Graph Neural Networks

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Outline

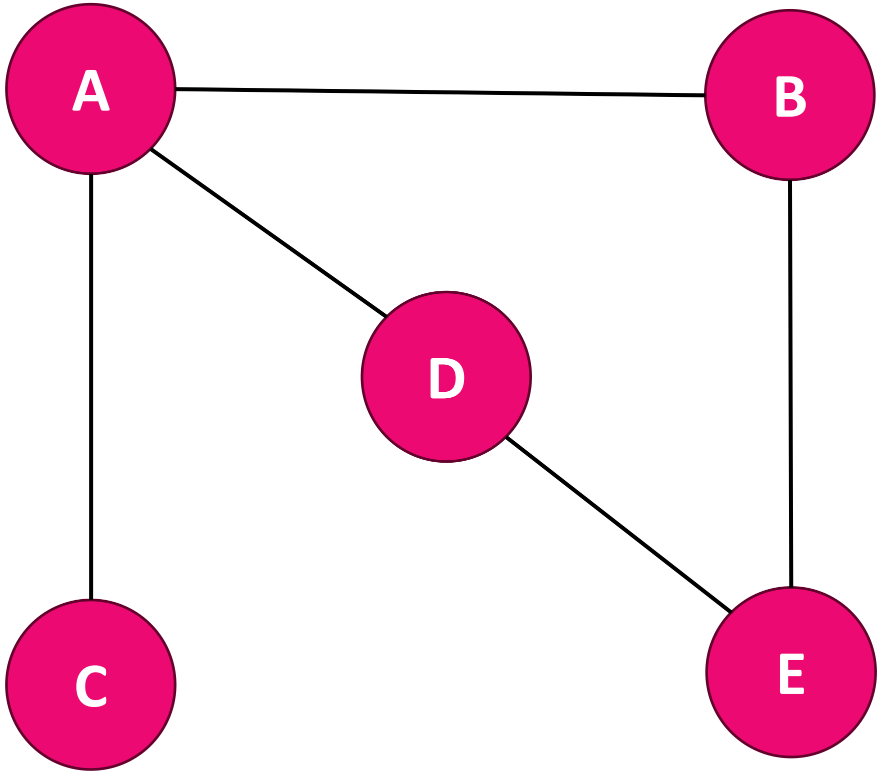
- Learning Goals
- Graph neural networks
  - What is graph-structured data
  - What sorts of problems can we solve using graph neural networks
  - How are graph neural networks designed
- Summary

Learning Goals

- Understand graph structured data and its differences from data we’ve seen so far
- What are some applications of GNNs
- Some of the core concepts of GNN implementation such as
  - Message passing
  - K-hop neighbourhood

What is a graph anyways?

- Graphs have **nodes** and **edges**
- Edges represent the relationship between any two nodes



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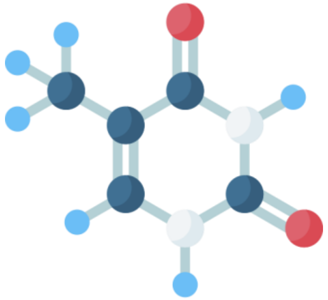
Graph structured data

Graphs can be used to represent data such as:

Social networks

[University of Kentucky]

Molecules

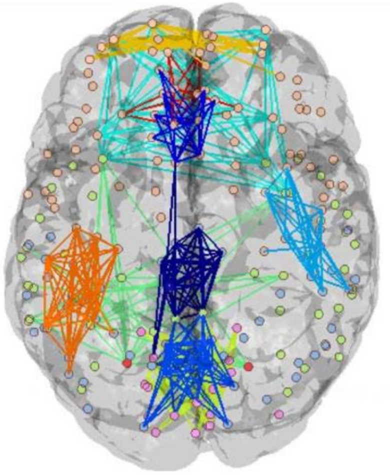


[flaticon.com]

Transit

[translink.ca]

Brain Connectivity



[spectrumnews.org]

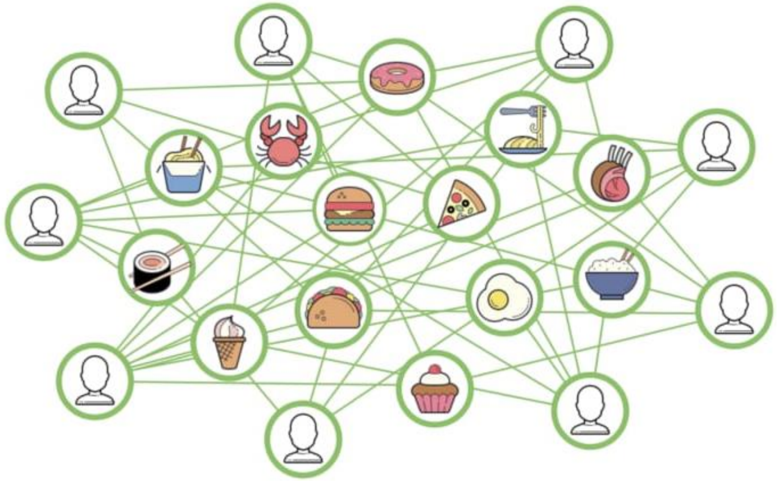
Citation Maps

[connectedpapers.com]

Graph structured data

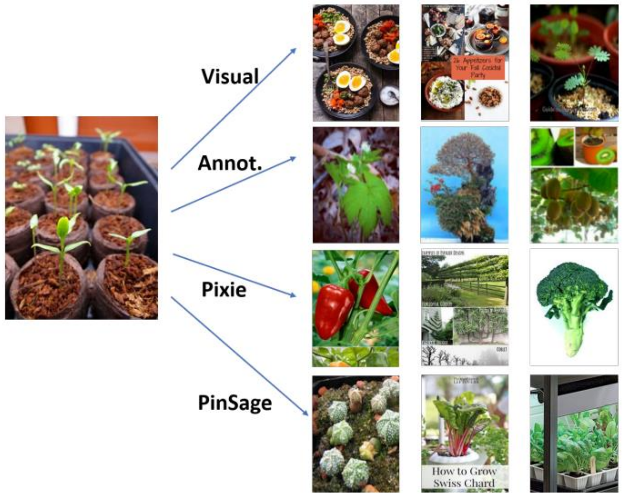
GNNs aren't just for niche applications-- they're trendy in industry too!

Uber Eats



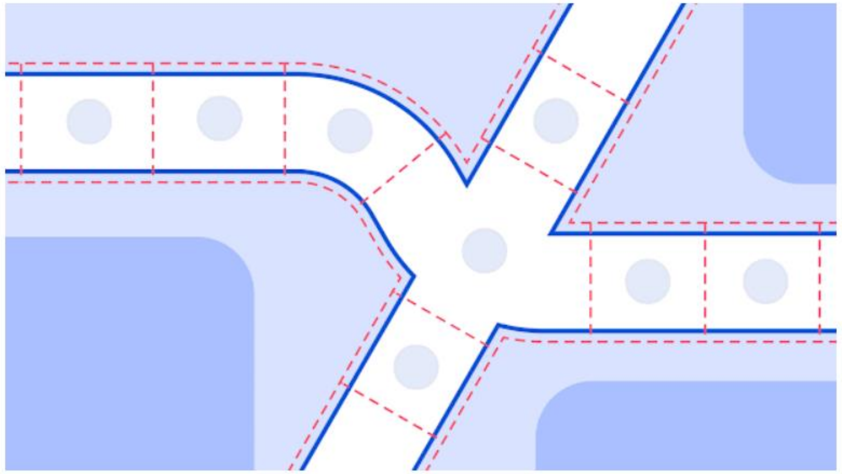
[uber.com]

Pinterest



[Ying et al. 2018]

Google maps



[deepmind.google.com]

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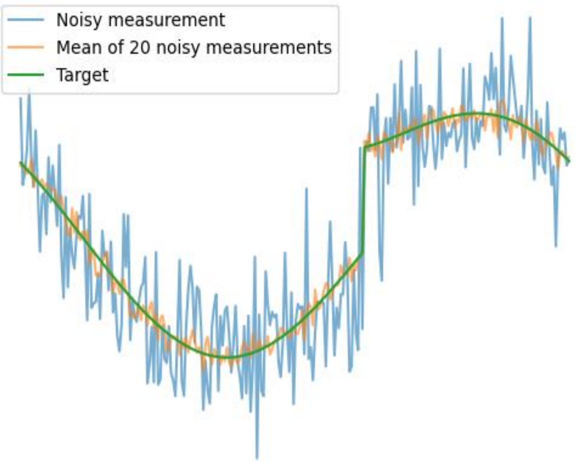
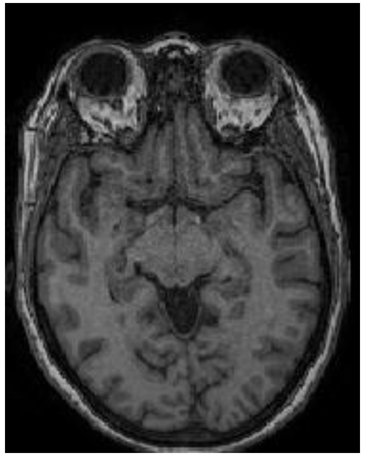
What we’ve seen so far

Signals



Images



Tabular

	age	workclass	fnlwgt	education	education-num	marital-status	occupation	relationship
0	39	State-gov	77516	Bachelors	13	Never-married	Adm-clerical	Not-in-family
1	50	Self-emp-not-inc	83311	Bachelors	13	Married-civ-spouse	Exec-managerial	Husband
2	38	Private	215646	HS-grad	9	Divorced	Handlers-cleaners	Not-in-family
3	53	Private	234721	11th	7	Married-civ-spouse	Handlers-cleaners	Husband
4	28	Private	338409	Bachelors	13	Married-civ-spouse	Prof-specialty	Wife

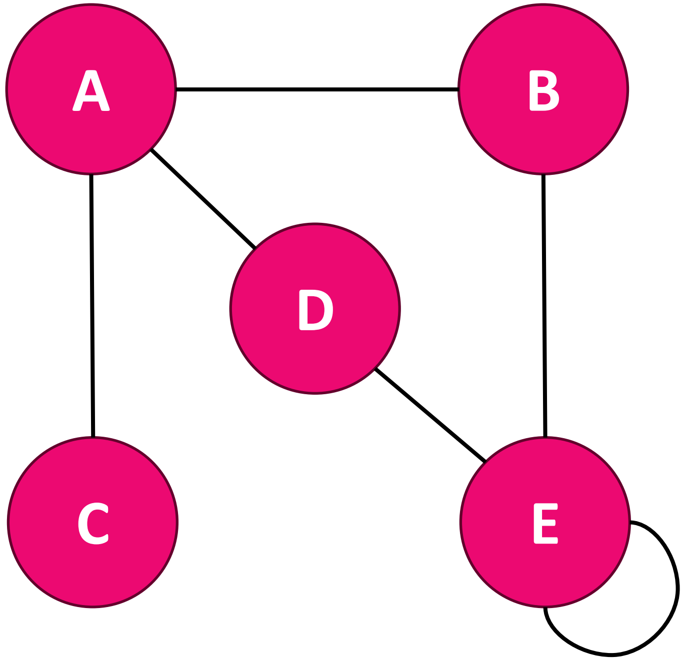
Text

Love looks not with the eyes, but with the mind; And therefore is wing'd Cupid painted blind. Nor hath love's mind of any judgment taste; Wings and no eyes figure unheedy haste: And therefore is love said to be a child, Because in choice he is so oft beguil'd.

- All of these can be represented as graphs!
- Graphs are one of the most general data structures

A bit more on graphs

- We can represent graphs as an adjacency matrix

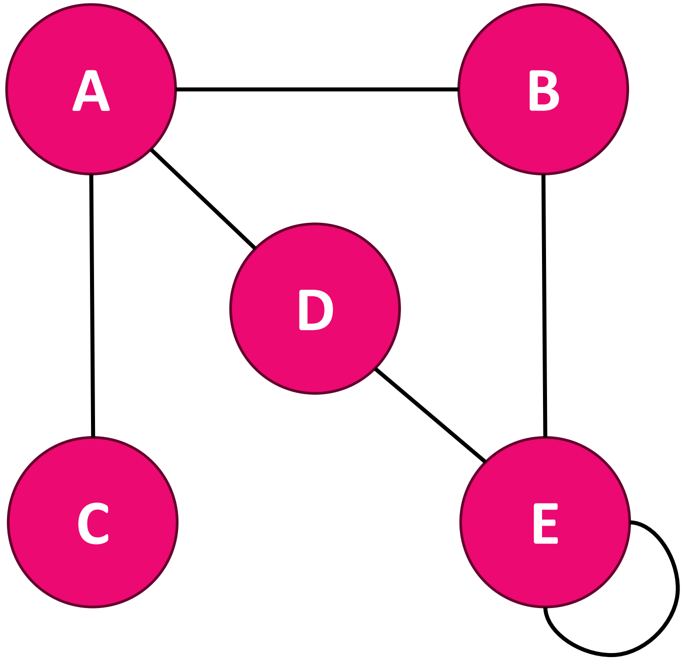


	A	B	C	D	E
A	0	1	1	1	0
B	1	0	0	0	1
C	1	0	0	0	0
D	1	0	0	0	1
E	0	1	0	1	1

A bit more on graphs

- We can represent graphs as an adjacency matrix
- Edges can be weighted and/or directional

Weighted edges



	A	B	C	D	E
A	0	0.4	1	0.2	0
B	0.4	0	0	0	1
C	1	0	0	0	0
D	0.2	0	0	0	1
E	0	1	0	1	1

A bit more on graphs

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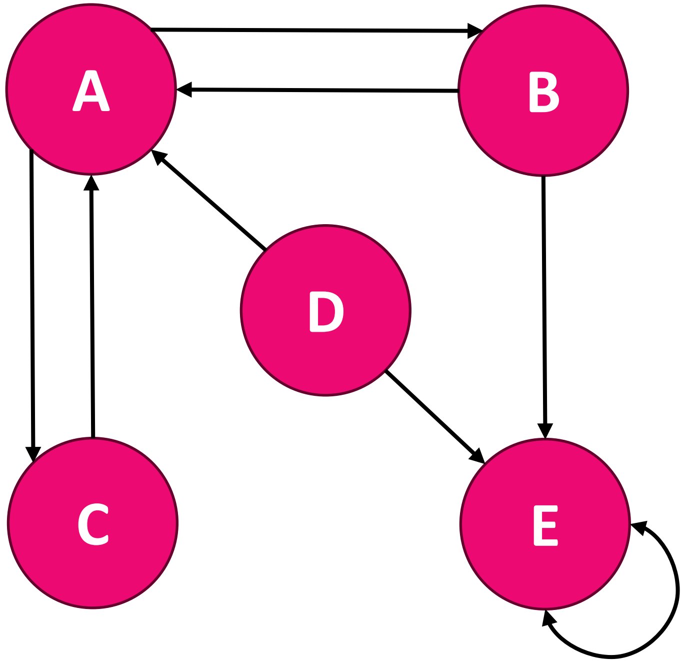
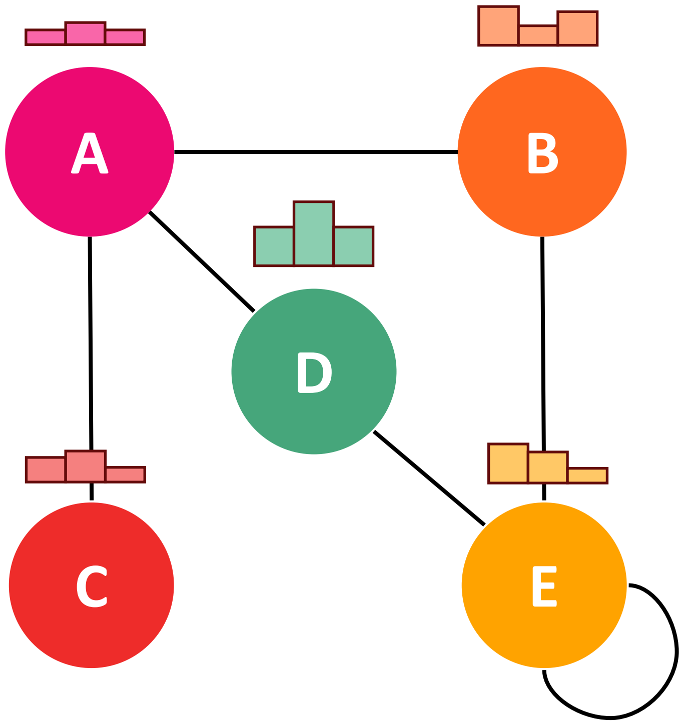
Directional edges



	A	B	C	D	E
A	0	1	1	0	0
B	1	0	0	0	1
C	1	0	0	0	0
D	1	0	0	0	1
E	0	1	0	1	1

A bit more on graphs

- We can represent graphs as an adjacency matrix
- Edges can be weighted and/or directional
- Can have features related to nodes, edges, or graph as a whole
  - Node features most common



	A	B	C	D	E
A	0	1	1	1	0
B	1	0	0	0	1
C	1	0	0	0	0
D	1	0	0	0	1
E	0	1	0	1	1

Working with sparse tensors

- Since they are often sparse, adjacency matrices are commonly represented as a list of edges

	A	B	C	D	E
A	0	1	1	1	0
B	1	0	0	0	1
C	1	0	0	0	0
D	1	0	0	0	1
E	0	1	0	1	1

Working with sparse tensors

- Since they are often sparse, adjacency matrices are commonly represented as a list of edges

	0	1	2	3	4
0	0	1	1	1	0
1	1	0	0	0	1
2	1	0	0	0	0
3	1	0	0	0	1
4	0	1	0	1	1

Working with sparse tensors

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$$
\begin{array}{c|ccccc}
 & 0 & 1 & 2 & 3 & 4 \\
\hline
0 & 0 & 1 & 1 & 1 & 0 \\
1 & 1 & 0 & 0 & 0 & 1 \\
2 & 1 & 0 & 0 & 0 & 0 \\
3 & 1 & 0 & 0 & 0 & 1 \\
4 & 0 & 1 & 0 & 1 & 1
\end{array}
\qquad
\begin{pmatrix} (0, 1) \\ \\ \\ \\ \\ \end{pmatrix}
$$

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\qquad
\begin{pmatrix}
(0, 1) \\
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$$\begin{pmatrix} (0,1) \\ (0,2) \\ (0,3) \\ (1,0) \\ (1,4) \\ \vdots \end{pmatrix}$$

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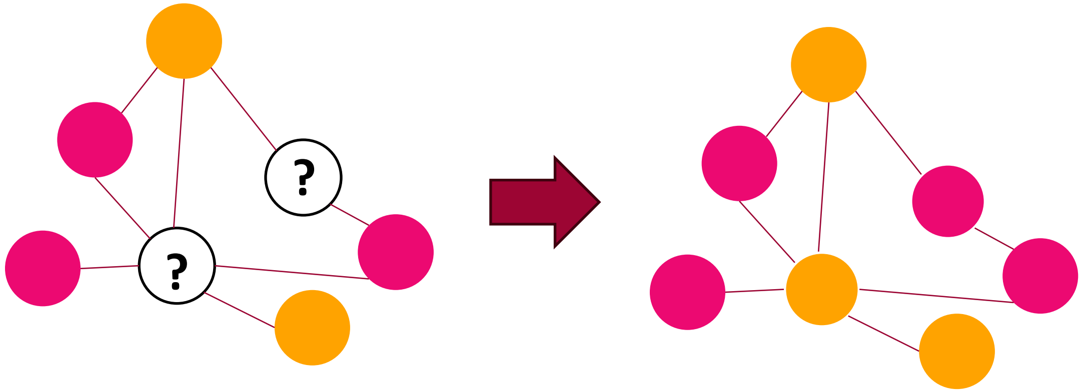
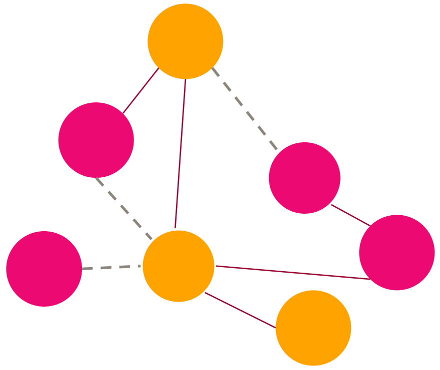
Tasks

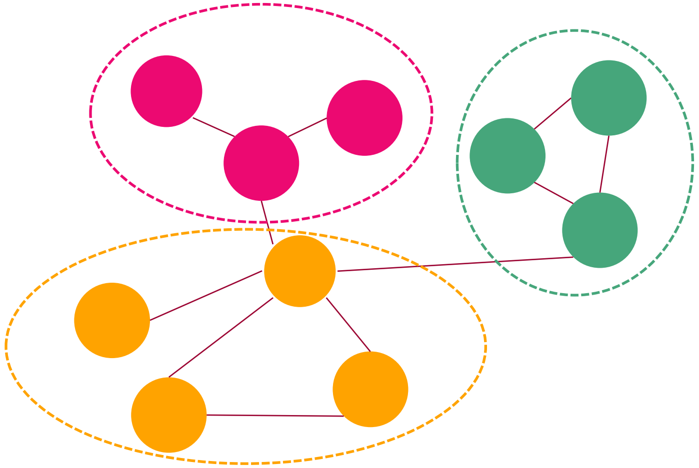
Node Classification



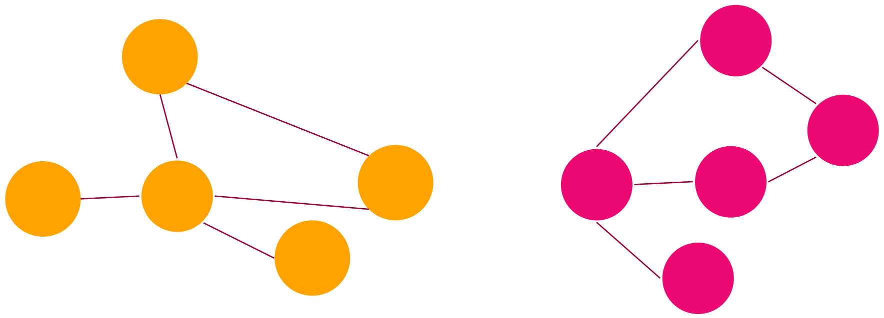
Edge prediction



Clustering

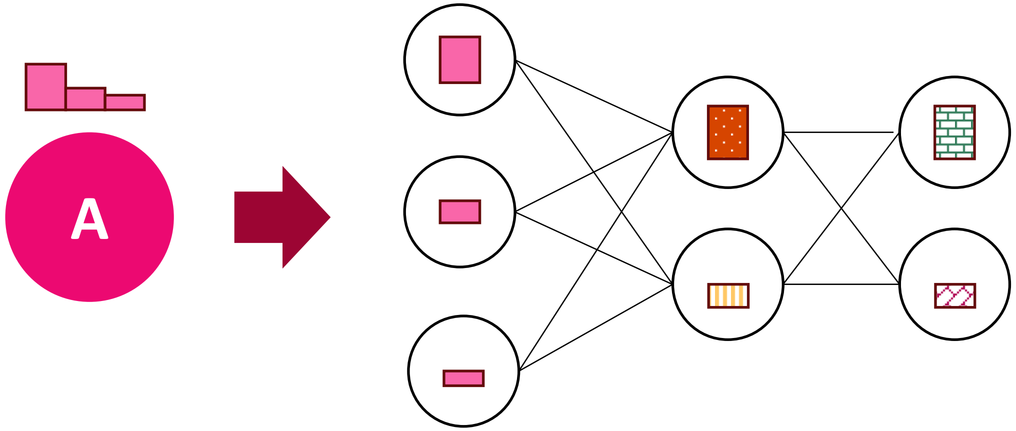


Graph Classification



Prelude to message passing

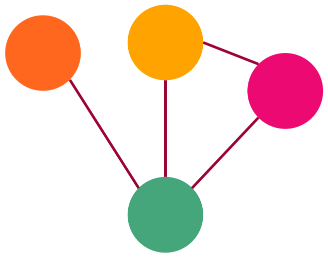
- How do we create models that can accommodate graph-structured data?
- Naïve approach: Feed a node and its features into an FCNN



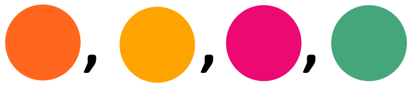
- **Question:** Are there any issues with this approach?

Prelude to message passing

- Unlike standard supervised learning, we do not have i.i.d. points!
  - Our nodes are connected to each other in unique ways



is not the same as



- We want to develop models that can exploit the relationships between the nodes
- We'll introduce **'message passing'** which allows for information to be propagated effectively throughout a neural network

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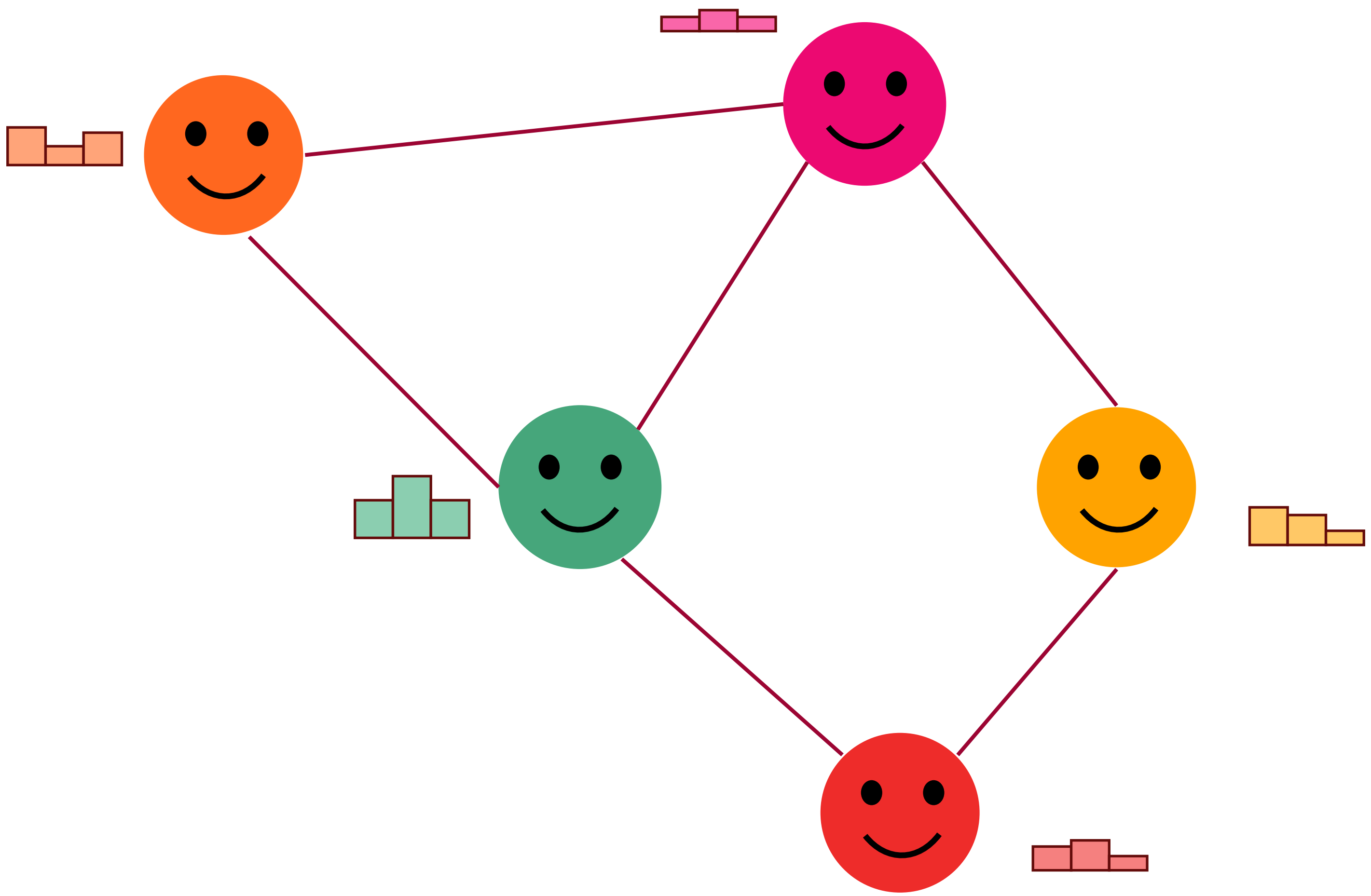
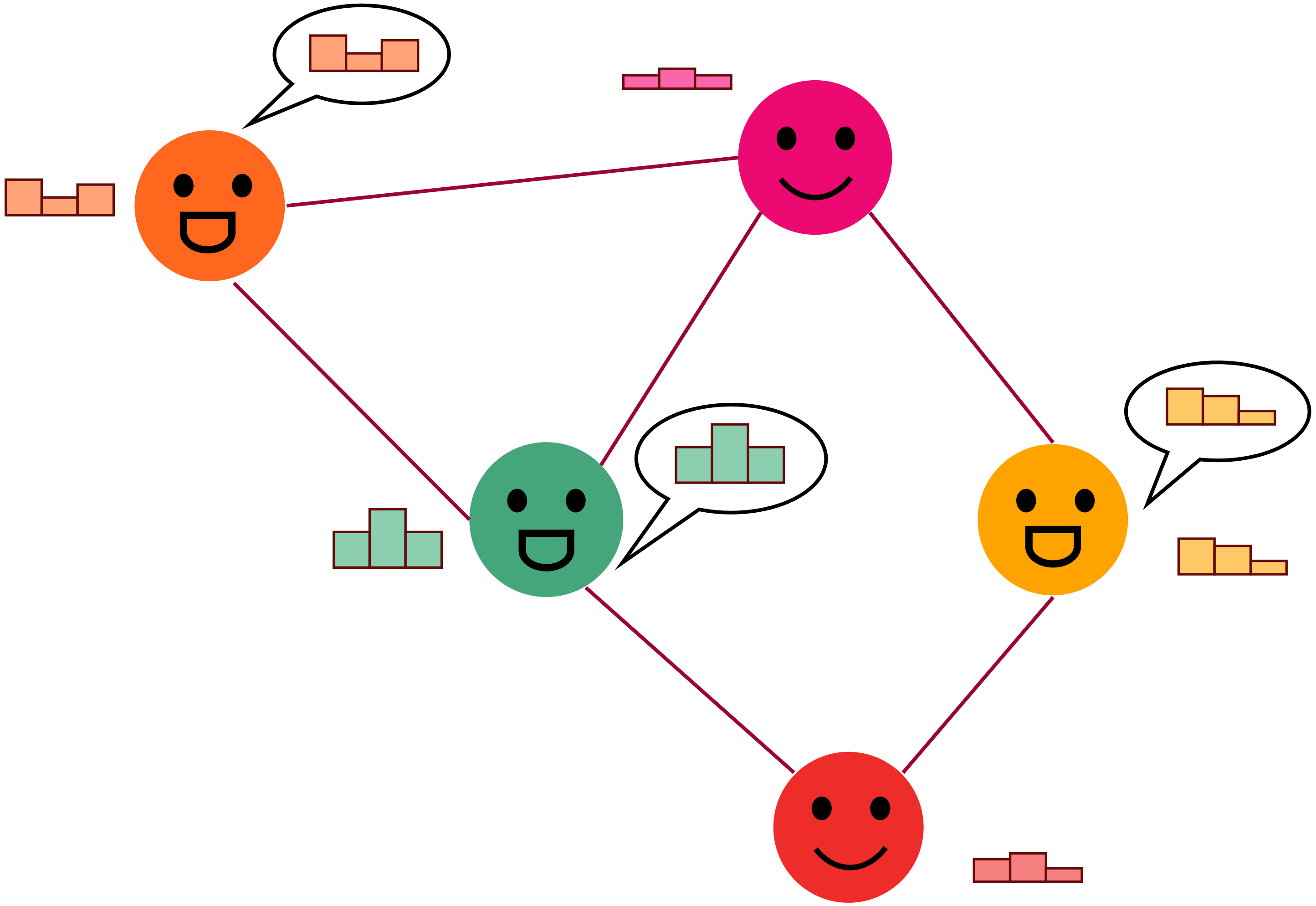
Message passing



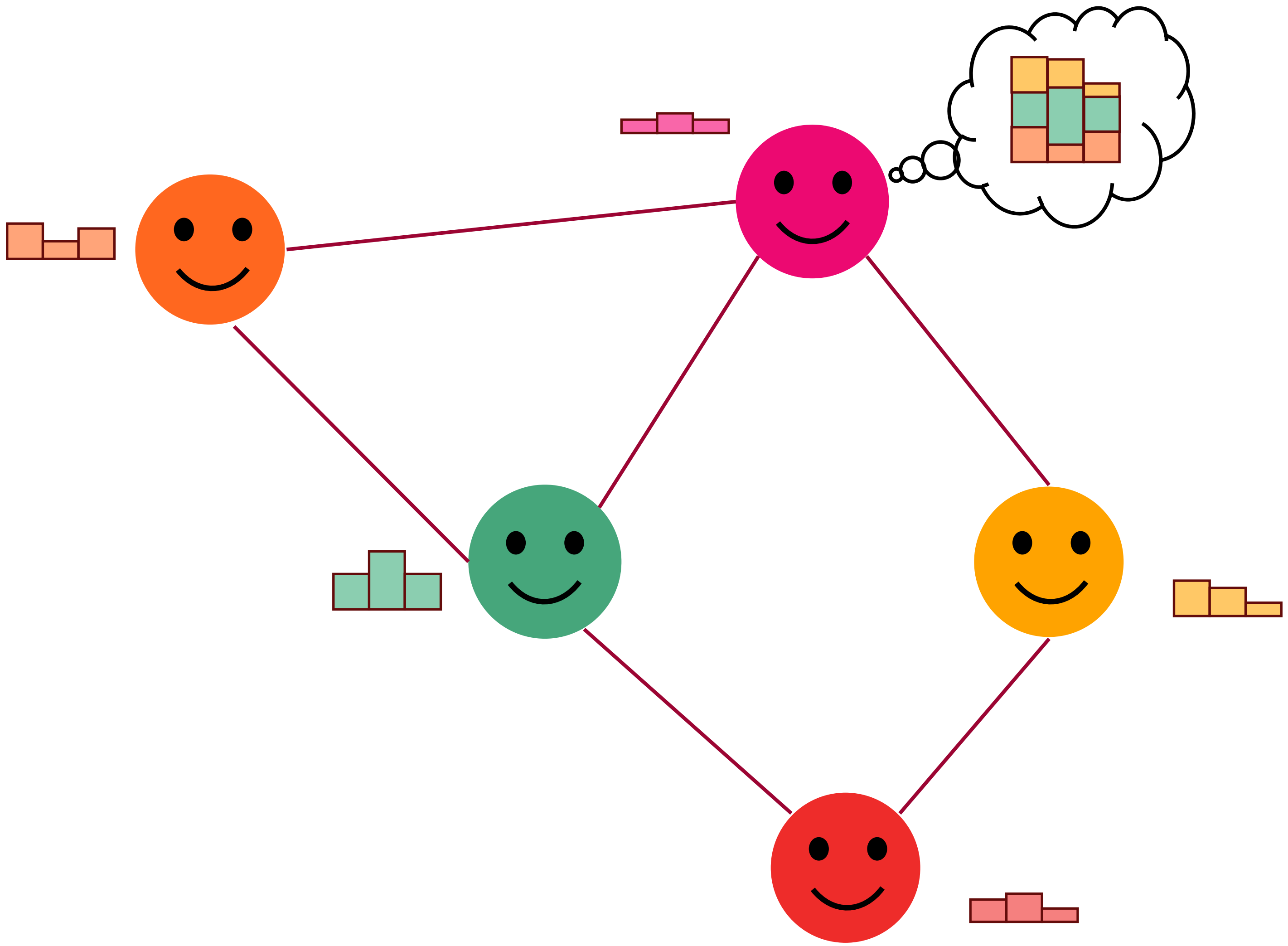
Message passing

1. **Message:** Nodes send messages to their neighbors



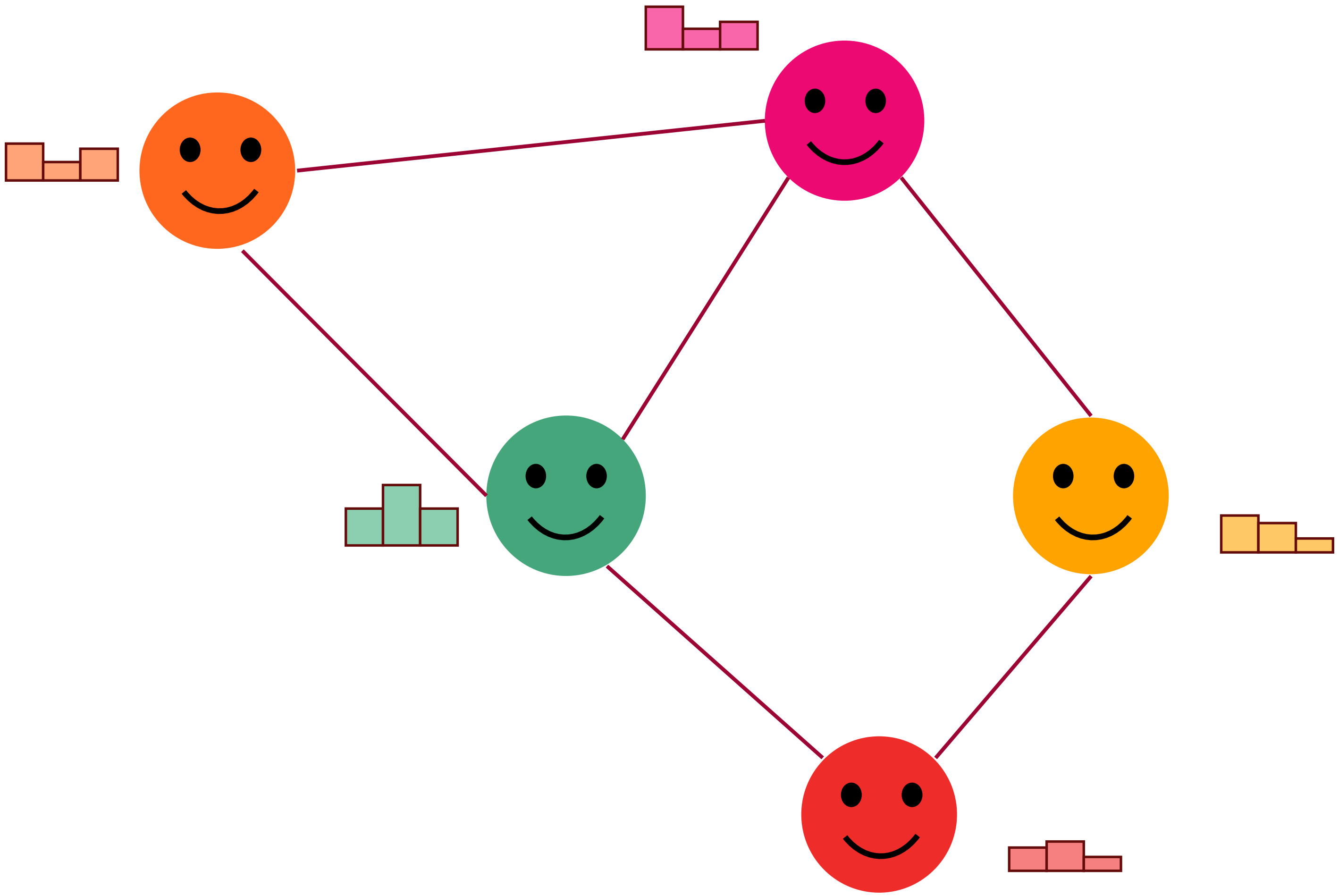
Message passing

1. **Message:** Nodes send messages to their neighbors
2. **Aggregate:** Messages are aggregated in a permutation-invariant way



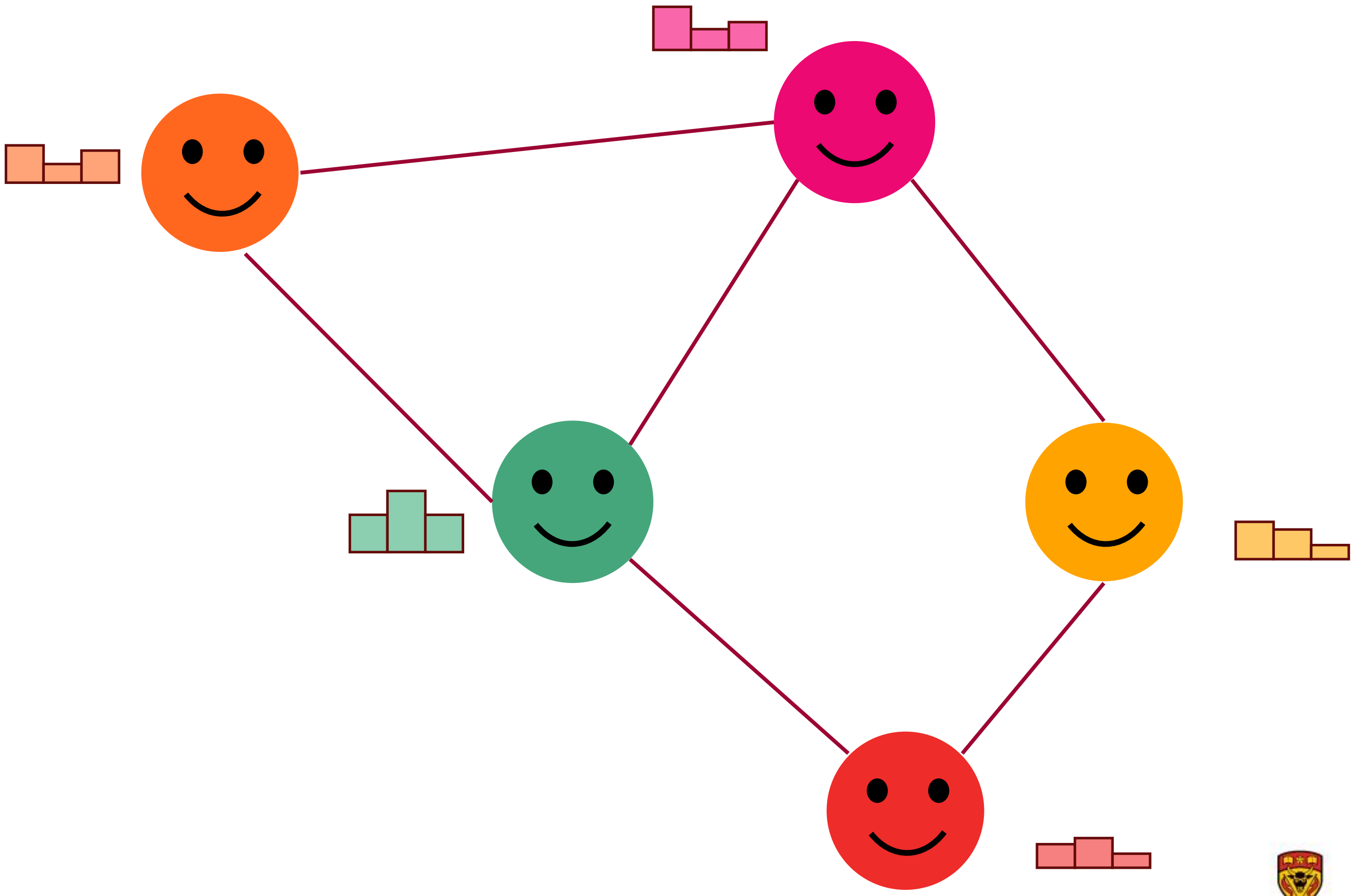
Message passing

1. **Message:** Nodes send messages to their neighbors
2. **Aggregate:** Messages are aggregated in a permutation-invariant way
3. **Update:** Node embeddings are updated



Message passing

- We just focused on updating the pink node, but in practice, all nodes are updated at the same time!



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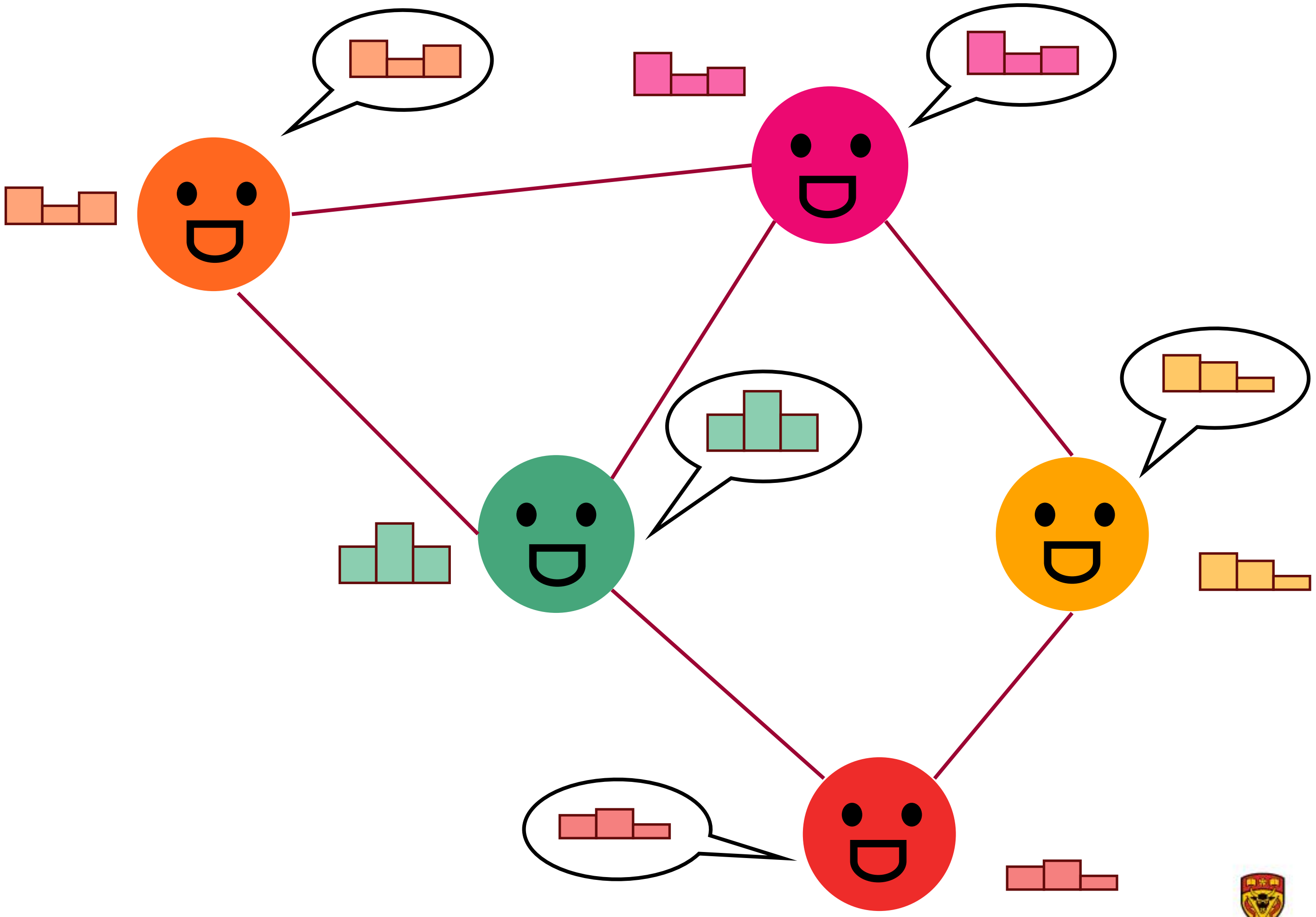

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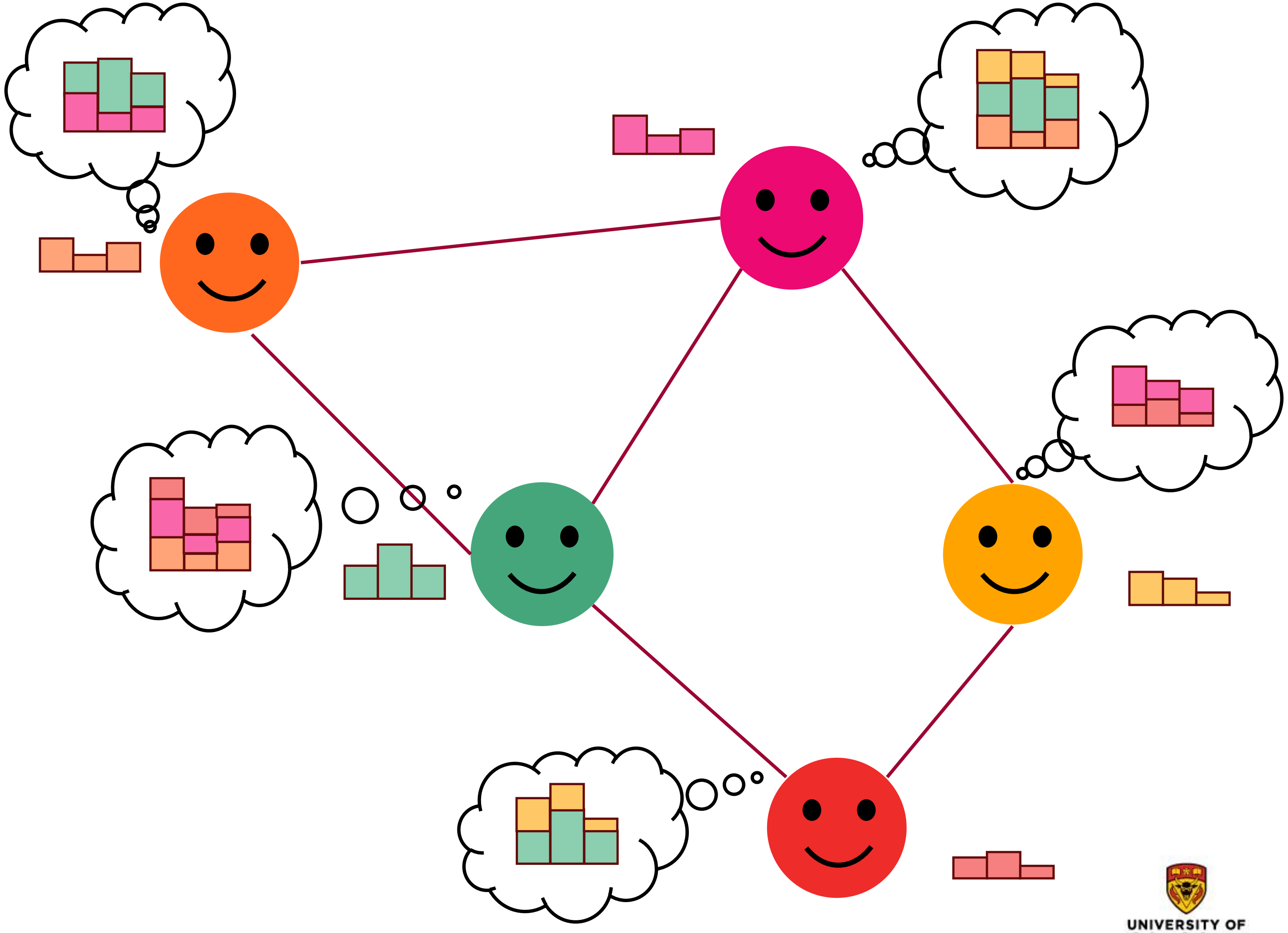

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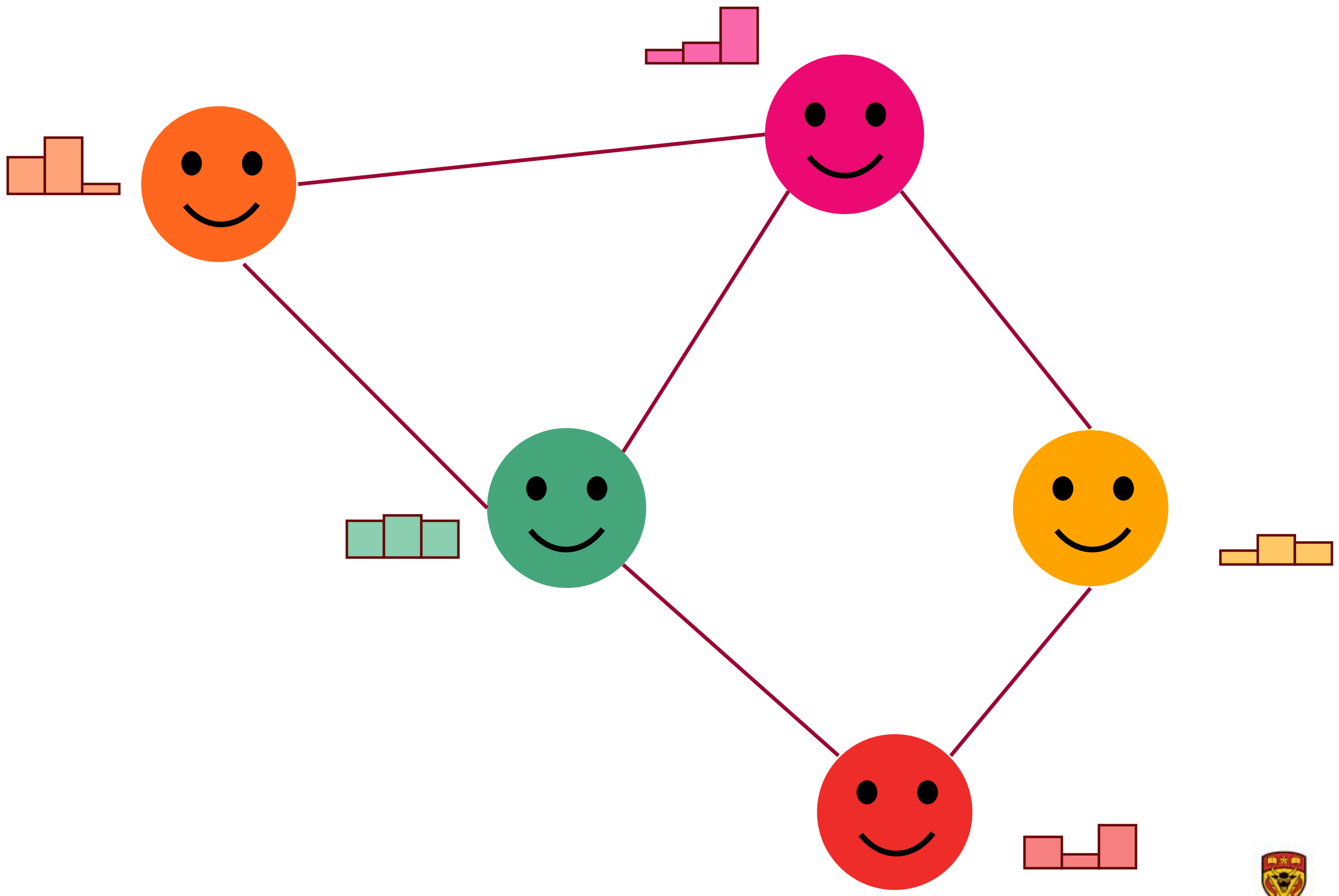
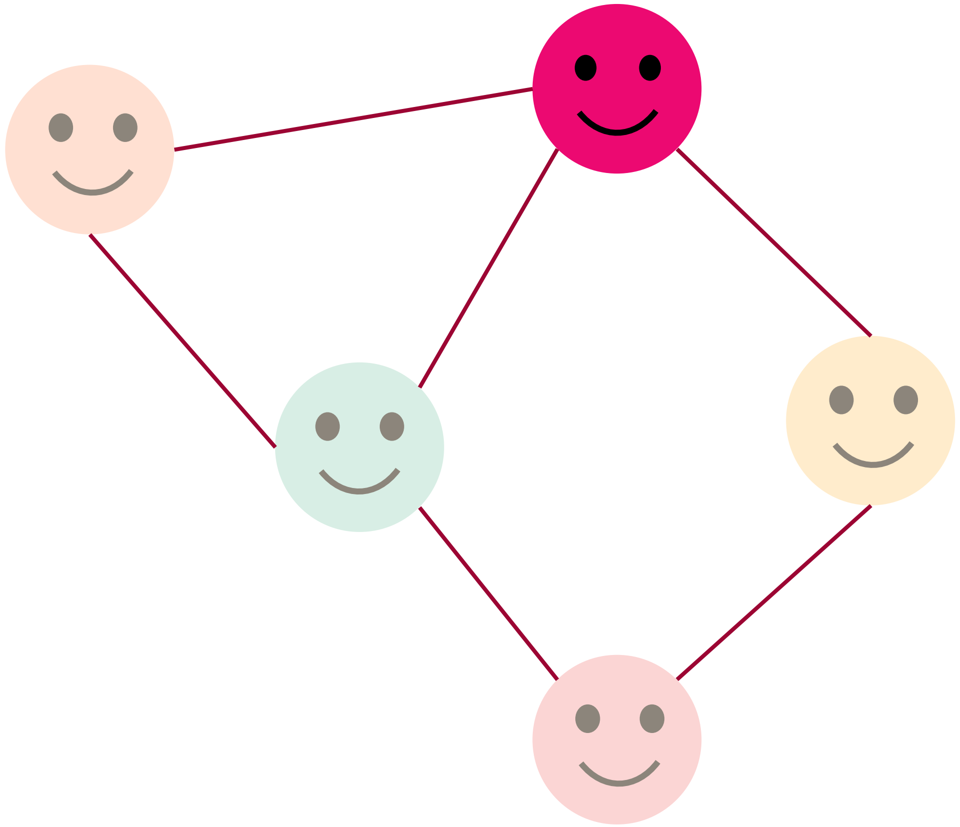


k-hop neighborhood

- The number of layers we have corresponds to the ‘k-hop’ neighborhood



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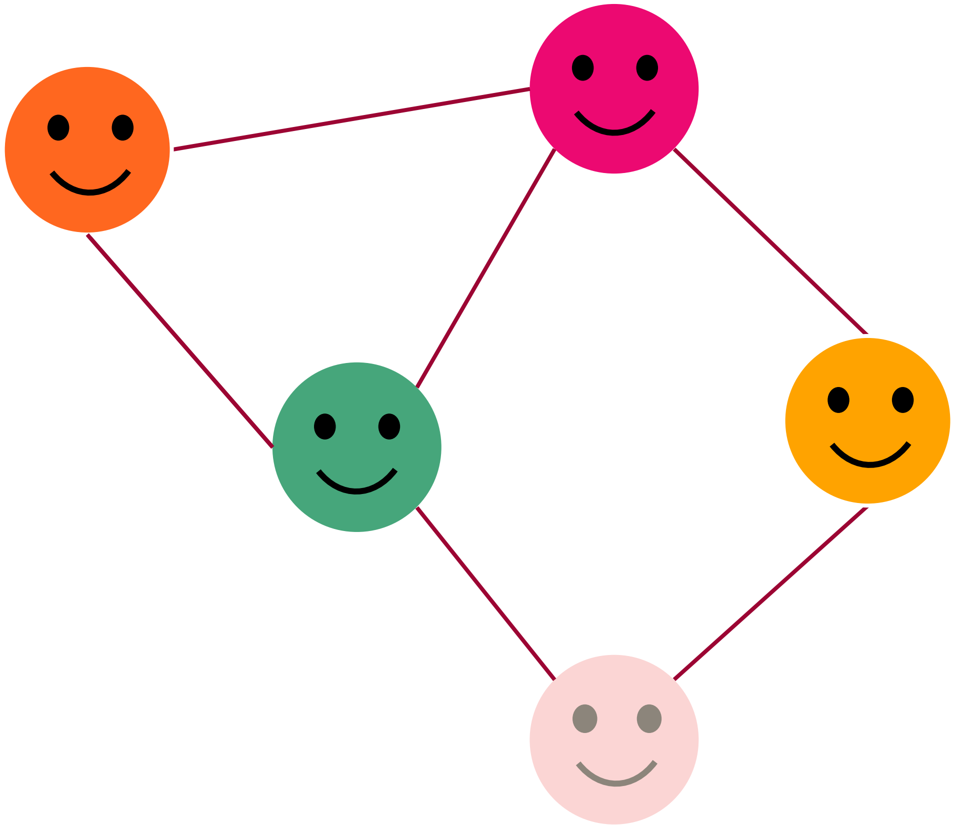

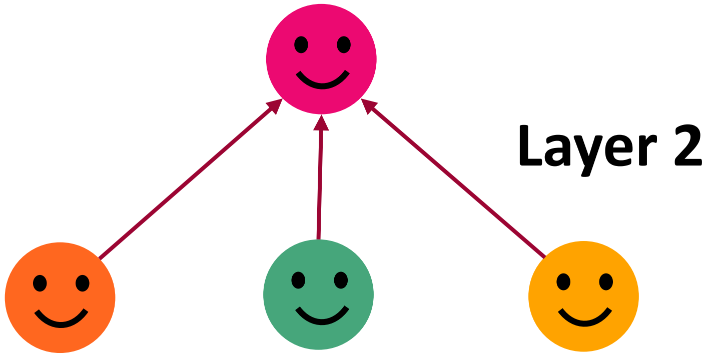

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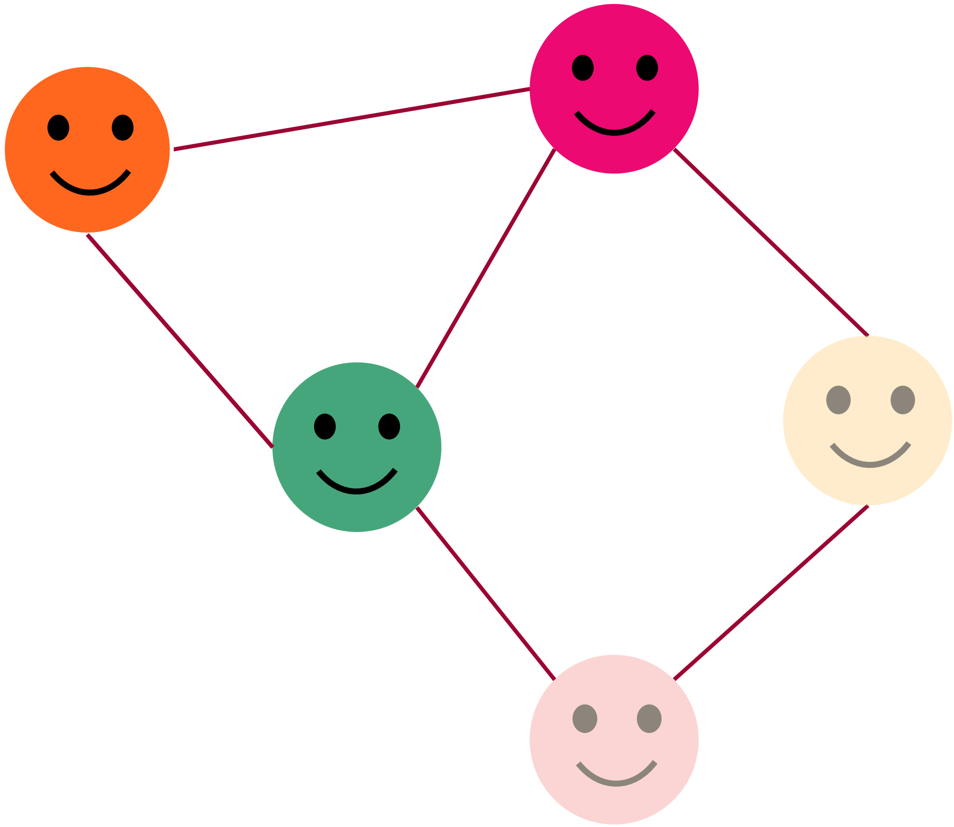

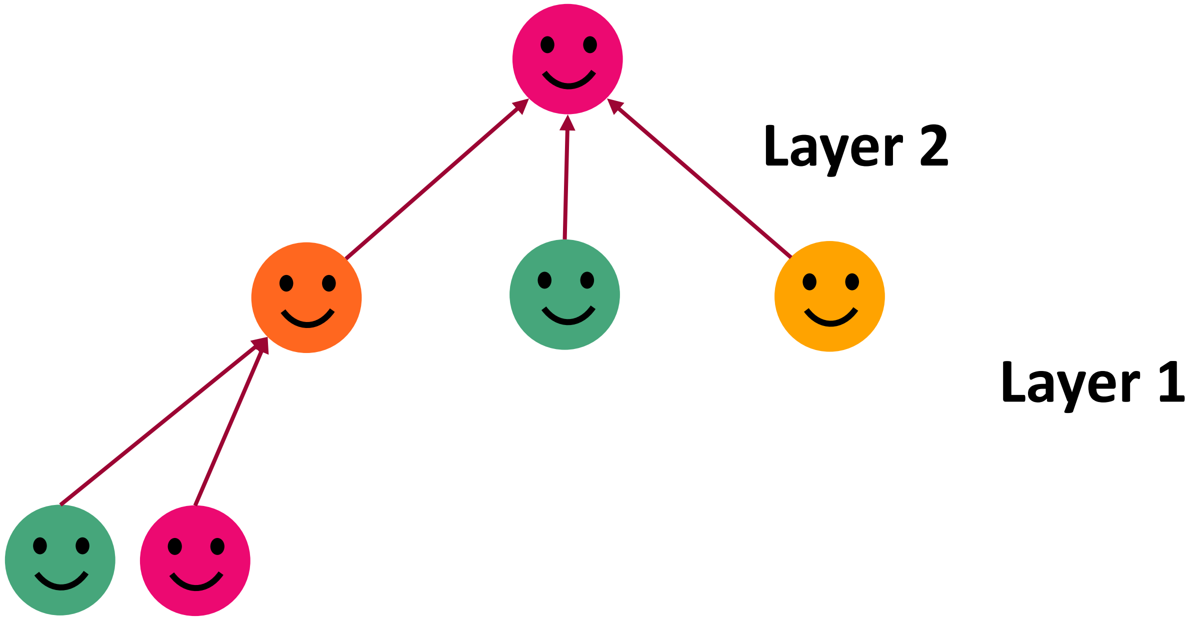

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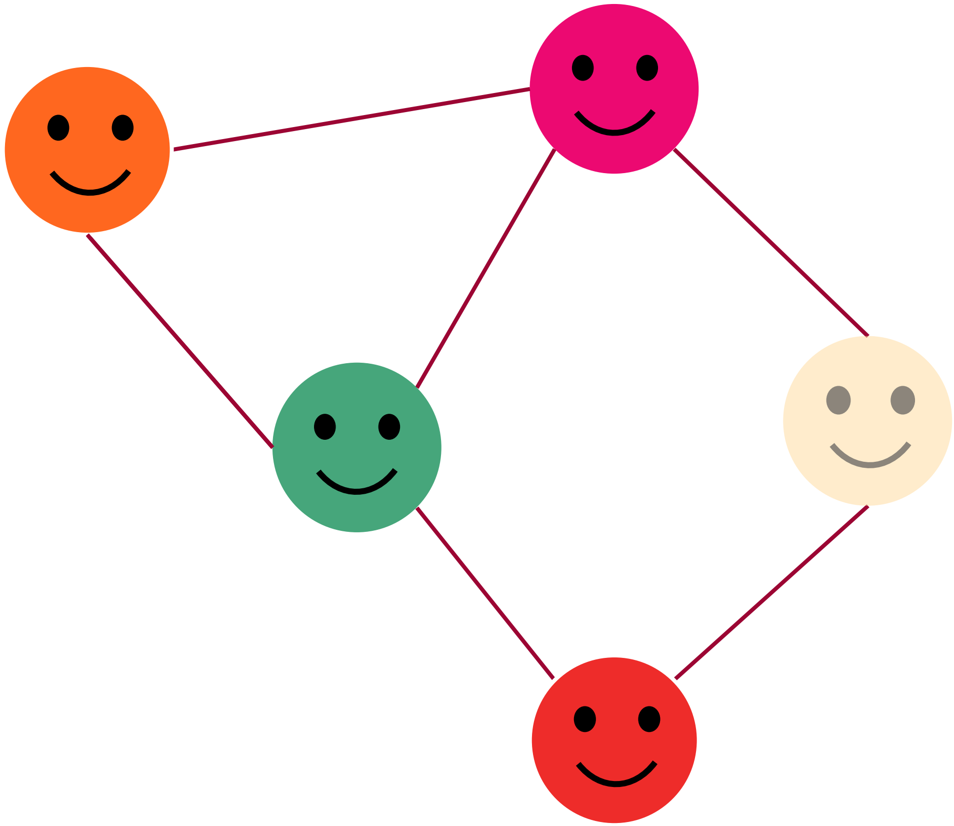

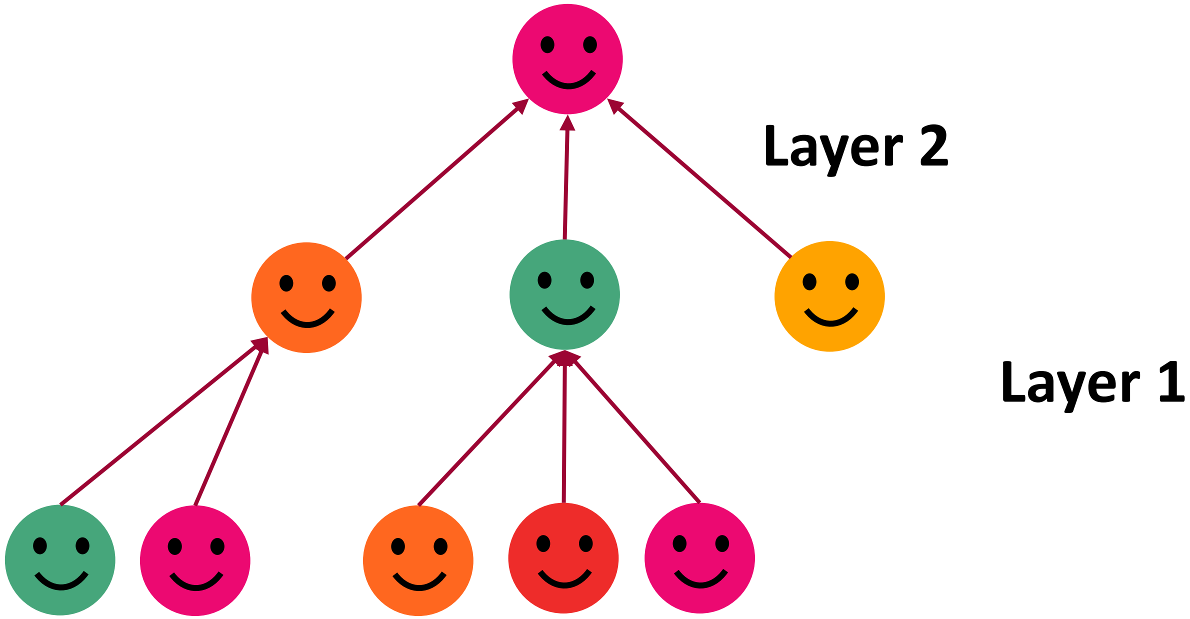

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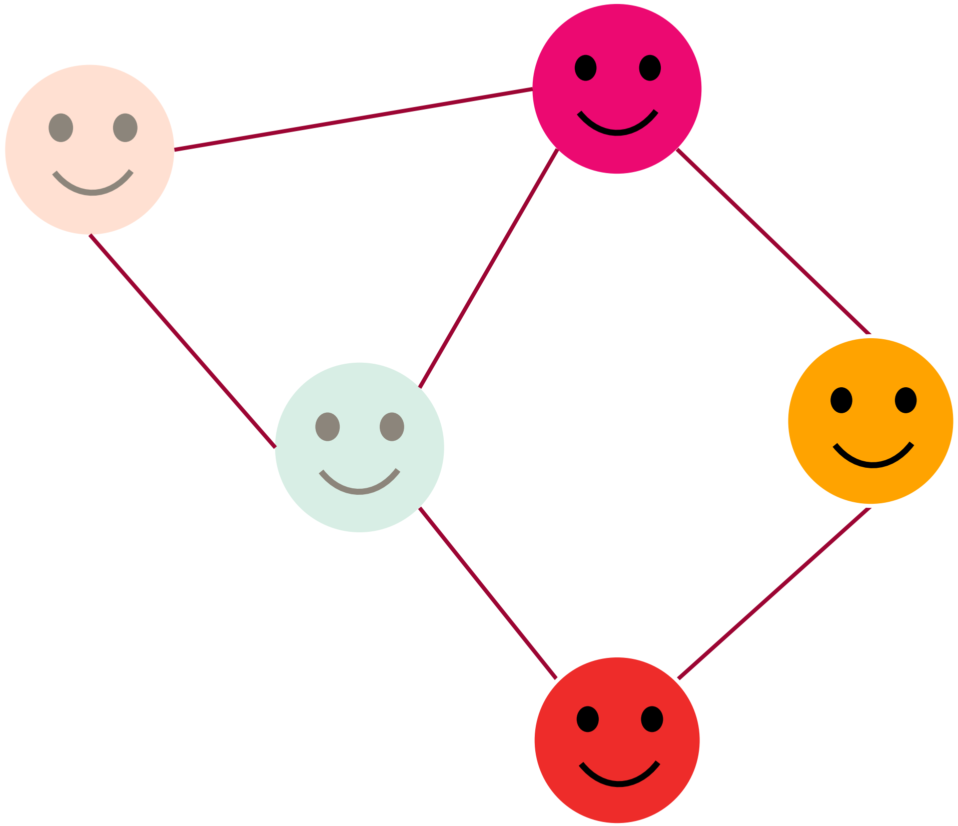
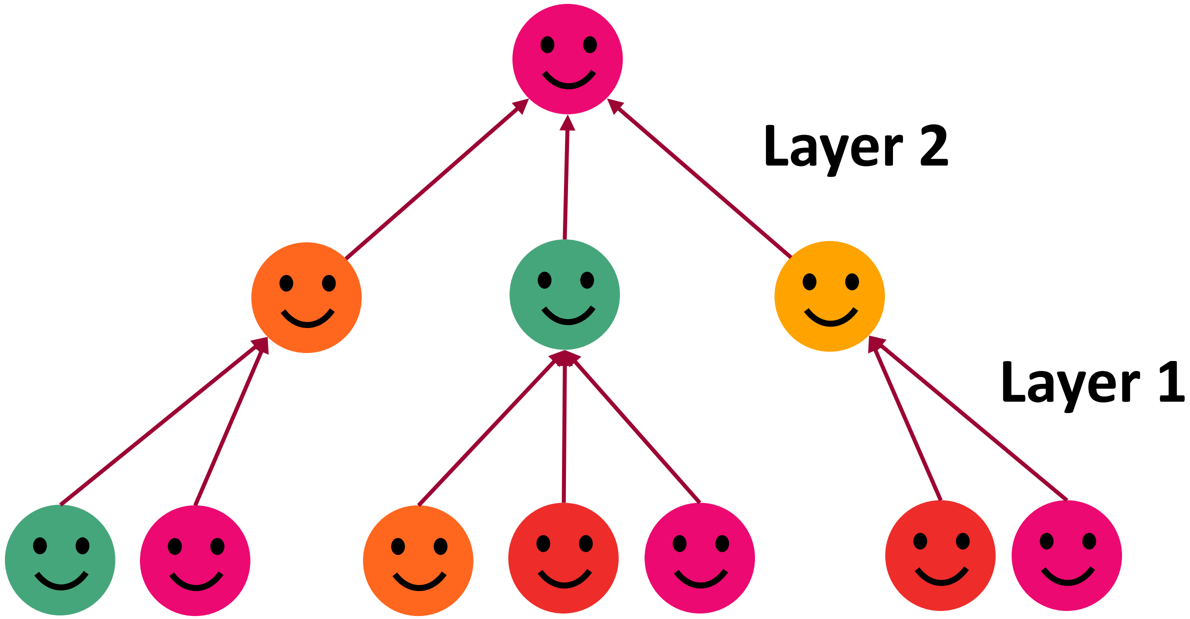
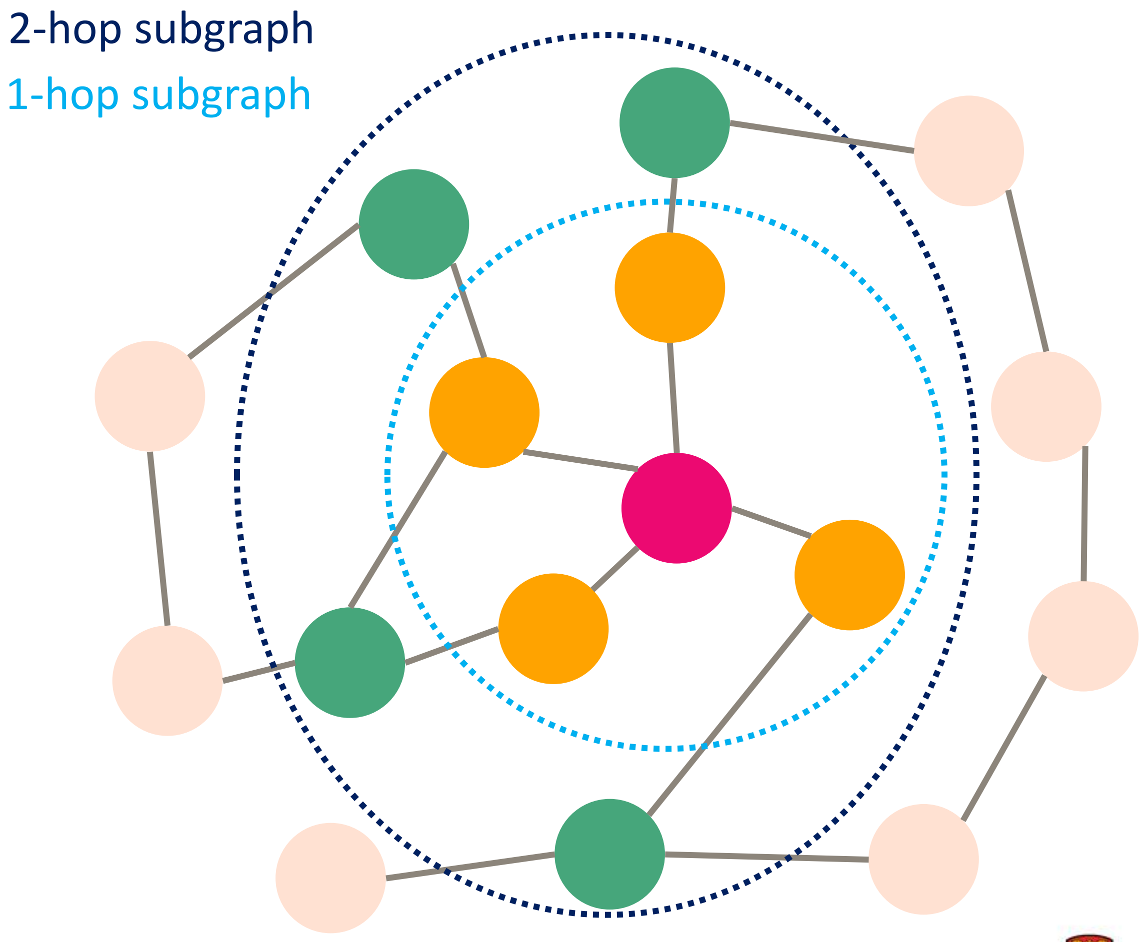




k-hop neighborhood

- The more hops, the more distant information each node gets
- More hops is good for global context
- …but too many hops will wash out local structural information



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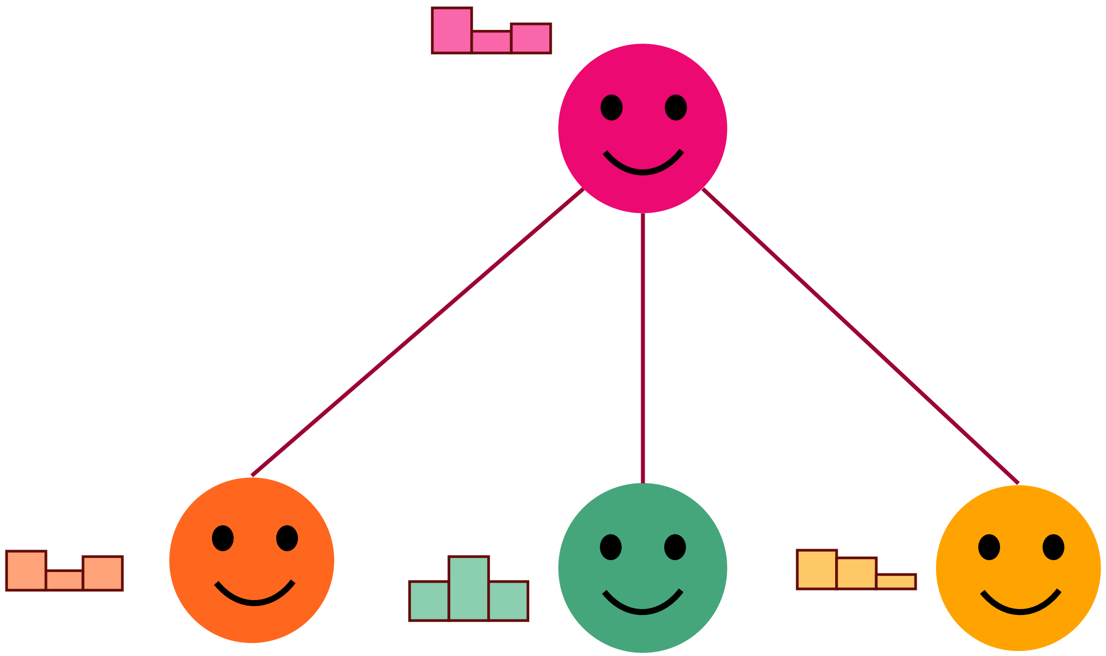
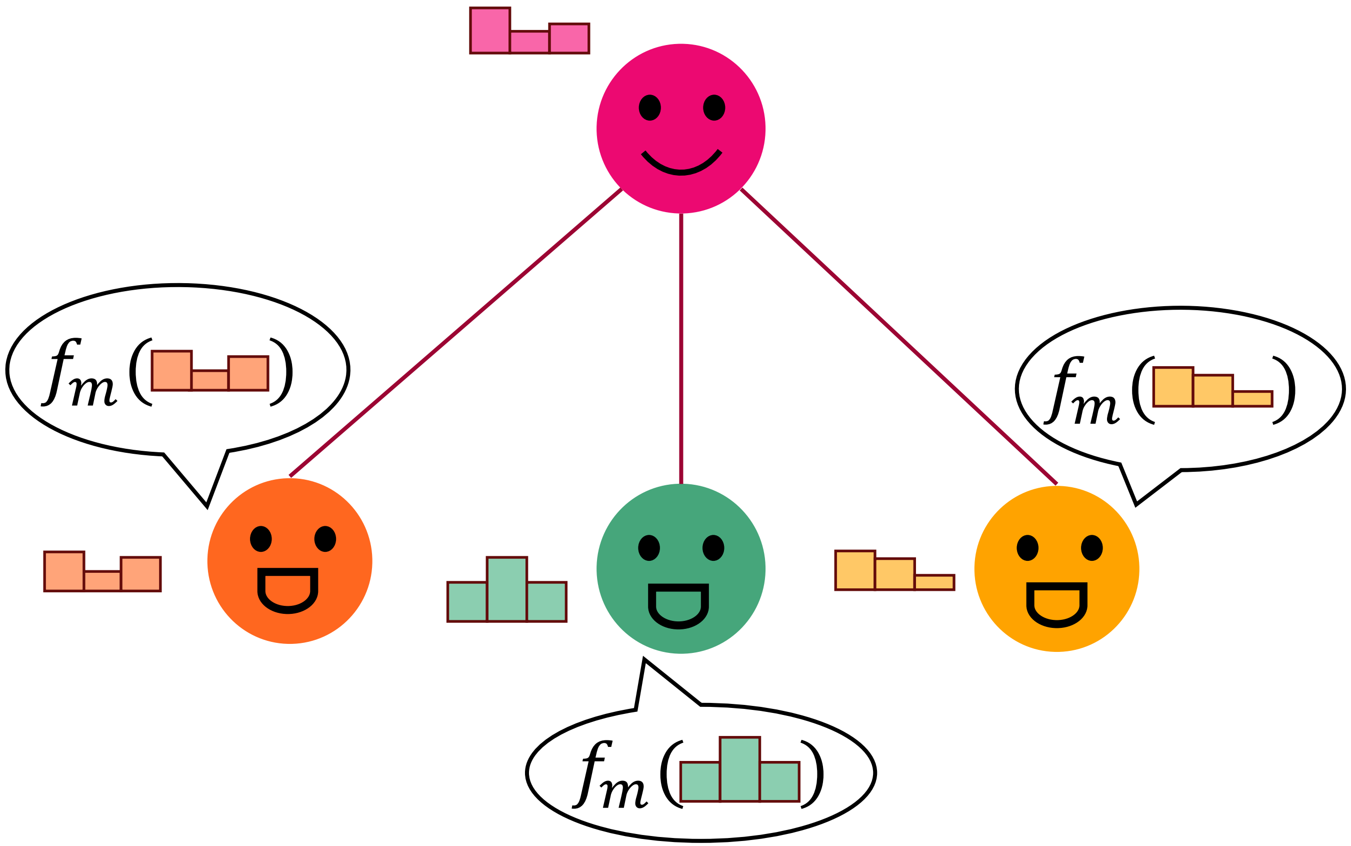
Trainable parameters

- Can think of it as two places we can have trainable parameters:



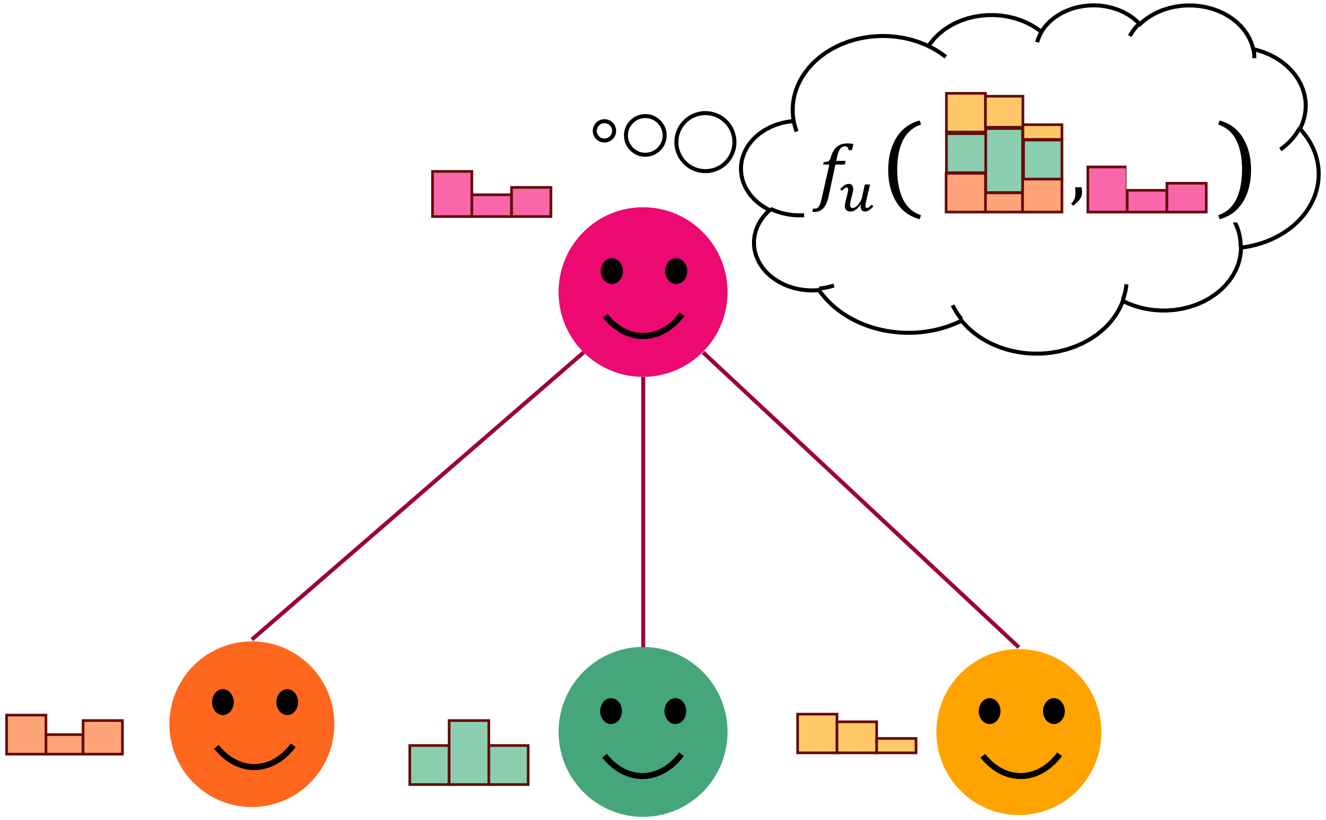
Trainable parameters

- Can think of it as two places we can have trainable parameters:
  - When passing a message



Trainable parameters

- Can think of it as two places we can have trainable parameters:
    - When passing a message
    - When updating an embedding



Trainable parameters

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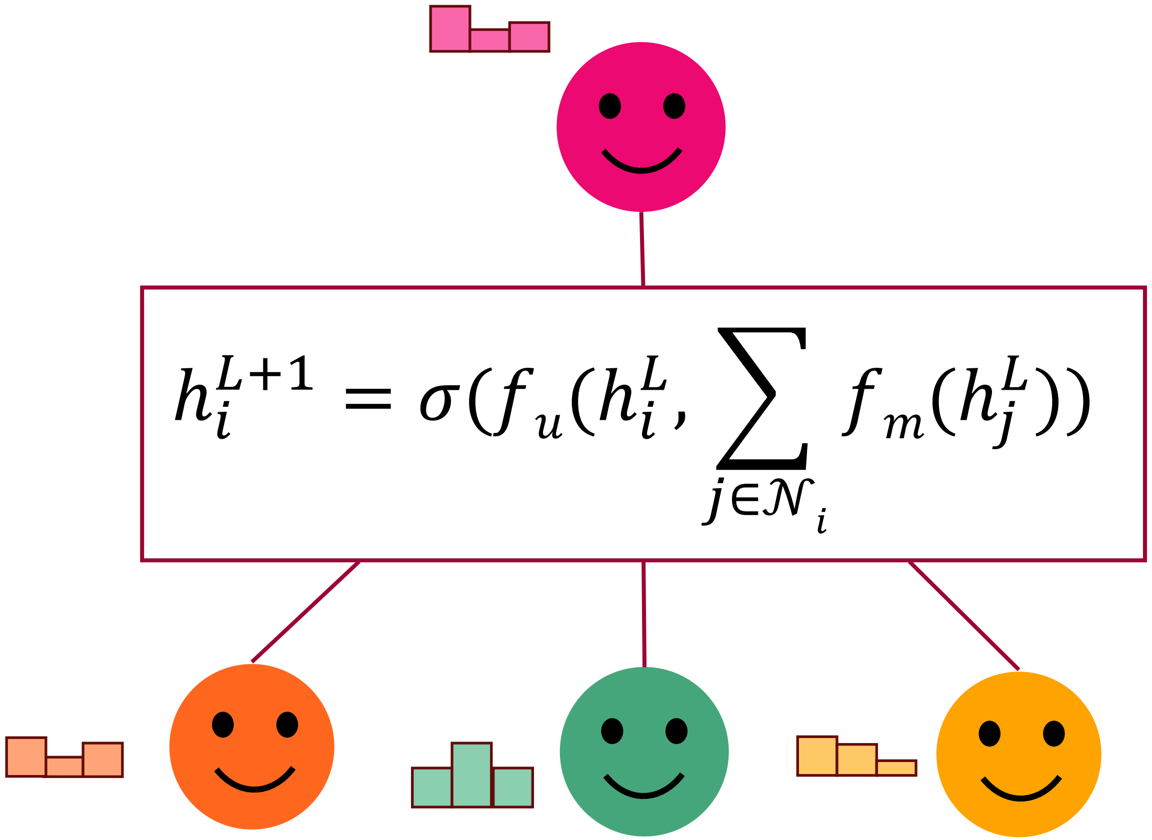
* Note: The trainable parameters are shared across ALL nodes!



$$h_i^{L+1} = \sigma(f_u(h_i^L, \sum_{j \in \mathcal{N}_i} f_m(h_j^L)))$$

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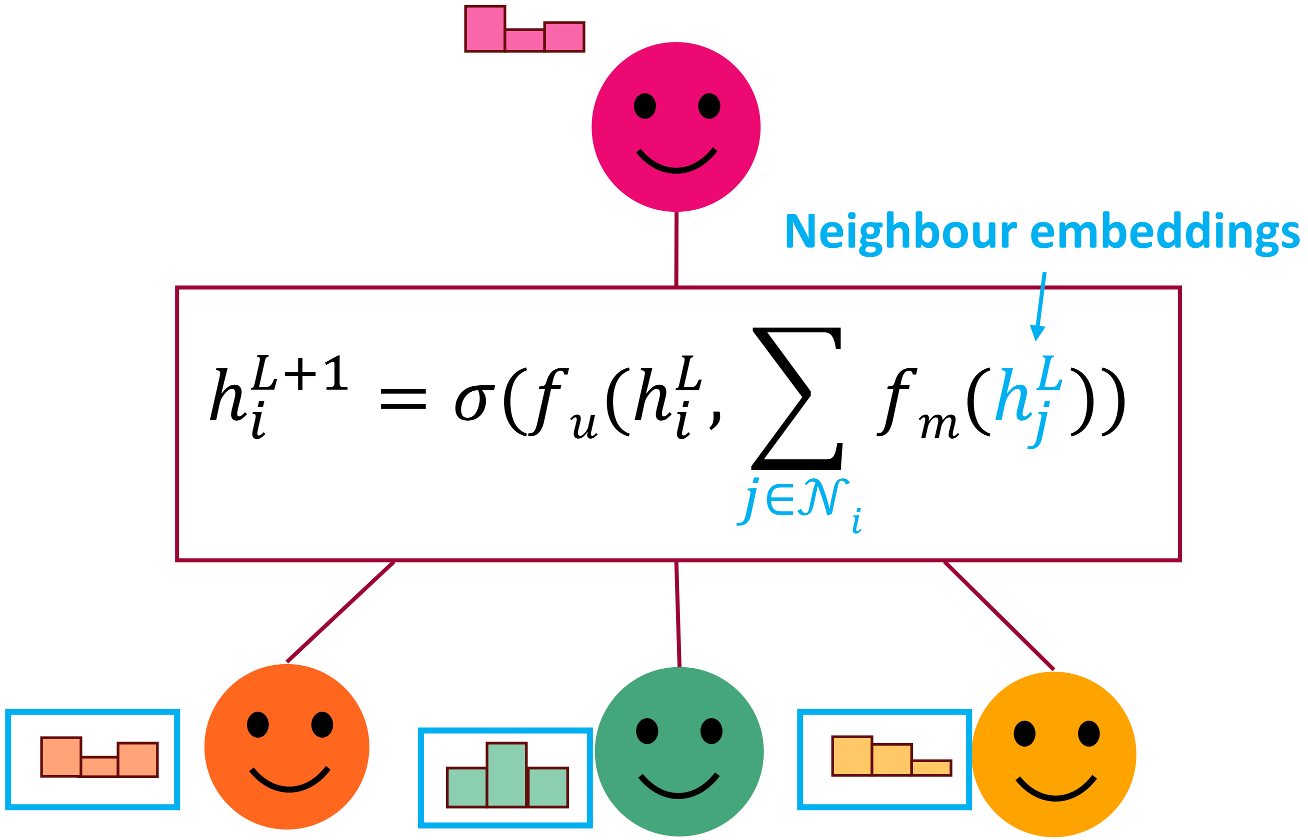

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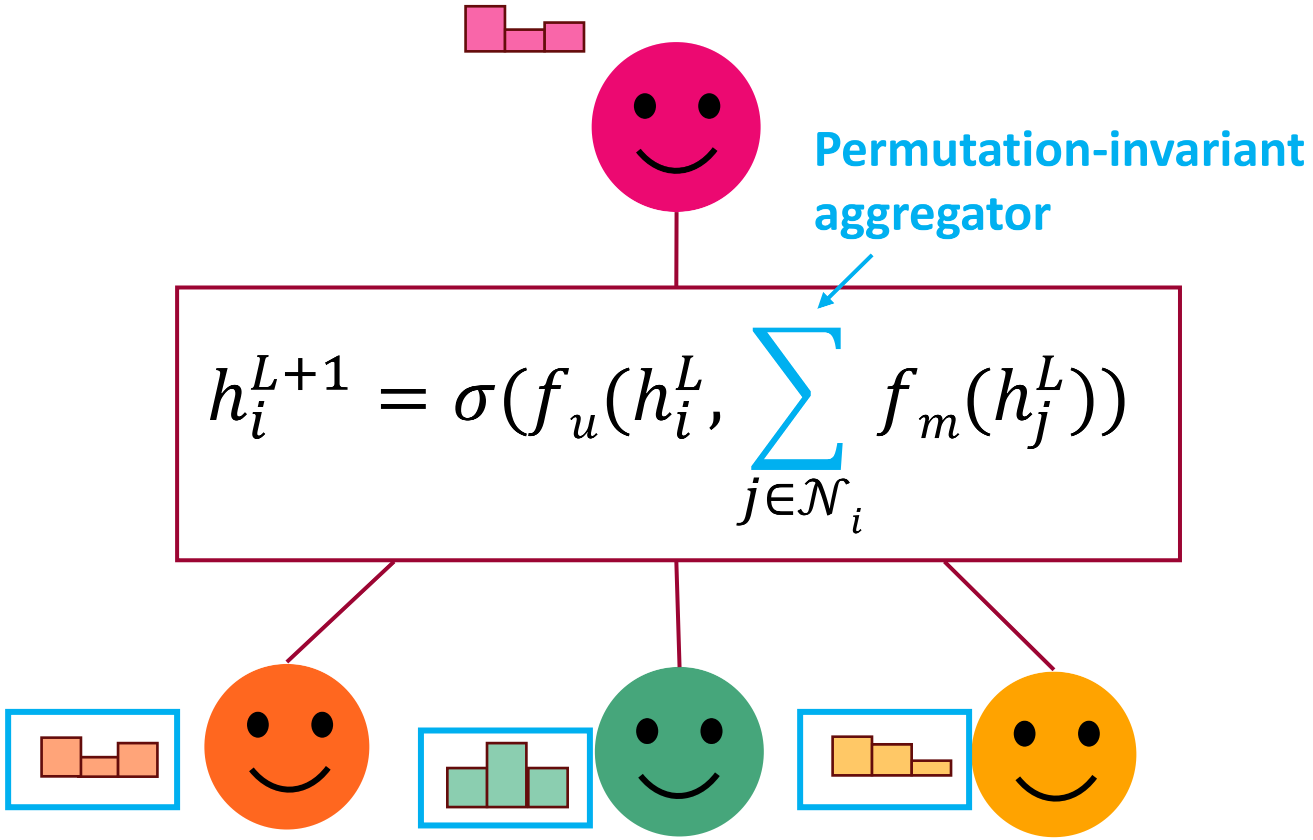

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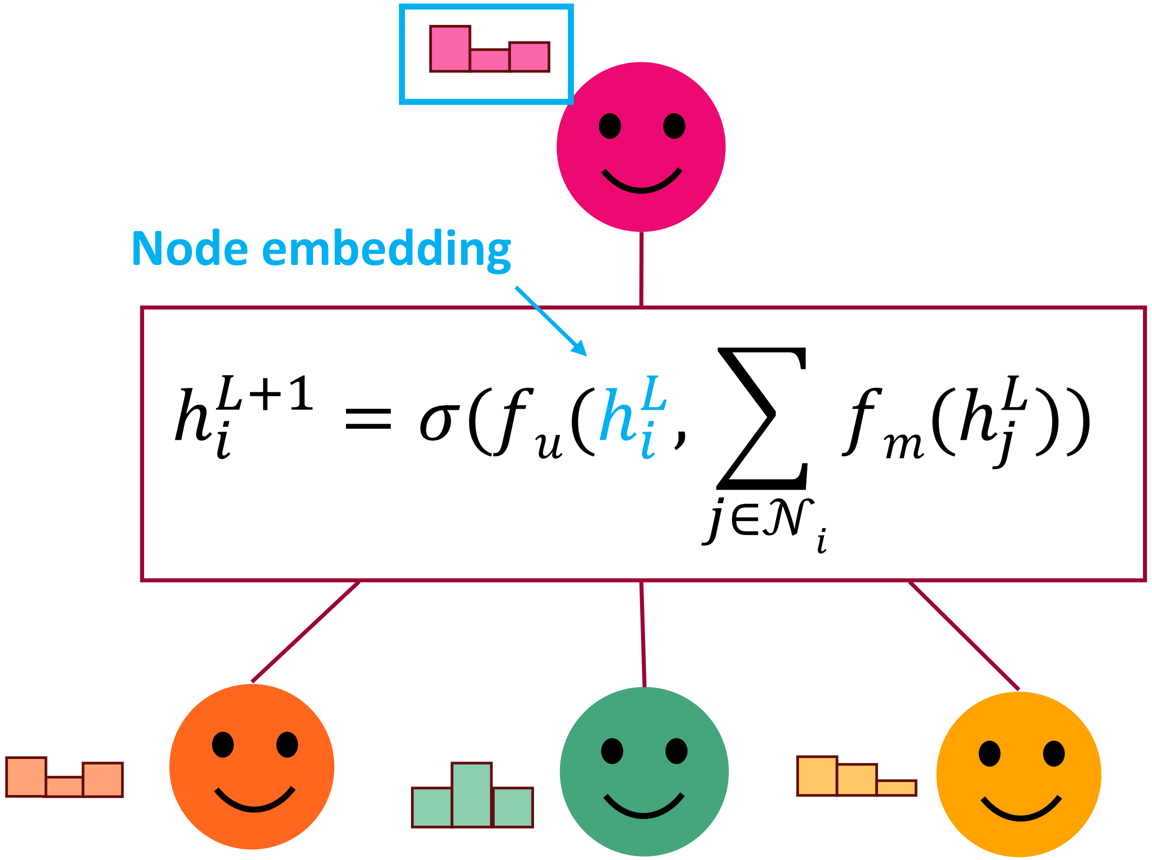

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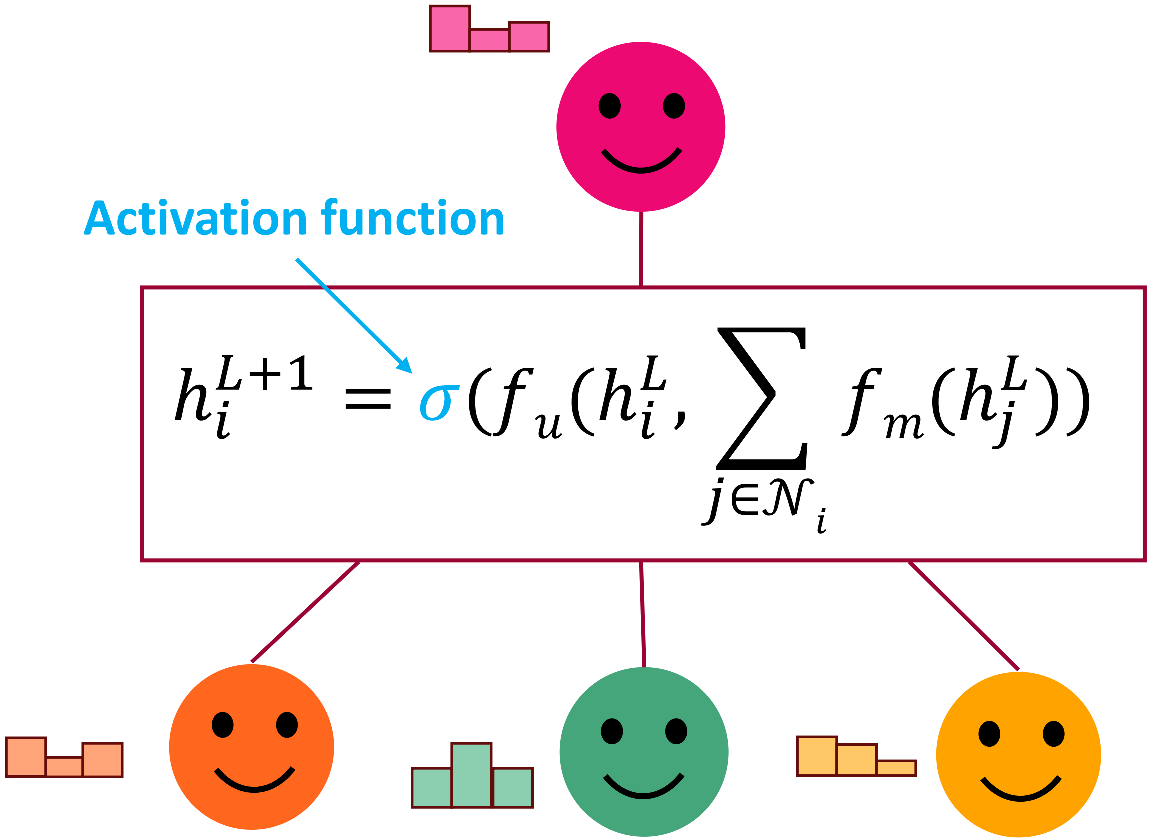

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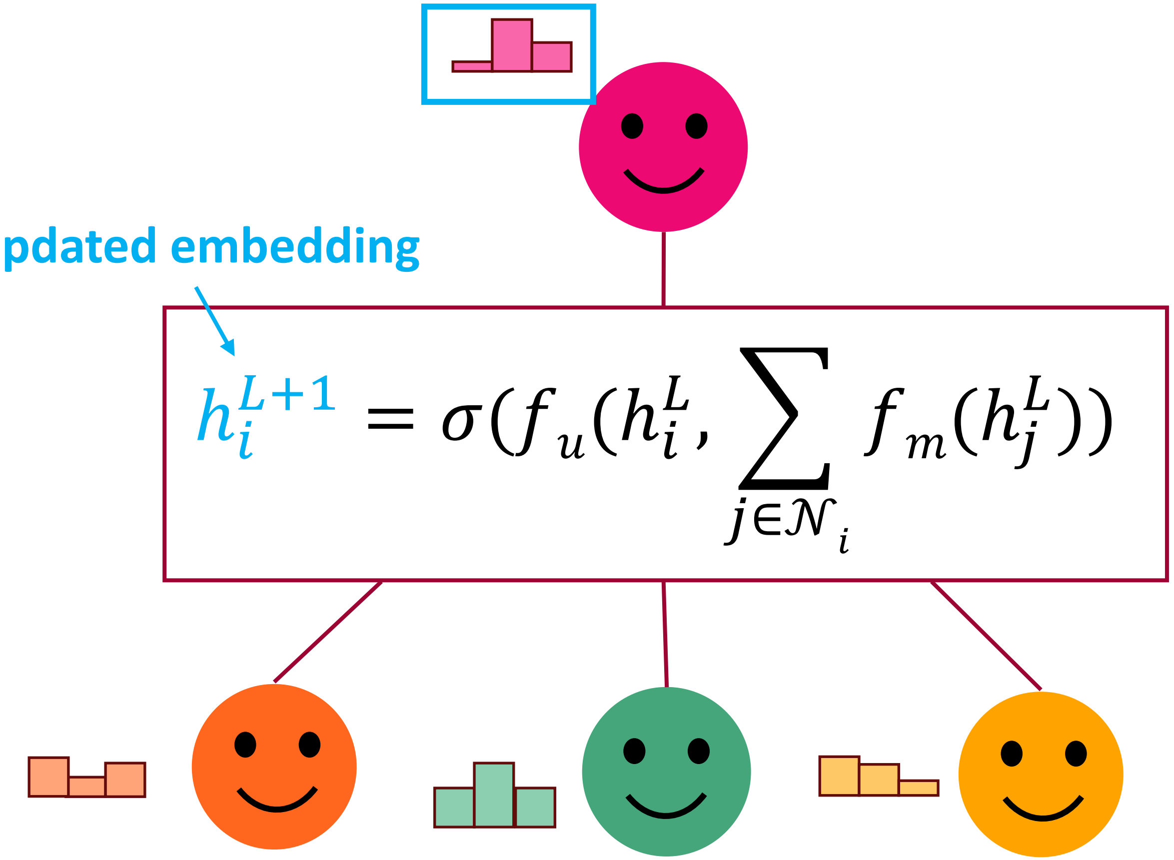
  - When updating an embedding

* Note: The trainable parameters are shared across ALL nodes!



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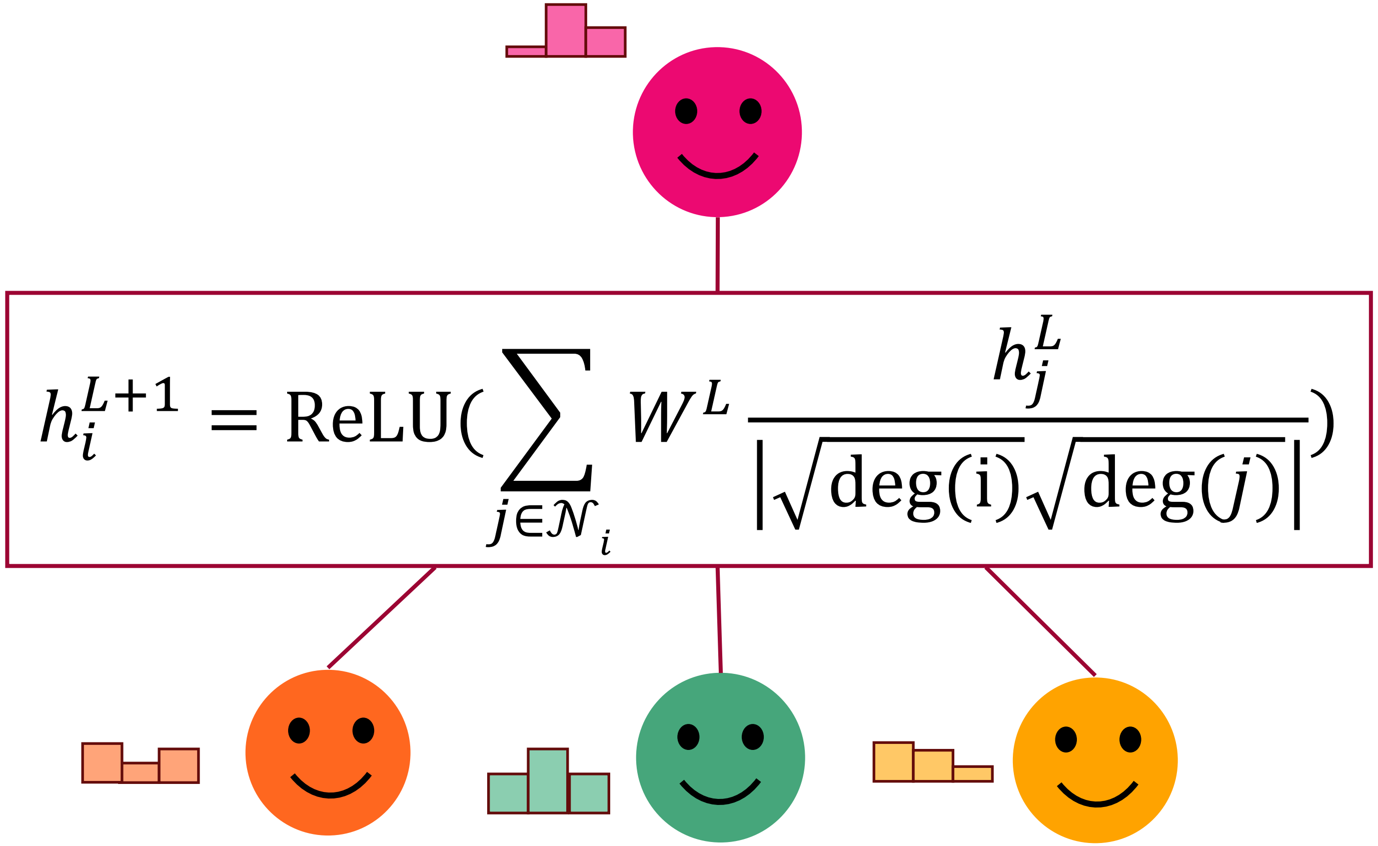
GNN layer example: Graph Convolutional Network

- Graph convolutional network (GCN) learns a simple matrix of weights
  - Can think of this matrix as a 'convolutional kernel' we use at each node instead of pixel



$$h_i^{L+1} = \mathrm{ReLU}\Big(\sum_{j\in\mathcal{N}_i} W^L \frac{h_j^L}{\left|\sqrt{\deg(\mathrm{i})}\sqrt{\deg(j)}\right|}\Big)$$

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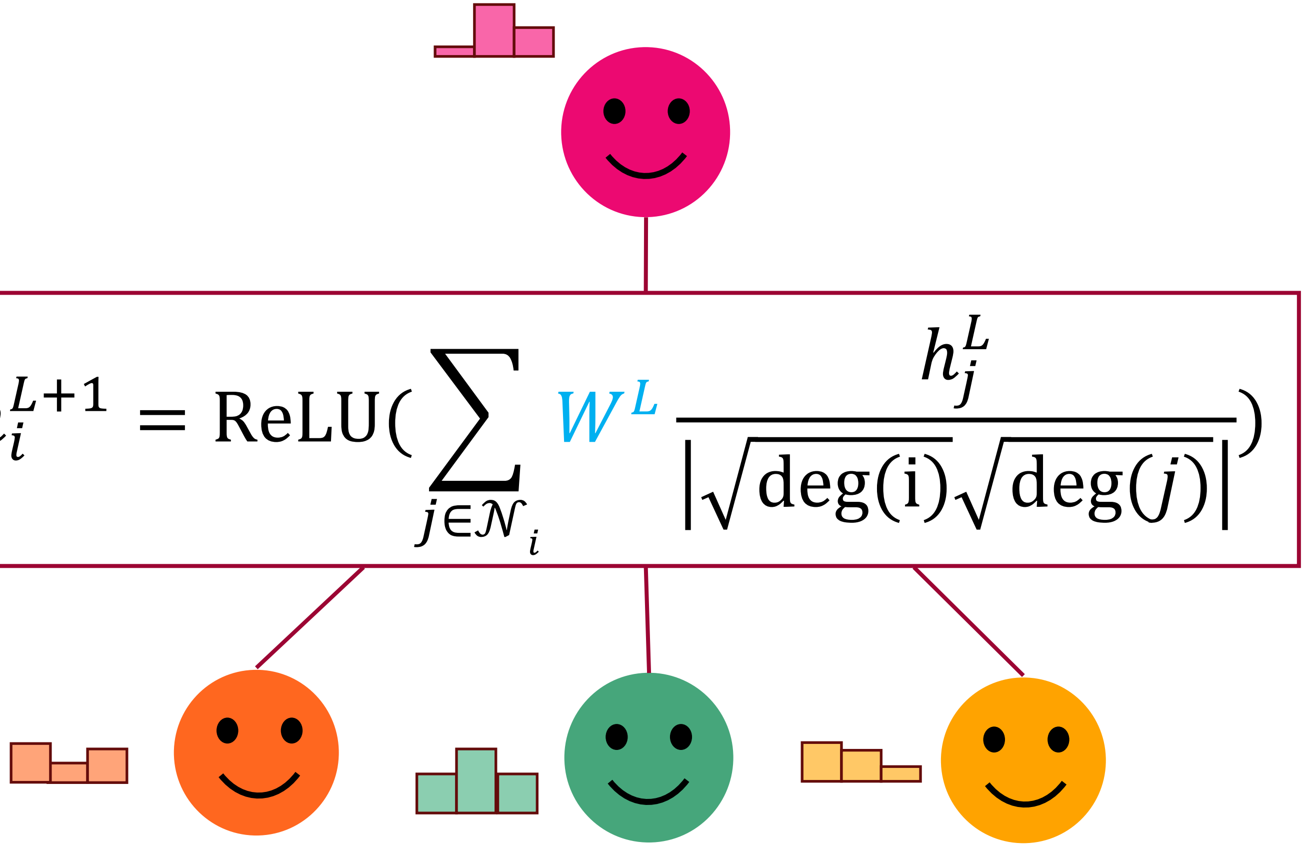

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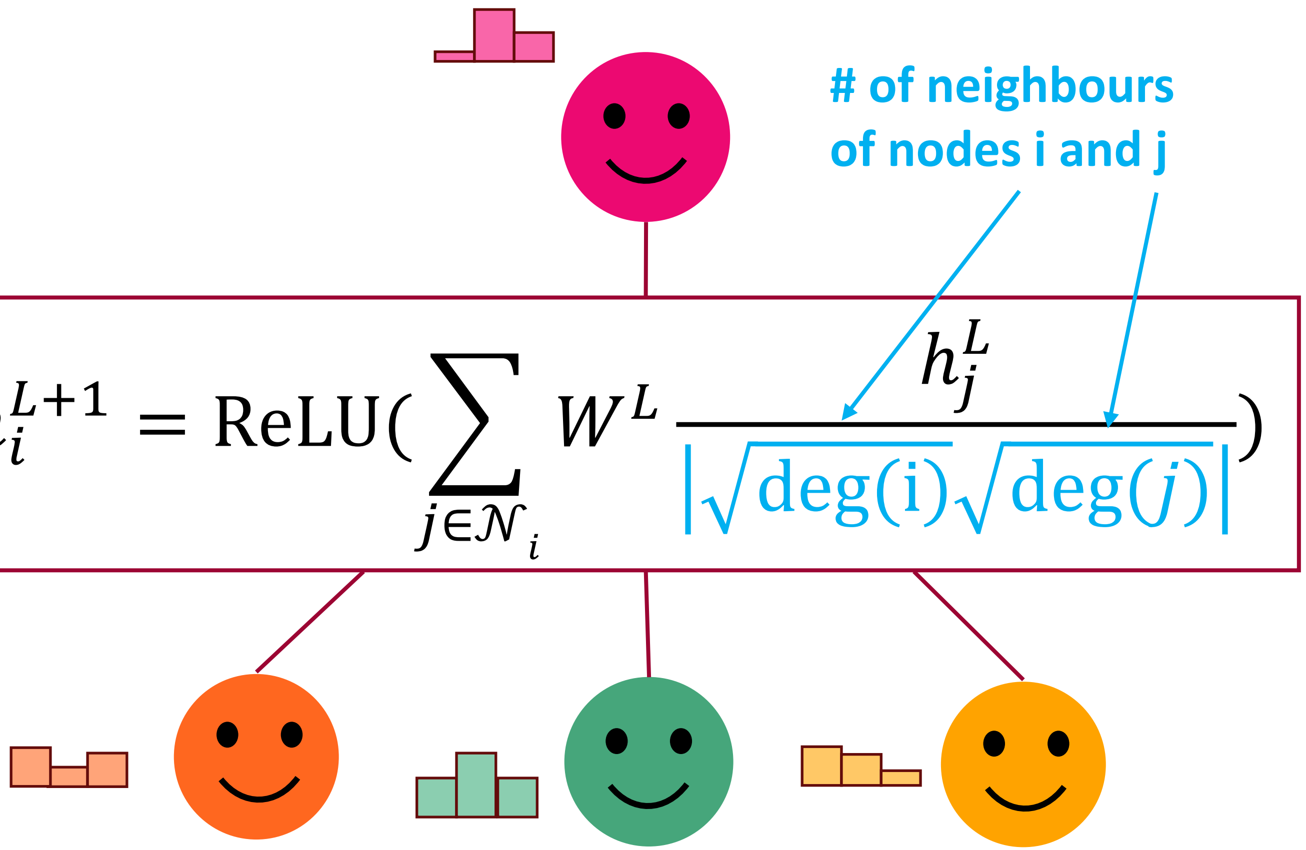

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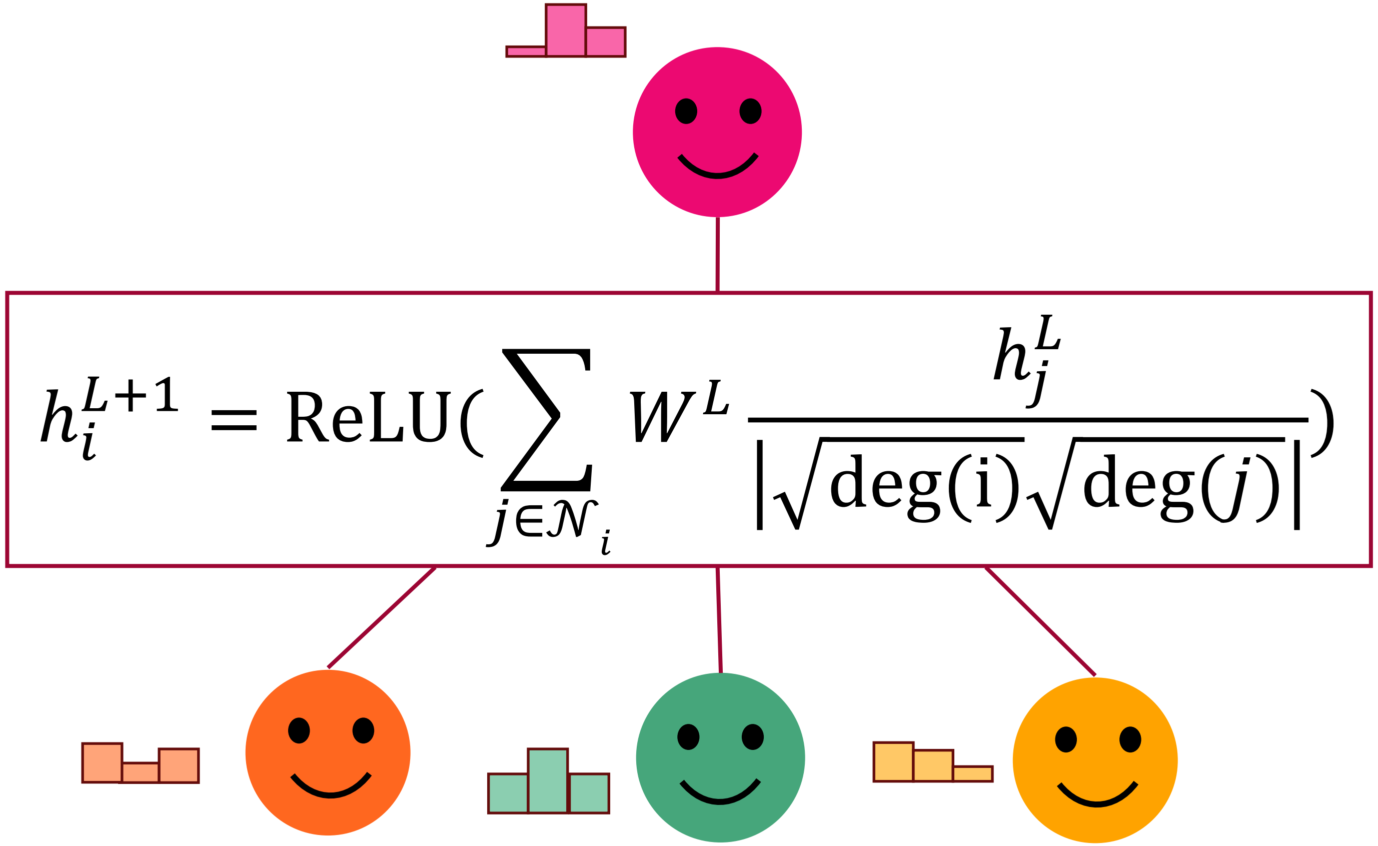
GNN layer example: Graph Convolutional Network

- Graph convolutional network (GCN) learns a simple matrix of weights
  - Can think of this matrix as a ‘convolutional kernel’ we use at each node instead of pixel
- GCN assumes self-edges!
  - So, each node is its own neighbor 🤔

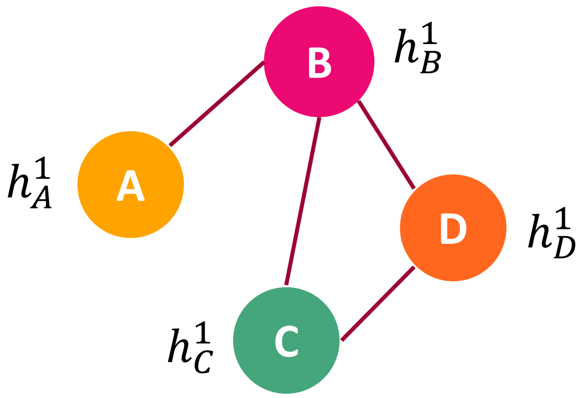


$$h_i^{L+1} = \mathrm{ReLU}\Big(\sum_{j\in\mathcal{N}_i} W^L \frac{h_j^L}{\left|\sqrt{\deg(\mathrm{i})}\sqrt{\deg(j)}\right|}\Big)$$

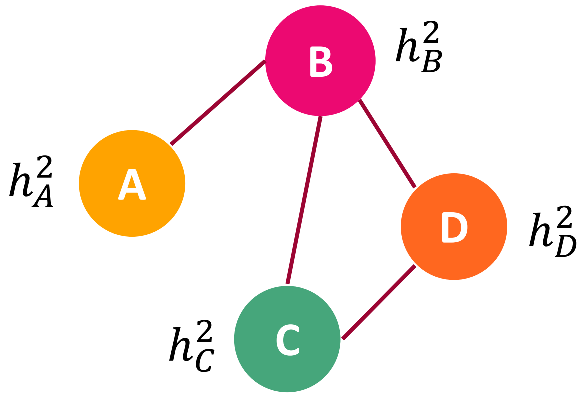
Putting it all together

- We *could* just learn node/edge/graph embeddings e.g. node2vec
- To tailor network for a specific task, we add an appropriate head
- E.g. Node classification:

Graph layer 1



Graph layer 2



Softmax

*Size of h_i^2 = # of classes

h_A^2 → [0.7, 0.3]

h_B^2 → [0.2, 0.8]

h_C^2 → [0.5, 0.5]

h_D^2 → [0.1, 0.9]

$$\frac{e^{h_i^2}}{\sum_j^K e^{h_j^2}}$$

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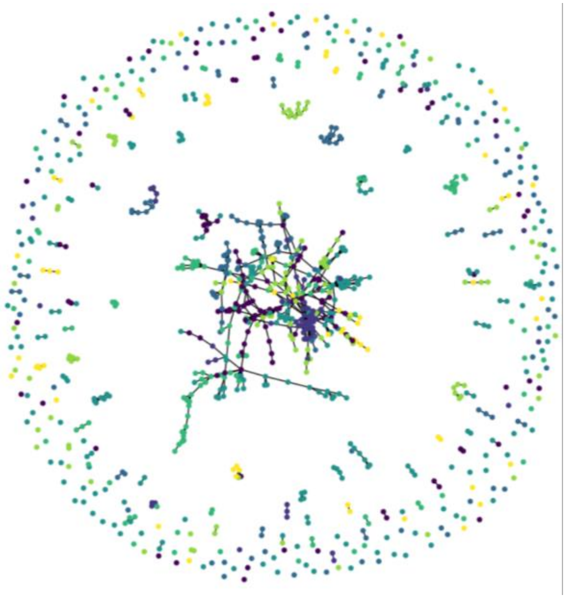
Summary

- Graph structured data is one of the most general types of data that encompasses a broad range of applications
- Graph neural networks can be used to solve a variety of tasks
- Since graph data is inherently different from other types of data, we need a unique framework to handle it
- Message passing allows for all the information in a graph to be effectively harnessed

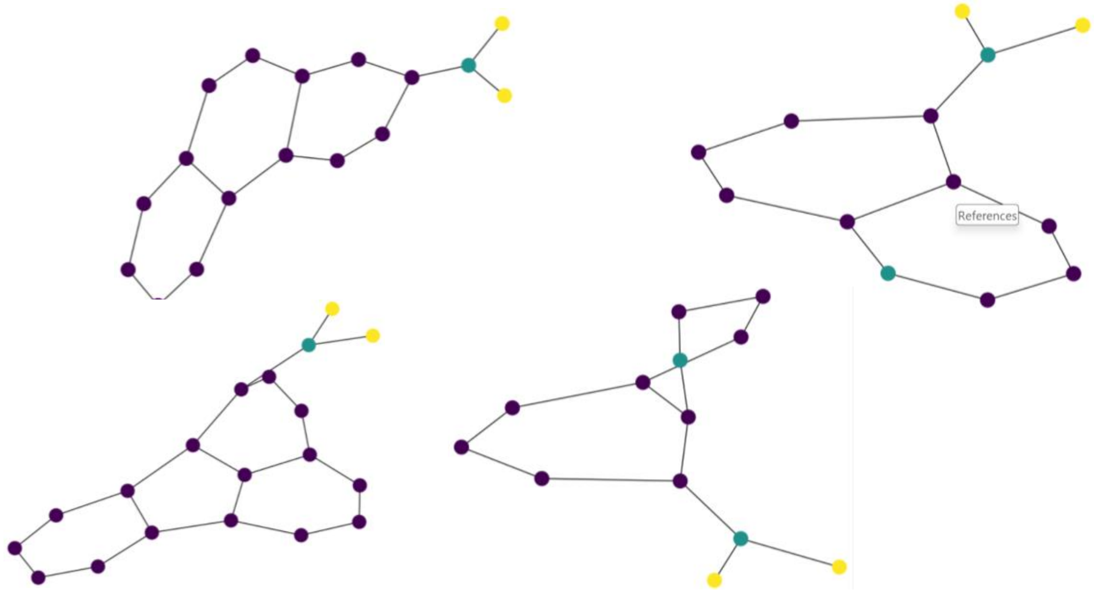
Next class:

- We will learn how to work with graphs and build models using pytorch-geometric!

Cora dataset (Citations)



TU MUTAG Dataset (Molecules)



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Thank you!