Graph Neural Networks

And a Myriad of Things that are Relevant

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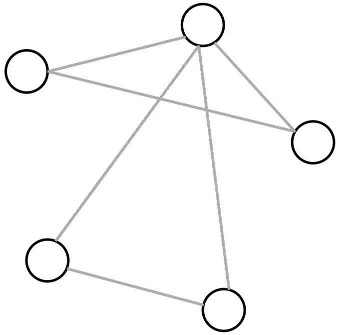
What is a Graph?

$$G = \{V, E\}$$

- A graph represents the relation (*edges*) between a collection of entities (*nodes*).

- V Vertices or nodes
- E Edges or links
- G Graph

What is a Graph?



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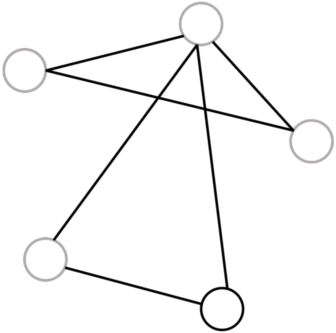

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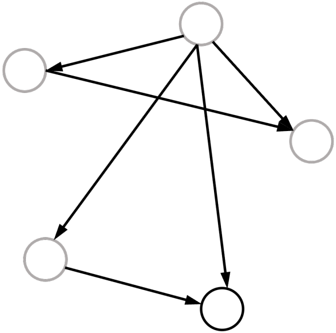

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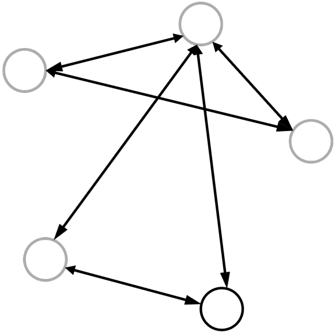
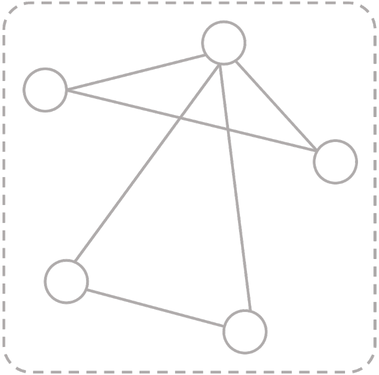


Attributes of Graph



V Vertex (or node) attributes

e.g., node identity, number of neighbors

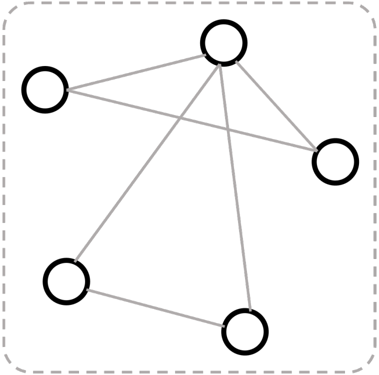
E Edge (or link) attributes and directions

e.g., edge identity, edge weight

U Global (or master node) attributes

e.g., number of nodes, longest path

Attributes of Graph



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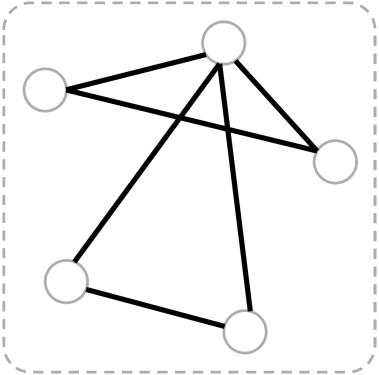

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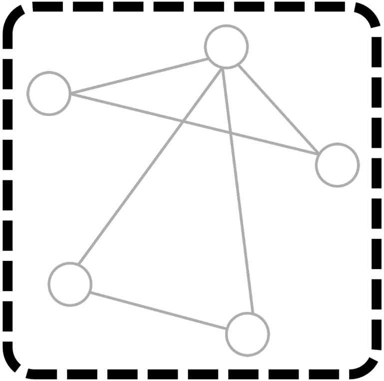

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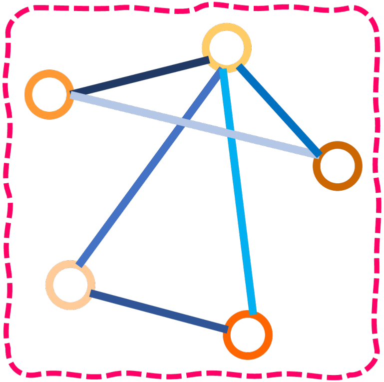


V Vertex (or node) embedding

~~e.g., node identity, number of neighbors~~

E Edge (or link) embedding

~~e.g., edge identity, edge weight~~

U Global (or master node) embedding

~~e.g., number of nodes, longest path~~

Where to Find them?

Graphs are all around us; real world objects are often defined in terms of their connections to other things.

Images as Graphs

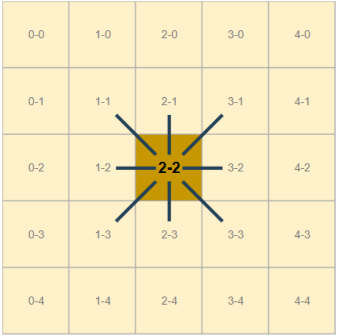
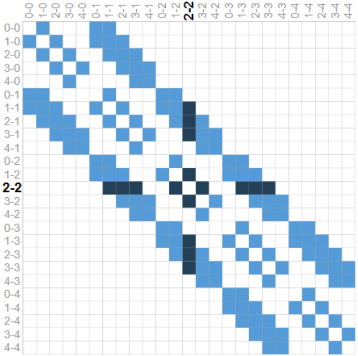
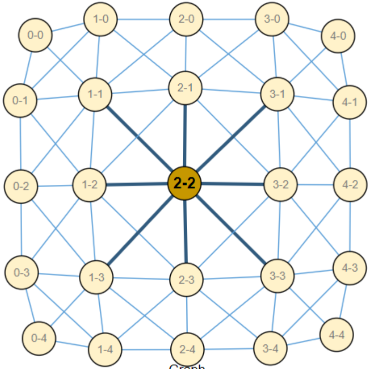


Image Pixels

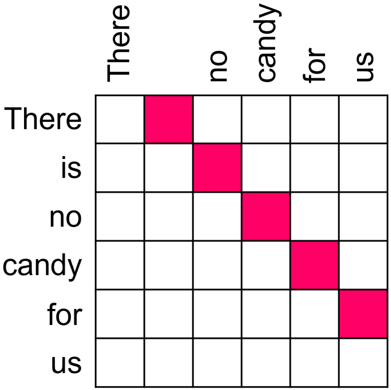


Adjacency Matrix



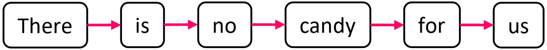
Graph

Text as Graphs



Adjacency Matrix

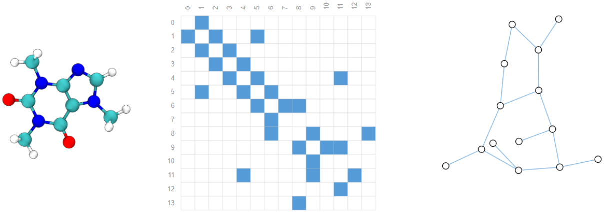
Text: There is no candy for us



Graph

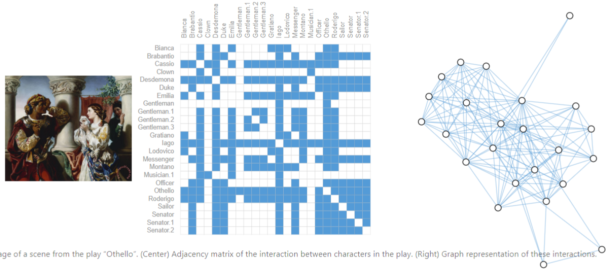
Graph-valued Data in the Wild

- Molecules



Graph-valued Data in the Wild

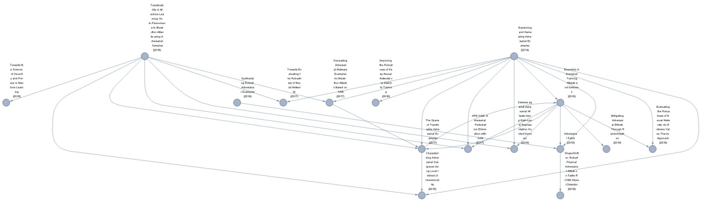
- Molecules
- Social networks



(Left) Image of a scene from the play "Othello". (Center) Adjacency matrix of the interaction between characters in the play. (Right) Graph representation of these interactions.

Graph-valued Data in the Wild

- Molecules
- Social networks
- Citation networks



Graph-valued Data in the Wild

- Molecules
- Social networks
- Citation networks
- etc

Dataset	Domain	graphs	nodes	edges	Edges per node (degree) min	mean	max
karate club	Social network	1	34	78		4.5	17
qm9	Small molecules	134k	≤ 9	≤26	1	2	5
Cora	Citation network	1	23,166	91,500	1	7.8	379
Wikipedia links, English	Knowledge graph	1	12M	378M		62.24	1M

Summary statistics on graphs found in the real world. Numbers are dependent on featurization decisions. More useful statistics and graphs can be found in KONECT [14]

What types of problems have graph structured data?

Graph-level Task

- Predicting the property of an entire graph

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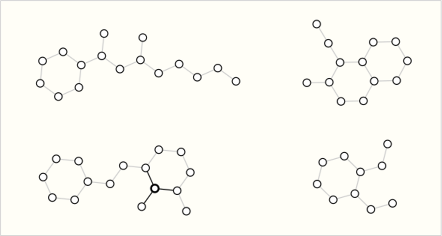
- Predicting the property of an entire graph

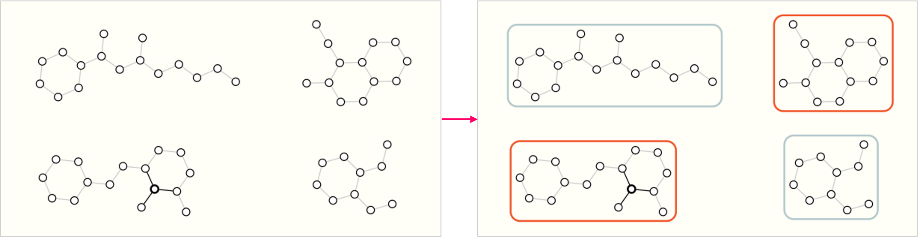


- **Input**: graphs

Graph-level Task

- Predicting the property of an entire graph

- **Input**: graphs
- **Output**: labels for each graph



Graph-level Task

- Predicting the property of an entire graph
  - the smell of the molecular
  - image classification
  - sentiment analysis of text

- **Input**: graphs
- **Output**: labels for each graph

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- Predicting the identity or role of each node

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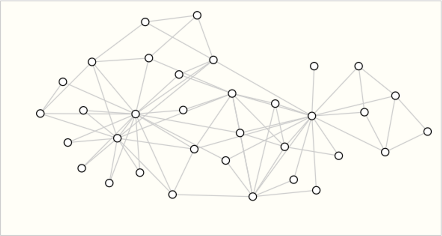

- **Input**: graphs (unlabeled nodes)

Node-level Task

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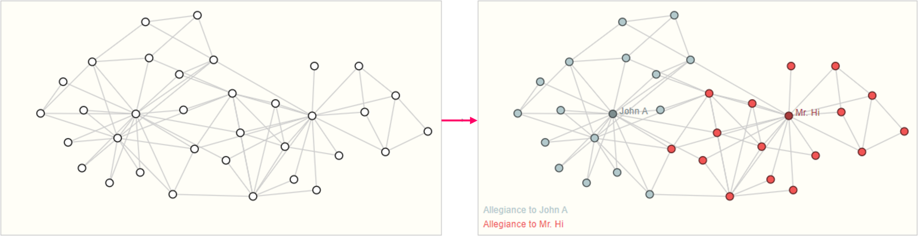

Node-level Task

- Predicting the identity or role of each node
    - image segmentation
    - PoS of each word

- **Input**: graphs (unlabeled nodes)
- **Output**: graph node labels

Edge-level Task

- Predicting the identity or role of each edge

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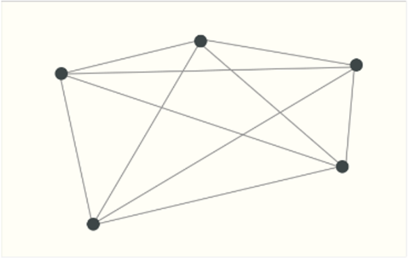
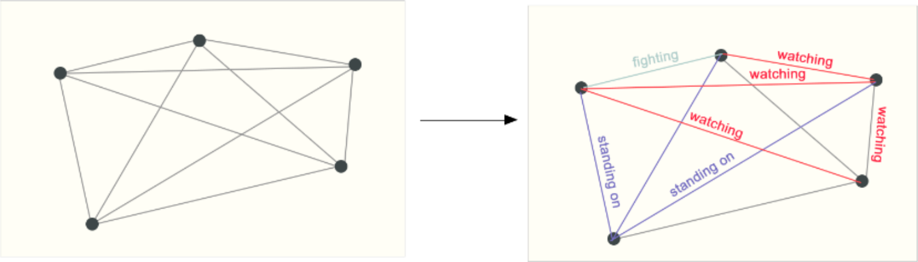


- **Input**: graphs (unlabeled edges)

Edge-level Task

- Predicting the identity or role of each edge

- **Input**: graphs (unlabeled edges)
- **Output**: labels for edges

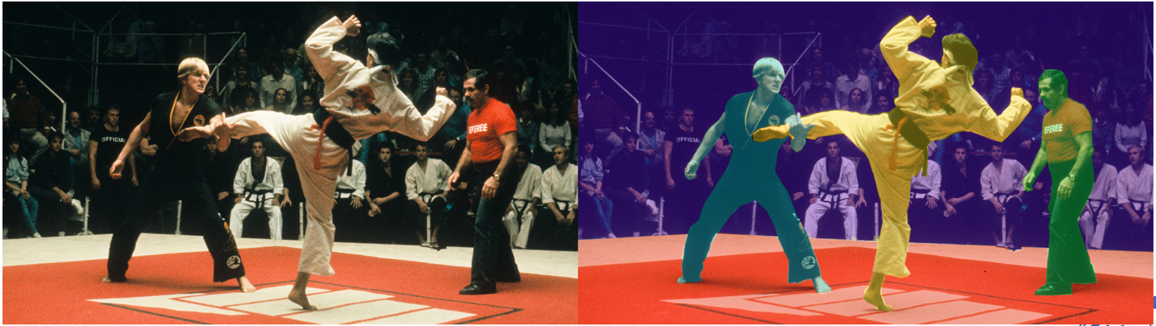


Edge-level Task

- Predicting the identity or role of each edge
  - scence understanding

- **Input**: graphs (unlabeled edges)
- **Output**: labels for edges

Edge-level Task



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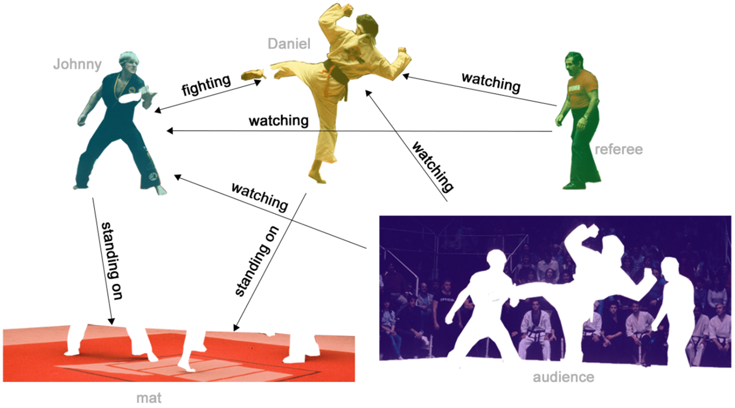


How do we go about solving these different graph tasks with neural networks?

How to Represent Graphs

Graphs have 4 types of information:

- nodes,
- edges,
- global-context,
- and connectivity!

How to Represent Graphs

Graphs have 4 types of information:

- nodes,
- edges,
- global-context,
- and **connectivity**!

$$N = \{node_i\} \quad [n_{nodes}, node_{dim}]$$
$$E = \{edge_i\} \quad [n_{edges}, edge_{dim}]$$
$$U = master\ node's\ embedding\ [, global_{dim}]$$

Representing Graph's Connectivity

- One elegant way to represent graphs is as **Adjacency lists**: These describe the connectivity of edge e_k between nodes n_i and n_j as a tuple (i, j) in the k-th entry of an adjacency list.
  - memory-efficient (even with sparse matrices),
  - permutation invariant.

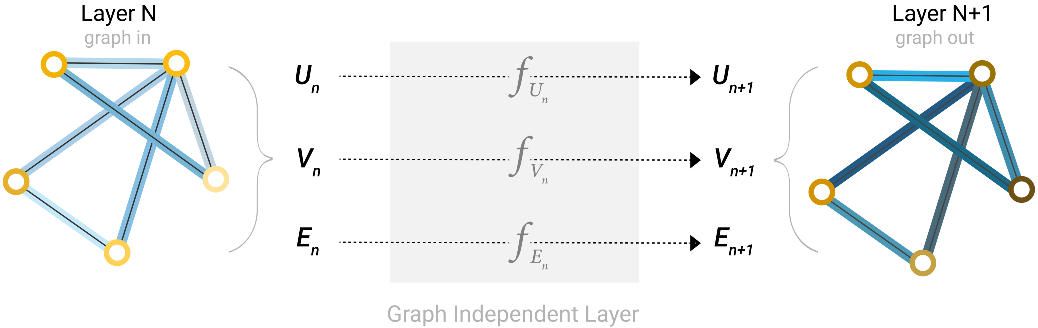
Representing Graph's Connectivity

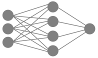
Images/adjacency-list.png

The simplest GNN

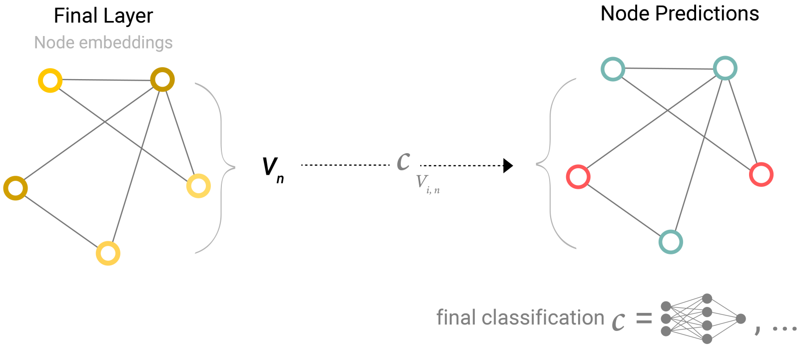
- **GNN**s = **G**raph **N**eural **N**etworks
- **A GNN is an optimizable transformation on all attributes of the graph** (i.e., nodes, edges, global-context) **that preserves graph symmetries** (connectivity or permutation invariances)
- *"graph-in, graph-out"* architecture

The Simplest GNN



update function $f =$  , ...

GNN Predictions



Pooling Information

- **Pooling**: Collecting information from 1 component and giving them to another.

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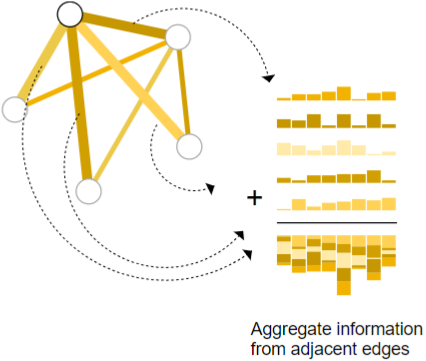
- Abbreviation: ρ e.g., gathering information from edges to nodes $\rho_{E_n \to V_n}$.

Pooling Information



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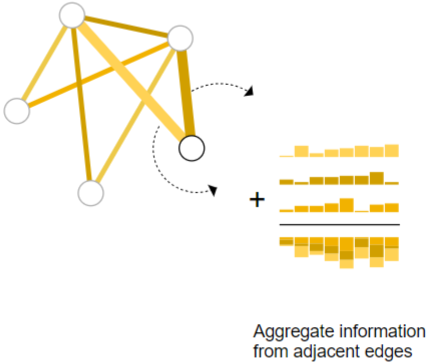
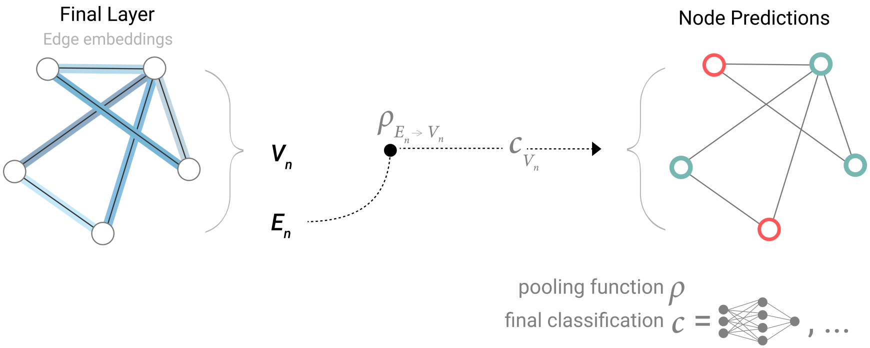


GNN Predictions by Pooling Information



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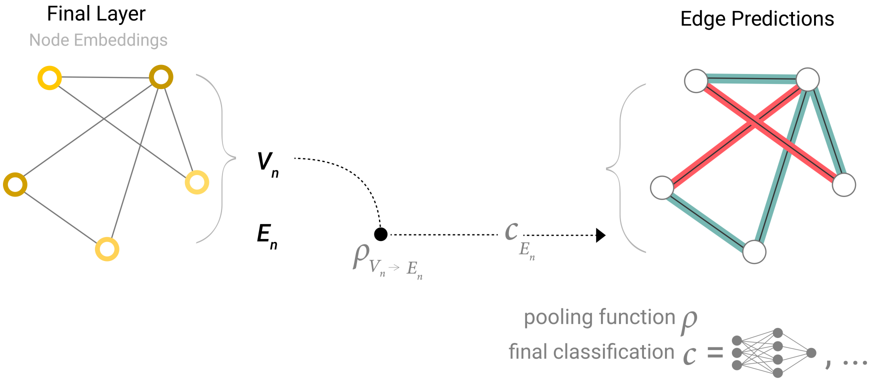

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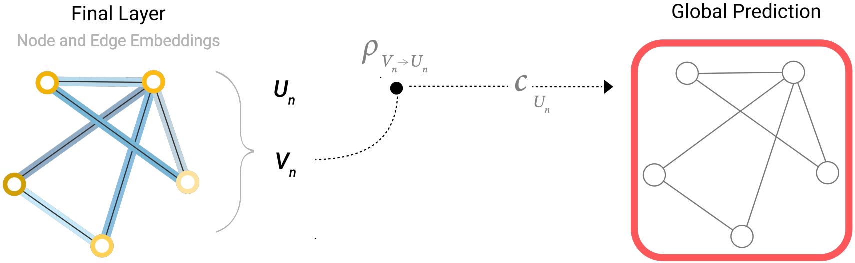
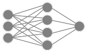
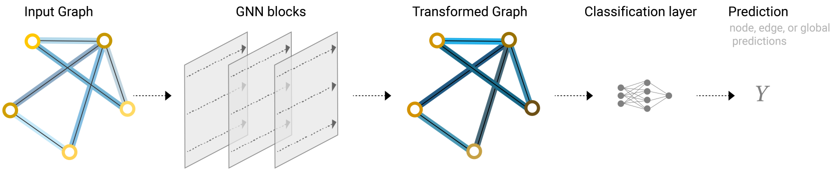


pooling function ρ

final classification c = , ...

End2End Prediction Task with a GNN Model



End2End Prediction Task with a GNN Model

- We still don’t use the connectivity of the graph
  - Each component is processed independently
  - ONLY use connectivity when prediction

Passing messages between parts of the graph

...What if we try using pooling inside GNN Layers?

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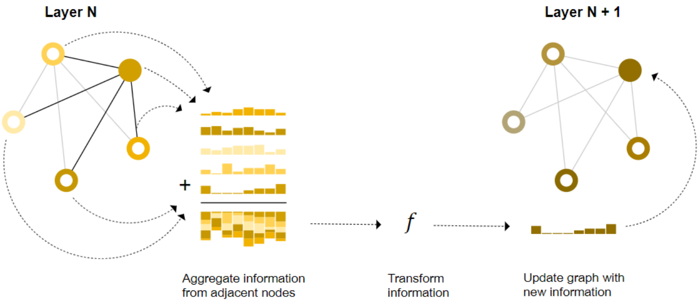
Or to make our learned embeddings aware of graph **connectivity**?

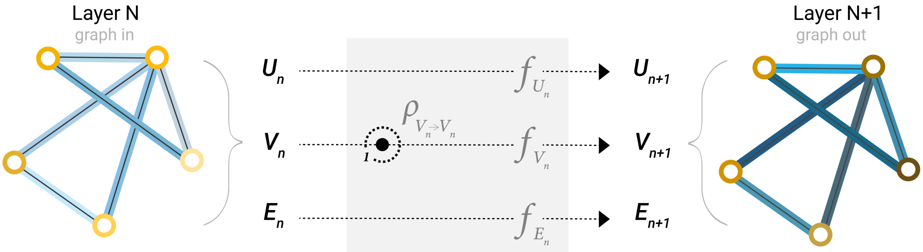
Message Passing

- **Message Passing:**
  1. For each node in the graph, *gather* all the neighboring node embedding (or messages), which is the g function described above.
  2. *Aggregate* all messages via an aggregate function (e.g, sum).
  3. All pooled messages are passed through an *update function*, usually a learned neural network.
- Just as pooling can be applied to either nodes or edges, message passing can occur between either nodes or edges.

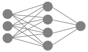
Message Passing



GCN architecture

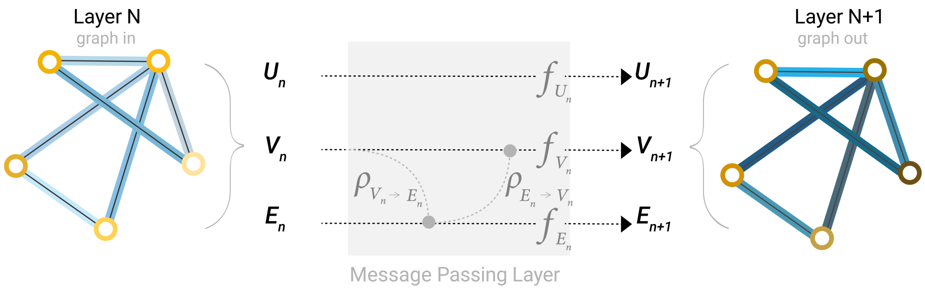


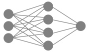
Graph Convolutional Layer

update function $f =$  , ...

pooling function ρ

Learning Edge Representations



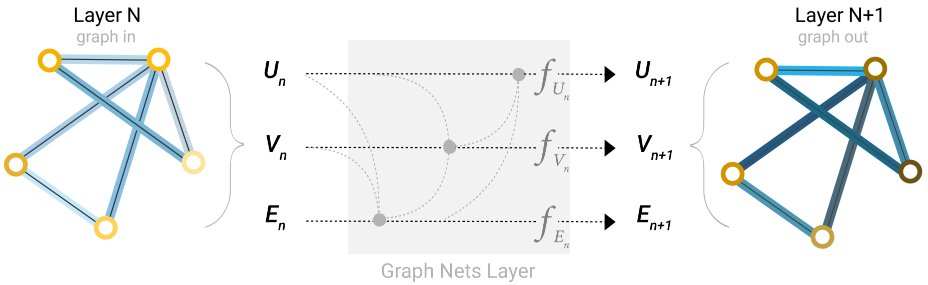
update function $f =$  , ...

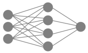
pooling function ρ

Adding Global Representations

- So far, there is still one flaw:
  - Nodes that far away from each other in the graph may never be able to efficiently transfer information to one another, even which several layers.
  - e.g., if we have *k*-layers, information will propagate at most *k*-steps away.
- One solution is by using the global representations or **master node**.

Adding Global Representations



update function $f =$  , ...

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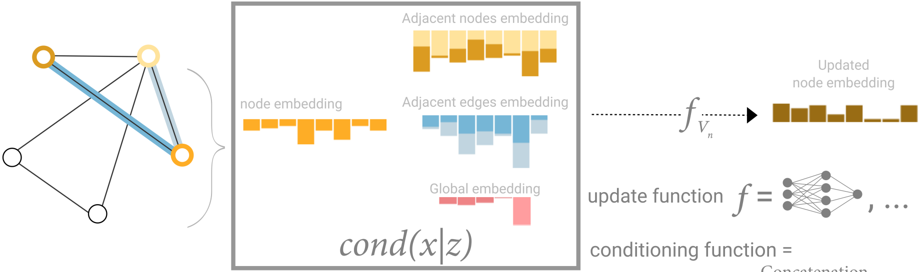
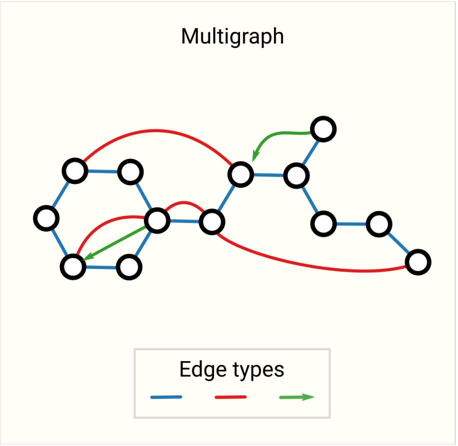
Adding Global Representations

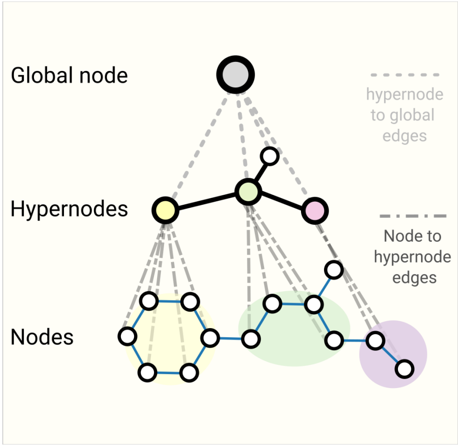


conditioning function =
Concatenation,
Linear Layer and Add,
FiLM Layer..

Into the Weeds

Other types of graphs





Sampling Graphs and Batching in GNNs

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Sampling Graphs and Batching in GNNs

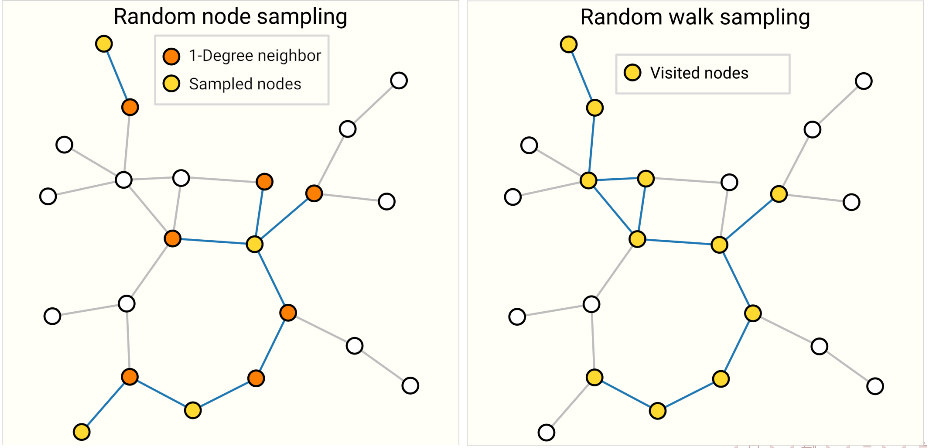
- For training neural networks, it's common to:
  - calculate on randomized but **constant** size subsets of the training data (mini-batches).
- Sometimes, a graph is too large that it cannot be fit in memory.
- However, the number of nodes and edges adjacent to each other are variable.

Sampling Graphs

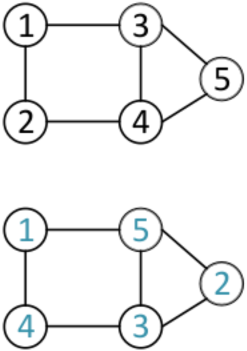
- To create subgraphs that preserve essential properties of the larger graph.
- This graph sampling operation is highly dependent on context,
  - some might make sense in some contexts (citation networks),
  - but might be too strong of an operation in others (molecule graph).

- Cluster-GCN, GraphSaint, Metropolis algorithm, etc...

Sampling Graphs



Generative Modelling



0	1	1	0	0
1	0	0	1	0
1	0	0	1	1
0	1	1	0	1
0	0	1	1	0

0	0	0	1	1
0	0	1	0	1
0	1	0	1	1
1	0	1	0	0
1	1	1	0	0

Same graph

Very different representations!

Generative Modelling

Example: Generate a ring graph on 6 nodes: