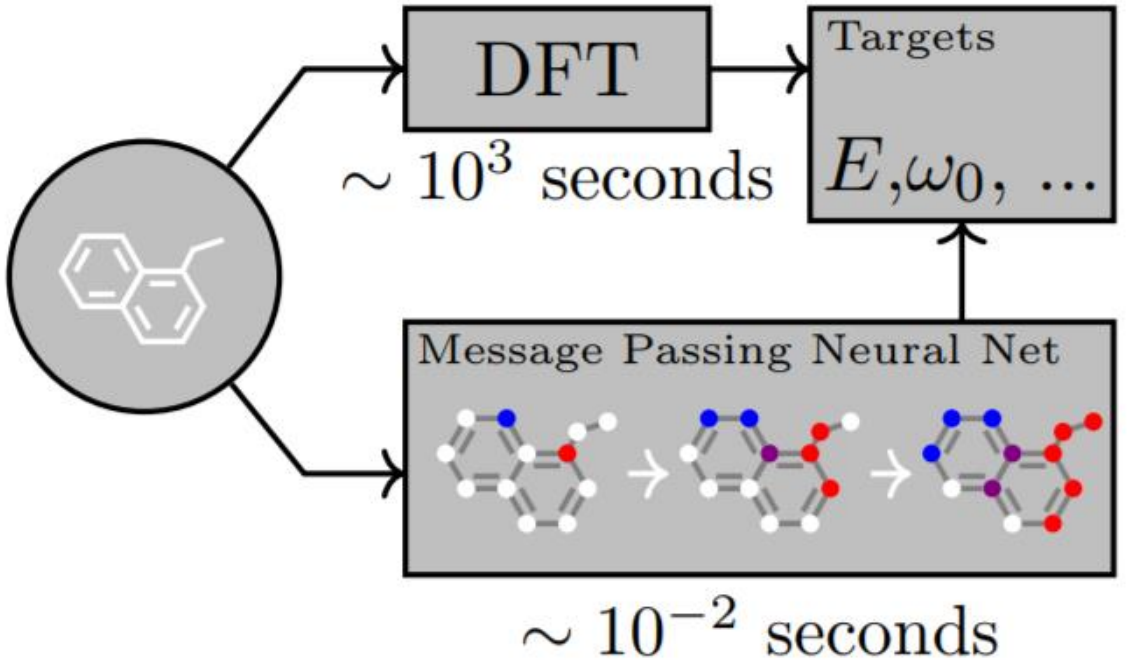


Figure 1. A Message Passing Neural Network predicts quantum properties of an organic molecule by modeling a computationally expensive DFT calculation.

How to start ?

Lib:

- GATED GRAPH NEURAL NETWORKS by microsoft
- Graph_nets by deepmind

Papers:

- The Graph Neural Network Model (Gori et al. 2005)
- GATED GRAPH SEQUENCE NEURAL NETWORKS (Li et al. ICLR 2016)
- Neural Message Passing for Quantum Chemistry (Gilmer et al. ICML 2017)
- HOW POWERFUL ARE GRAPH NEURAL NETWORKS? (at ICLR 2019)
- Relational inductive biases, deep learning, and graph networks (at CoRR 2018)

References:

- The Graph Neural Network Model (Gori et al. 2005)
- GATED GRAPH SEQUENCE NEURAL NETWORKS (Li et al. ICLR 2016)
- Representation Learning on Networks tutorial for GNN by Jure Leskovec.
- Graph neural networks: Variations and applications by Alexander Gaunt

Thank You for your Attention