Hands-on Introduction to Deep Learning

Graphs are everywhere

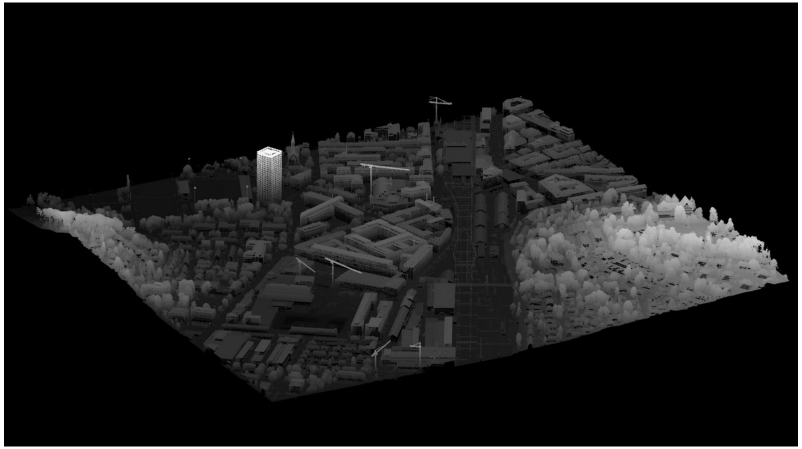
Data structures: Euclid and Text

Highly ordered data

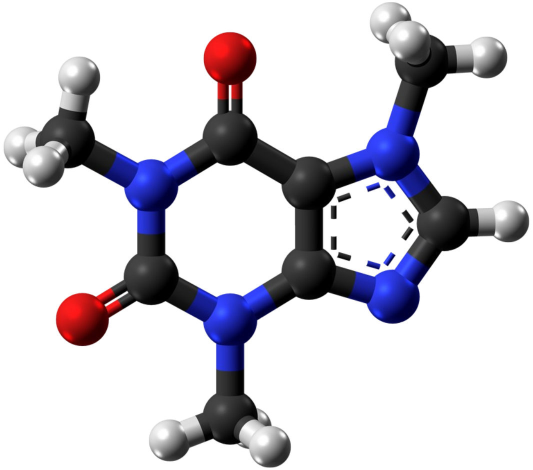
Rebirth of Deep learning was thanks to pictures, text and speech recognition

Data structures: Data is not always euclidean

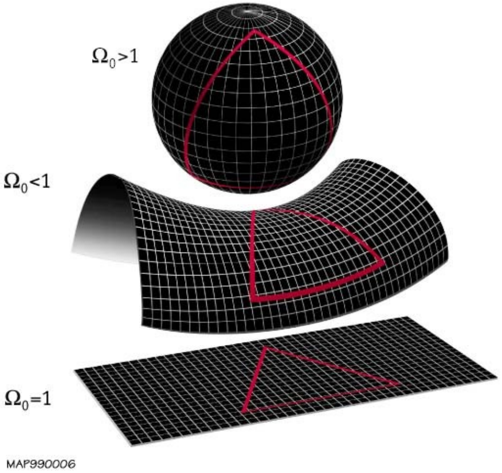
LIDAR



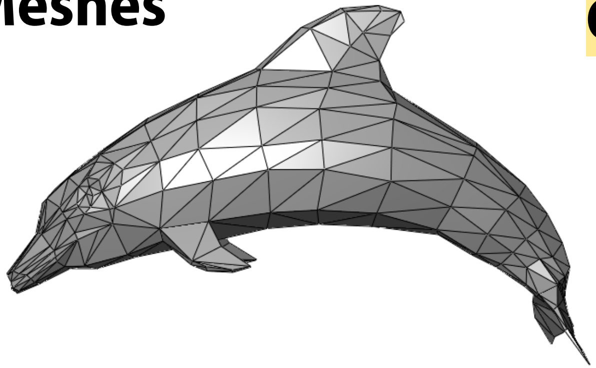
Molecules



Complex geometries

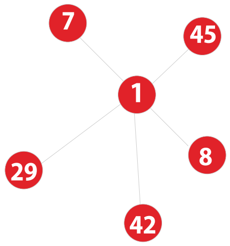


Meshes



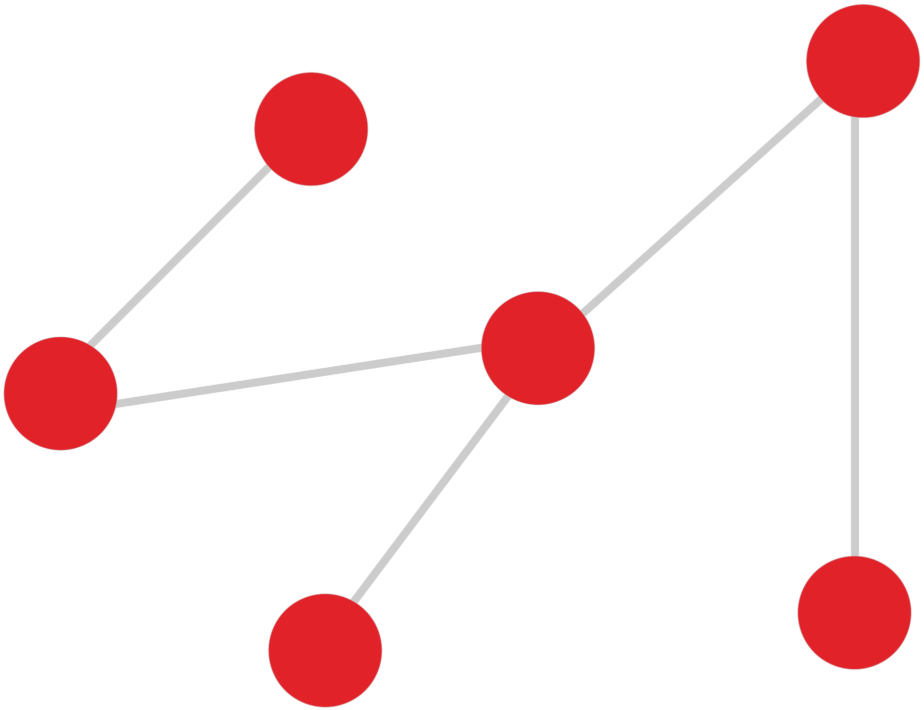
Geometric deep learning

Neighborhood:



Michael M. Bronstein, Joan Bruna, Taco Cohen, Petar Veličković, Geometric Deep Learning: Grids, Groups, Graphs, Geodesics, and Gauges https://arxiv.org/abs/2104.13478

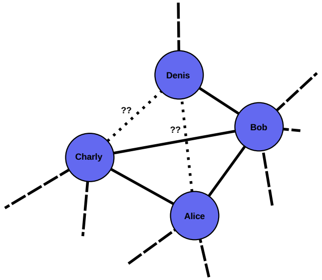
Graphs are everywhere



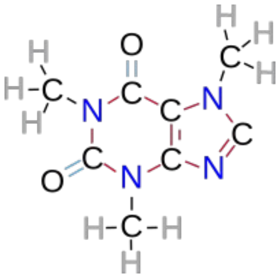
Data as a set of interconnected entities

Graphs are everywhere

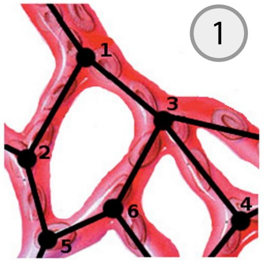
Social networks



Molecules

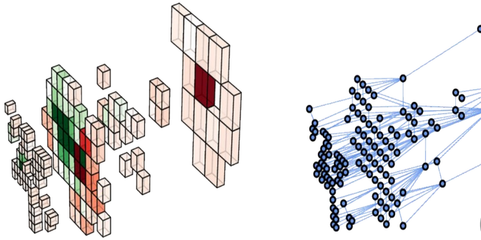


Capillary networks



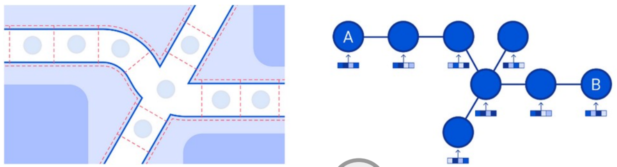
1

Particle physics



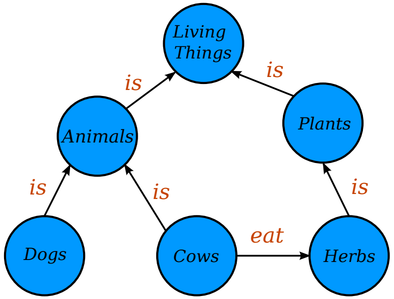
2

Directions recommendation



3

Knowledge graphs



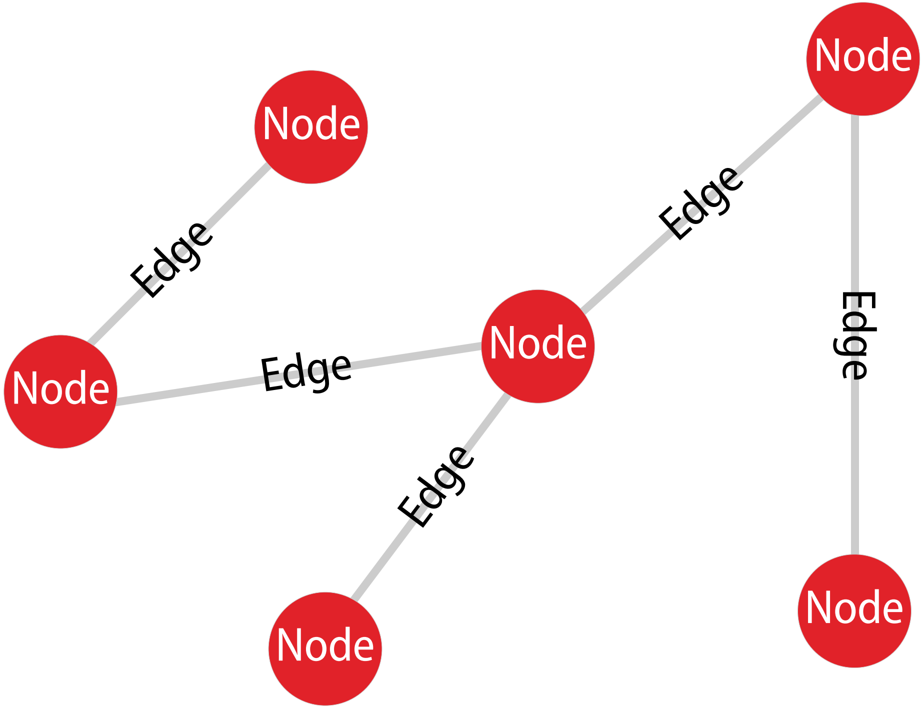
Many other fields

- Biology
- Recommendation systems
- Computer vision
- Medical diagnosis
- Robotics
- ...

[1] Erbertseder, K., Reichold, J., Flemisch, B., Jenny, P., & Helmig, R. (2012). A coupled discrete/continuum model for describing cancer-therapeutic transport in the lung. PLoS One, 7(3), e31966.
[2] J. Shlomi, P. Battaglia, and J.-R. Vlimant, "Graph neural networks in particle physics," Mach. Learn.: Sci. Technol., vol. 2, no. 2, p. 021001, Jan. 2021, doi: 10.1088/2632-2153/abbf9a.
[3] A. Derrow-Pinion et al., "ETA Prediction with Graph Neural Networks in Google Maps," in Proceedings of the 30th ACM International Conference on Information & Knowledge Management
New York, NY, USA, Oct. 2021, pp. 3767–3776. doi: 10.1145/3459637.3481916.

Vocabulary

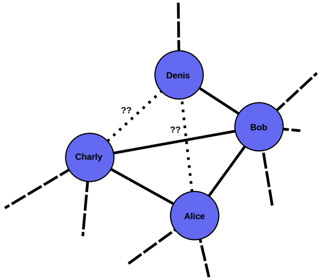
Graph



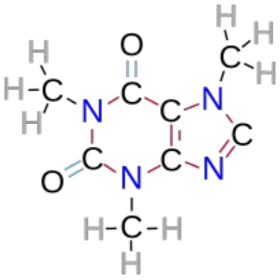
Node/vertex

Some example of nodes

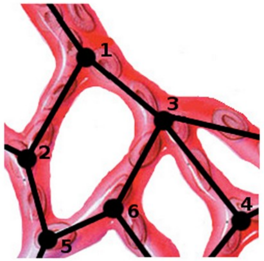
Persons



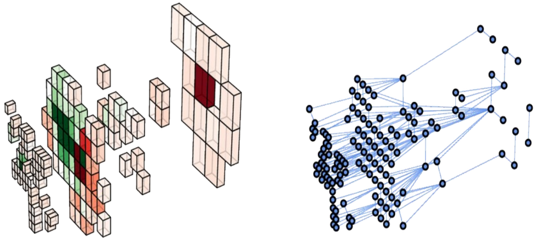
Atoms



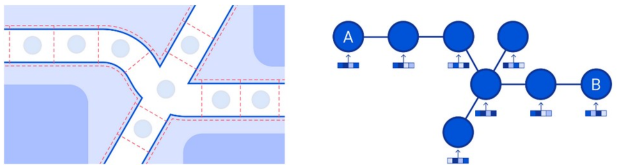
Intersections



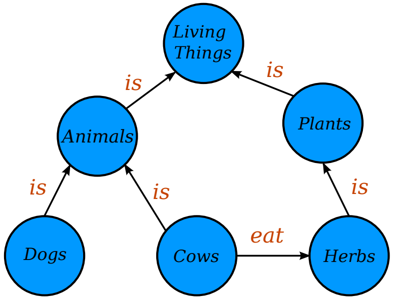
Particles



Road sections



Concepts



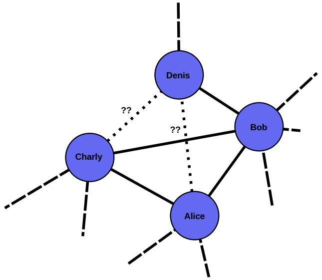
Many other fields

- Biology: An aminoacid in a protein
- Recommendation systems: A customer
- Computer vision: An object in a picture
- Medical diagnosis: Brain region (MRI)
- Robotics: Joints
- ...

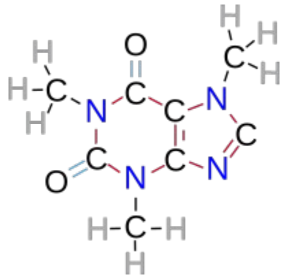
Edge

Some example of edges

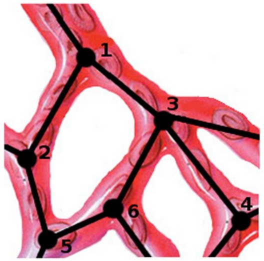
Relationship



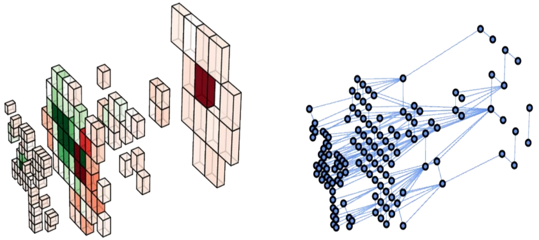
Type of bond



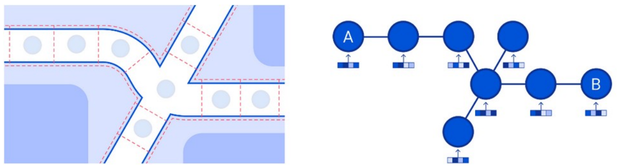
Vessel



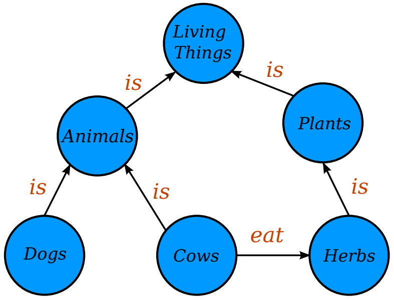
Decayed to



Time



Statement



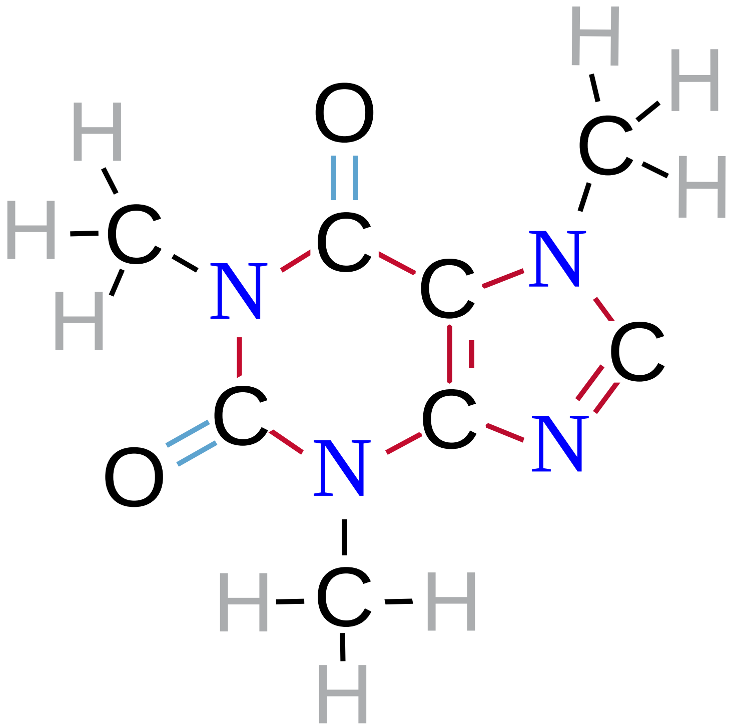
Many other fields

- Biology: Distance between residues
- Recommendation systems: Connected customers
- Computer vision: Interaction between objects
- Medical diagnosis: Interaction between brain region (MRI)
- Robotics: connection between joints
- ...

Edge: orientation

A relationship can be symmetrical or not between nodes

Undirected graphs

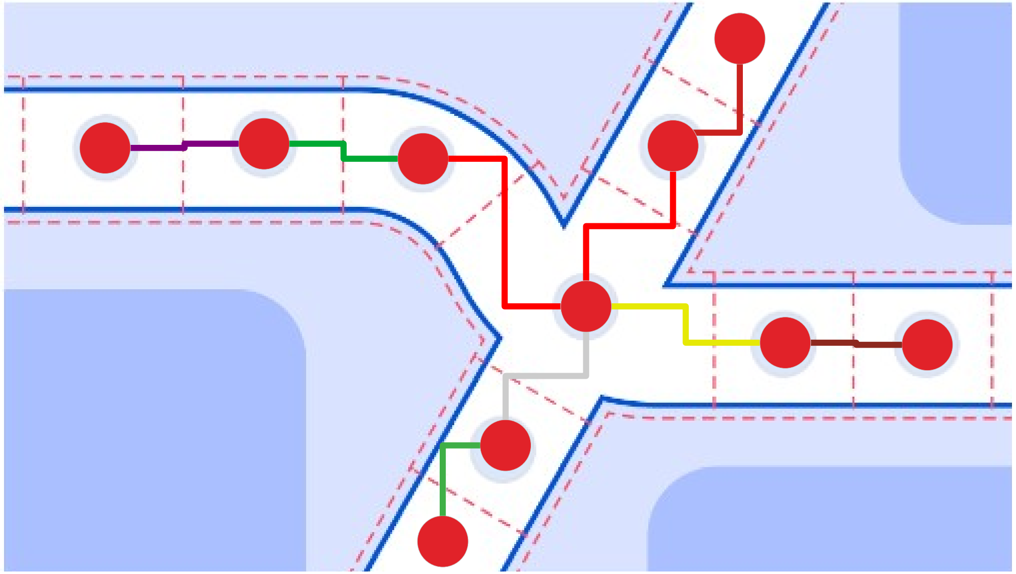


Directed graphs

Alterna2 http://www.alterna2.com, CC BY 2.0 <https://creativecommons.org/licenses/by/2.0>, via Wikimedia Commons

Edge: weight

Edges can carry information → **edge weight**



Graphs store information: Features

Graphs can store information on **nodes**, **edges** and **globally**

	Globally	Nodes	Edges
Social Network	Group of interest,...	Name, age, job,...	Is friend, follows, family,...
Molecule	Is a drug, energy,...	Atomic number,...	Bond order,...
Citations	Field,...	Article,...	Was cited,...
Particle physics	Experiment,...	Particle,...	Decayed to,...
Motion capture	Character,...	Joints,...	Is connected to,...
Natural language	Paragraph,...	Group of words,...	Refers to,...

It can be a number, a concept, ...

Formal definition

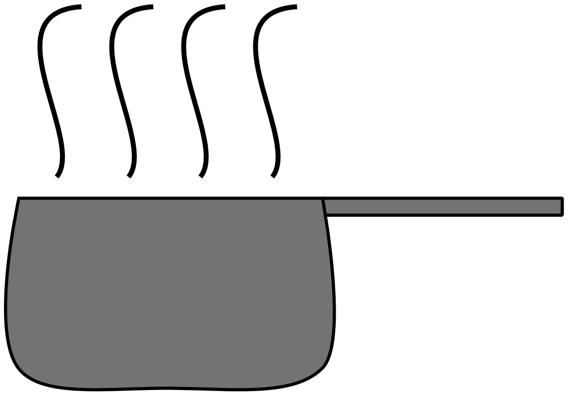
G = (V, E): a set of nodes and edges

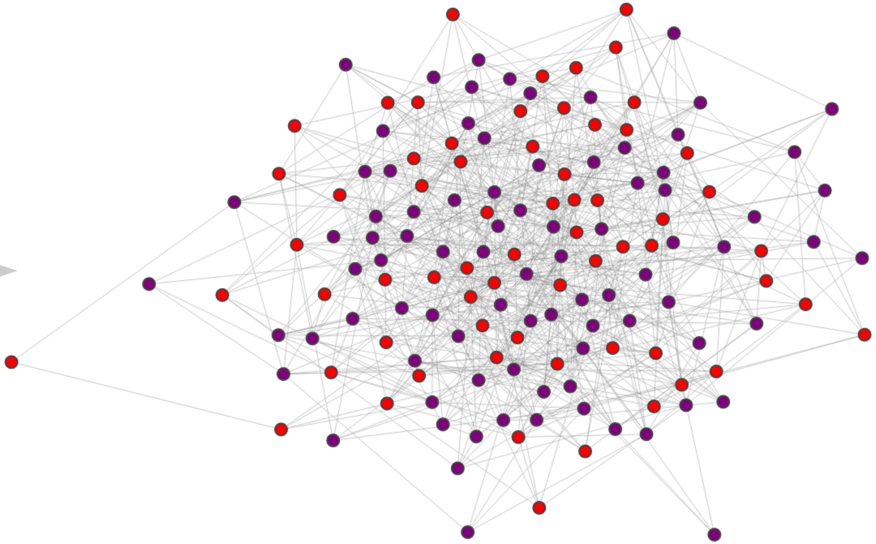
Features

$\{y_i^V\}$ $\{y_i^E\}$ $\{y_i^G\}$

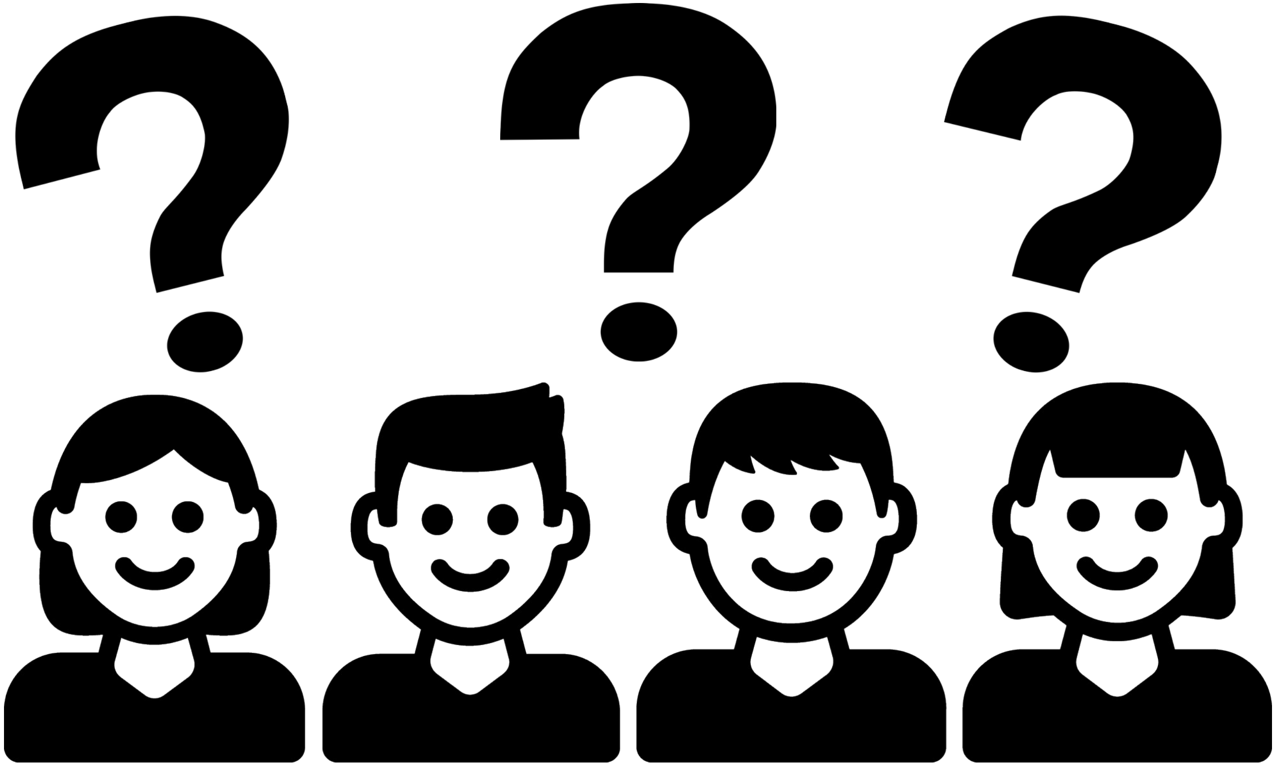
$\{v_i\}_{i\in V}$

$\{e_i\}_{i\in E}$

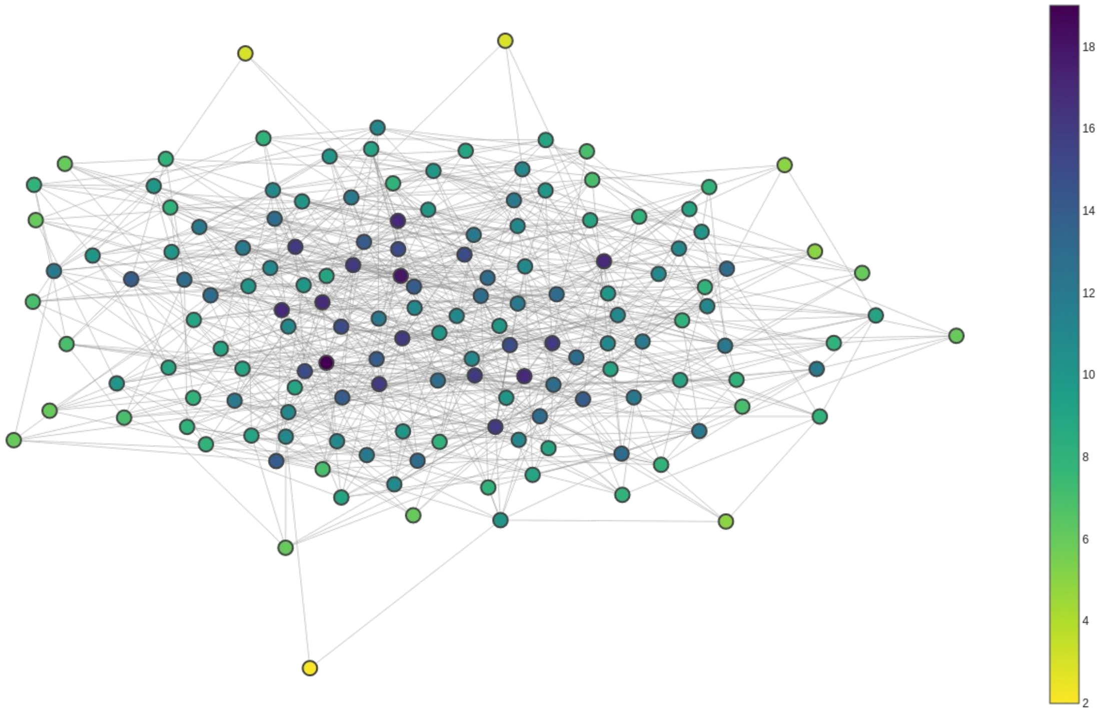




Question break



Graph: Complexity



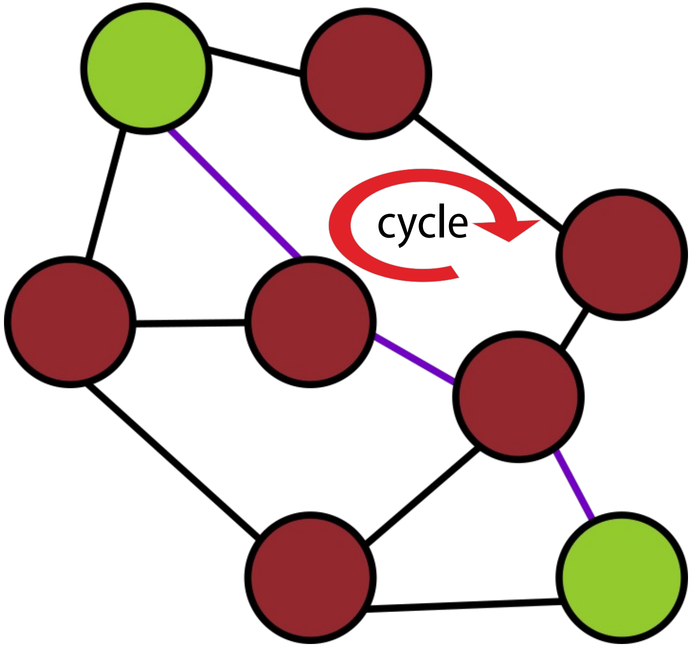
Number of neighbors

- The inner structure of a graph can vary a lot
- The number of edges/nodes might vary a lot from one graph to another
- One single graph can contain several thousand of nodes/edges
- ...

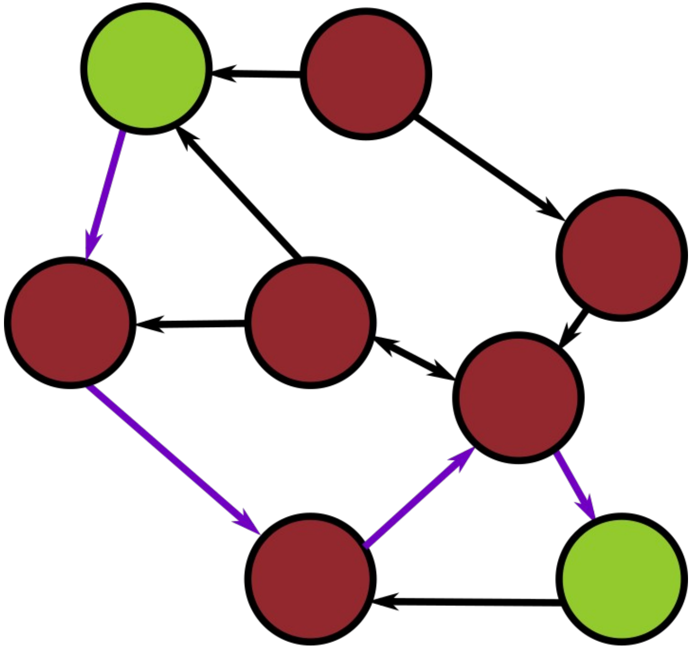
Graph: Paths

A **path** is a sequence of edges connecting 2 nodes

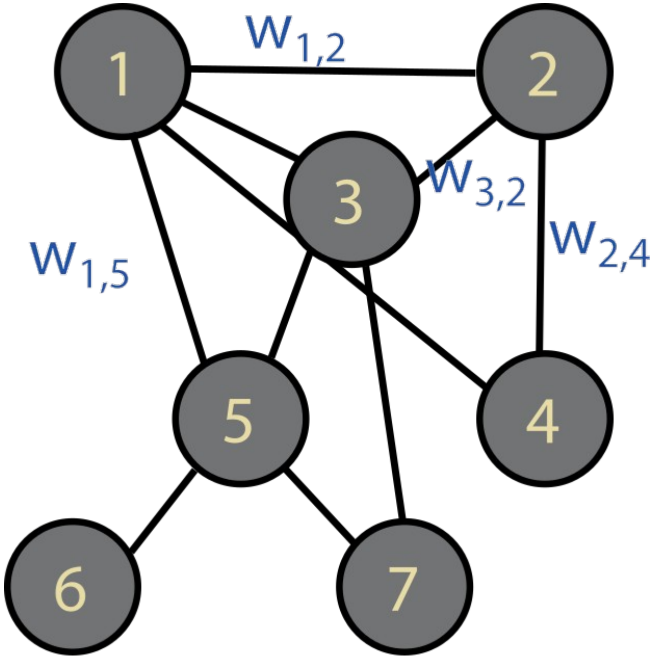
Undirected graph



Directed graph



Graph: Node proximity and centrality



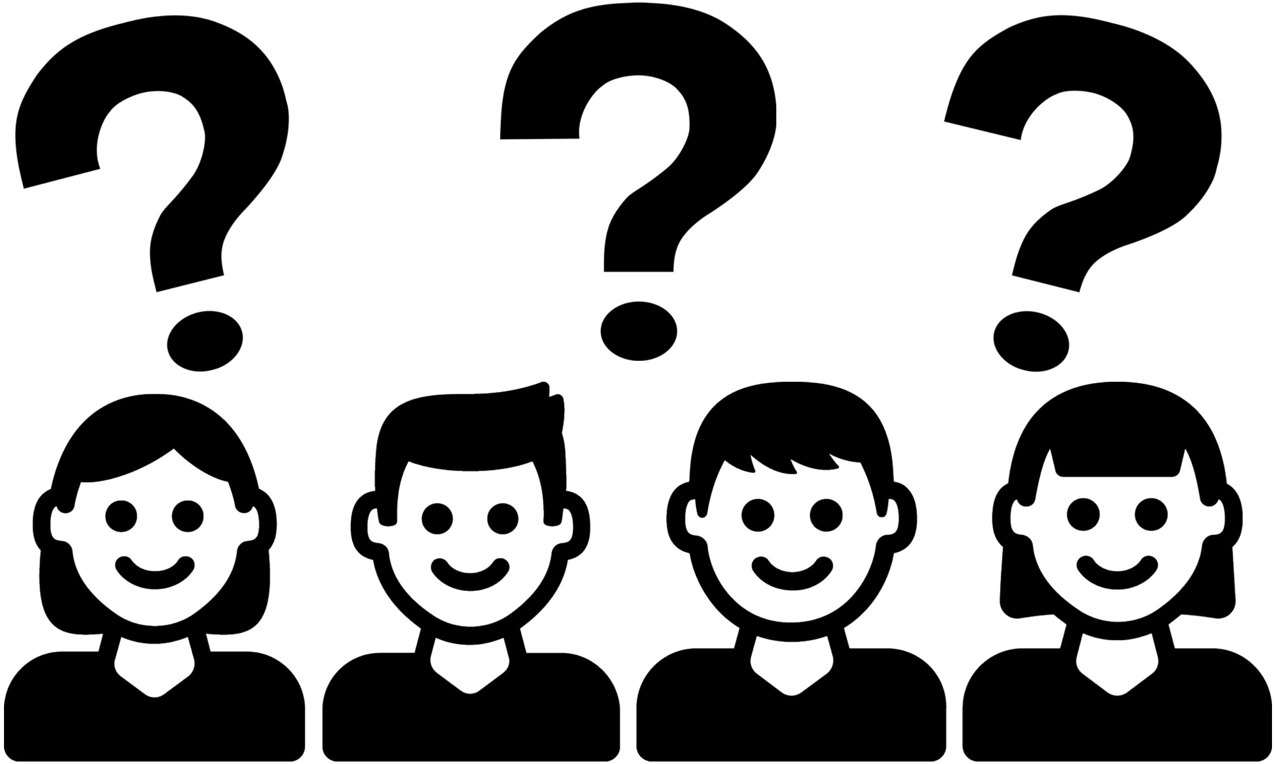
Node centrality

Measure how many paths goes through the node

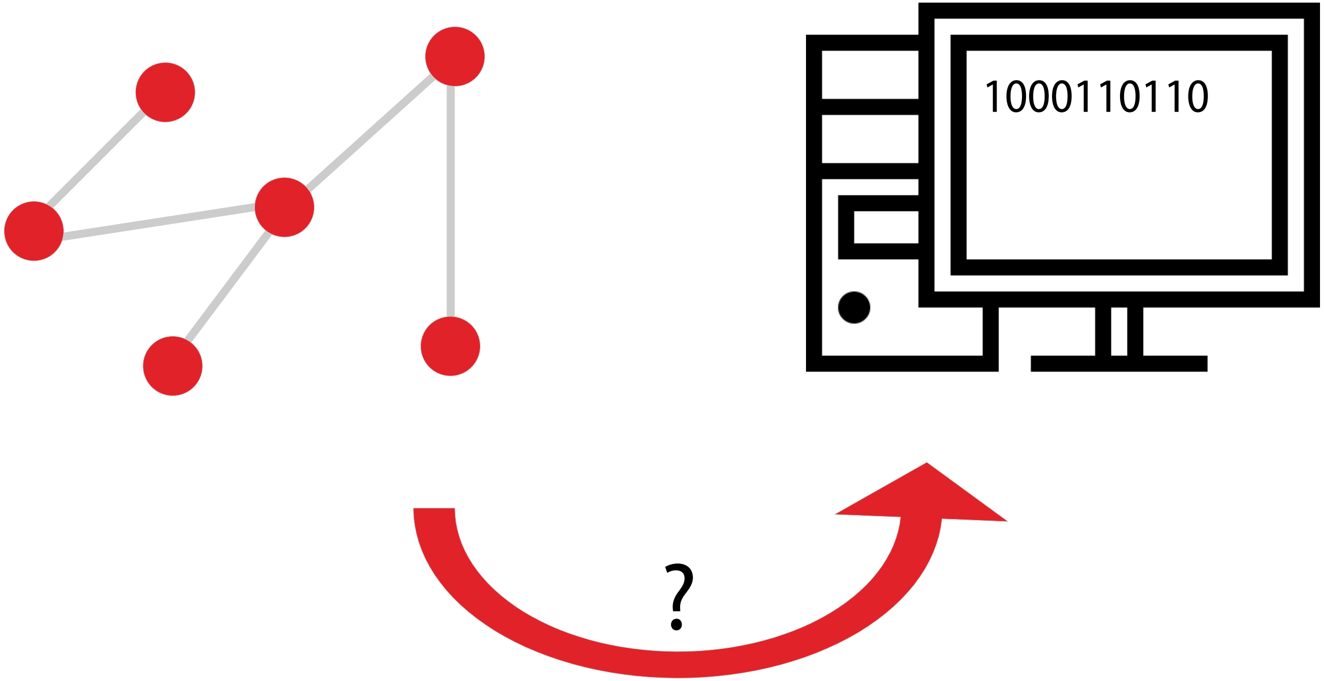
Node proximity

- 1st order: $\mathbf{w}_{i,j}$ between node i and j
- 2nd order: similarity of neighborhood structure
- Higher orders possible

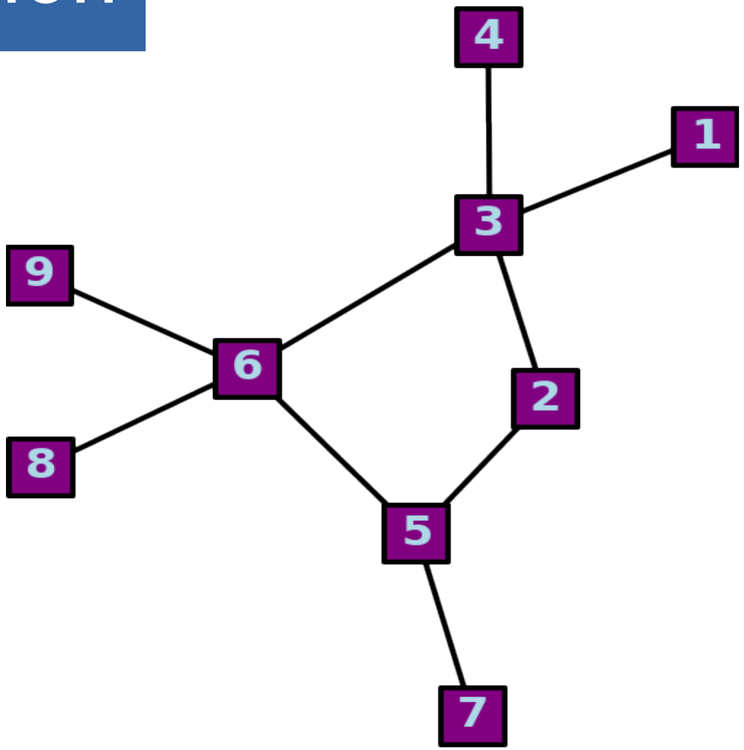
Question break



Graph representation



Graph representation

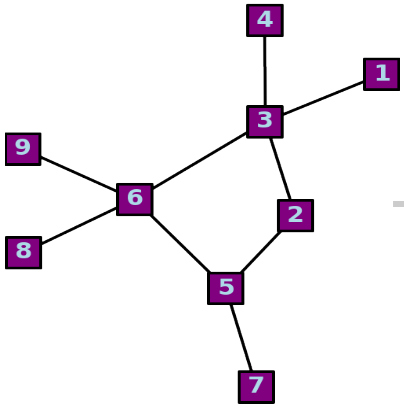


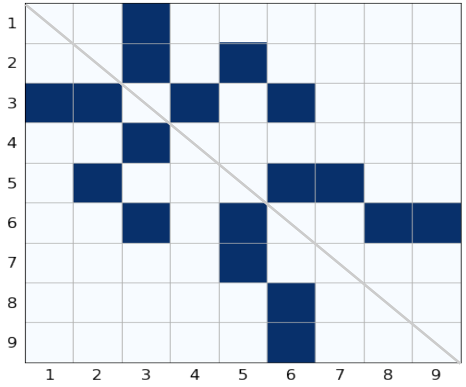
Random numbering of nodes

Graph representation

Adjacency matrix $W_{(i,j)} = \begin{cases} w_{i,j} \, if \, there \, is \, an \, edge \\ 0 \, if \, not \end{cases}$

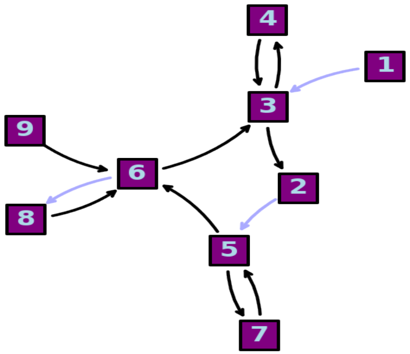
Undirected

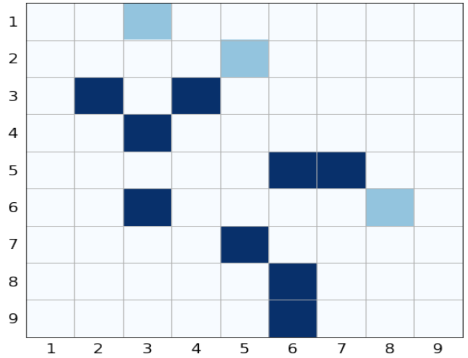




Symmetric

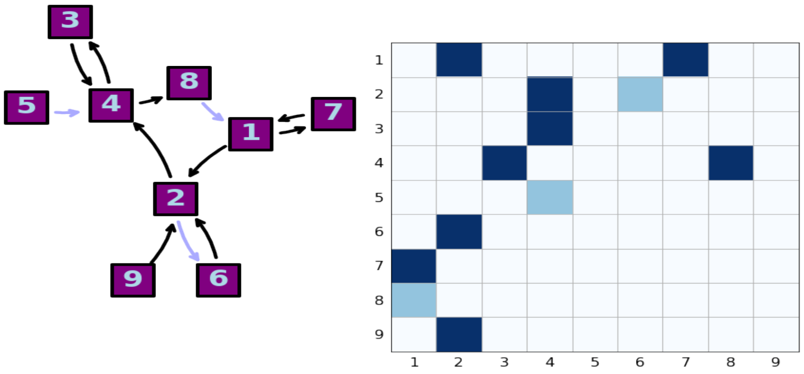
Directed





Graph representation

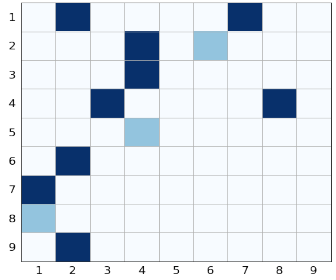
Adjacency list



Adjacency list: [[5, 4],
[8, 1],
[4, 8], [4,3],
[3, 4],
[1, 7], [1, 2],
[2, 4], [2, 6],
[7,1],
[6, 2],
[9, 2]]

Edges: [0.4, 0.4, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0,
0.4, 1.0, 1.0, 1.0]

Graph representation



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[2, 4], [2, 6],
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[6, 2],
[9, 2]]

Edges: [0.4, 0.4, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0,
0.4, 1.0, 1.0, 1.0]

- Scale V^2 → lot of space
- Might be sparse
- Easy to find an edge

- Scale E → less space
- Might be difficult to find an edge

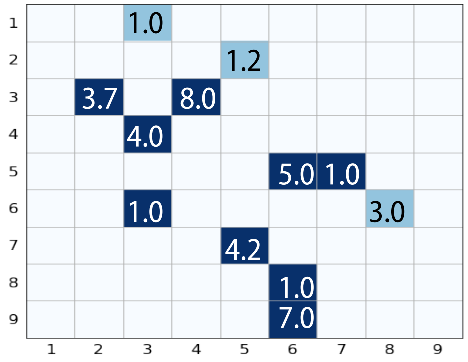
V = number of nodes/vertices
E = number of edges

https://www.geeksforgeeks.org/comparison-between-adjacency-list-and-adjacency-matrix-representation-of-graph/

Graph representation

- Edge weights are stored either directly in the adjacency matrix, or in an independent tensor.

Adjacency matrix



Adjacency list: [[5, 4],
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[3, 4],
[1, 7], [1, 2],
[2, 4], [2, 6],
[7,1],
[6, 2],
[9, 2]]

Edges: [0.4, 1.4, 2.4, 9.0, 1.0, 5.0, 1.7, 3.0, 0.4, 1.3, 7.0, 6.2]

- Information (features) on nodes and graphs will also be stored in independent tensors.

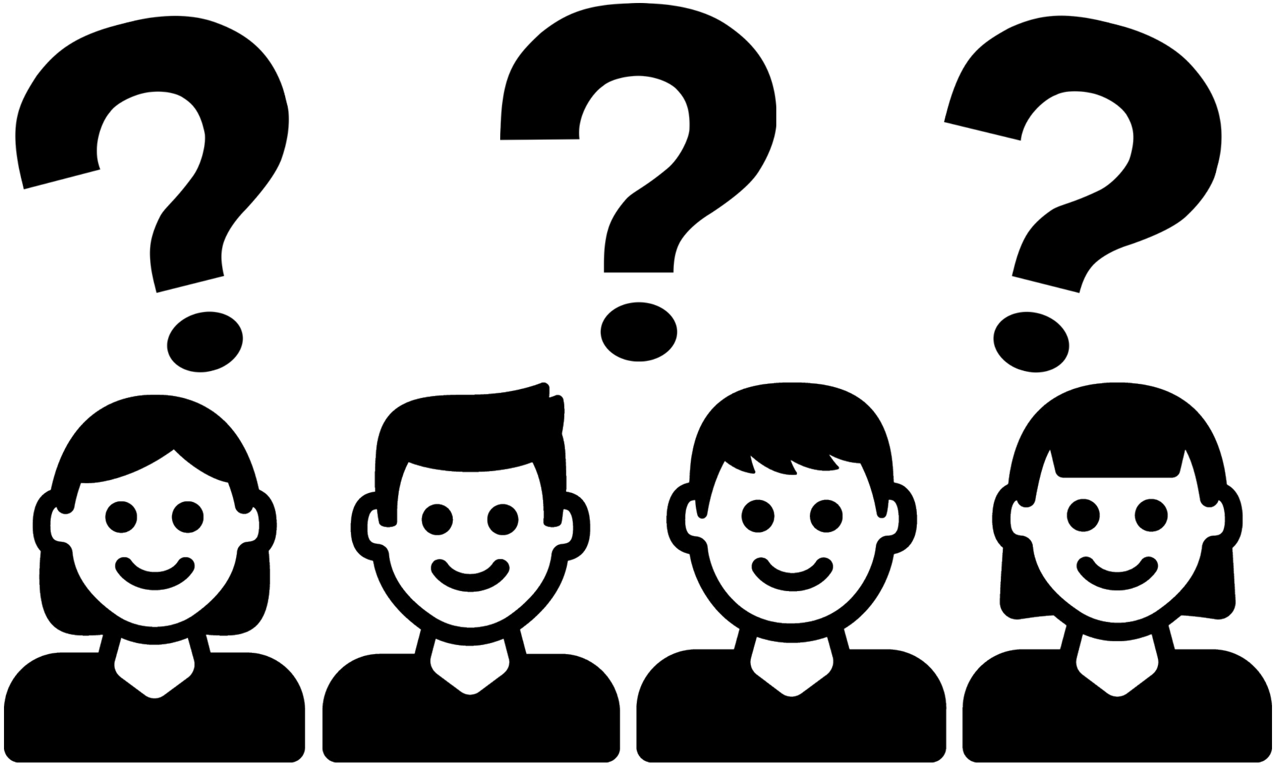
Nodes: [4.1, 4.2, 6.4, 1.0, 1.0, 5.0, 1.7, 3.0, 5.0]

Graph: [8.0]

Useful Matrices

Adjacency	**W**	Weight of edges
Degree	**D**	Diagonal matrix with number of edges for each node
Laplacian	**L**	**D - W**
Node Features	**X**	Information stored

Question break



Roadmap

10

Graph Neural Network

GNN

9.1 **Graphs are everywhere**

- Complex data structures
- Basics of graph theory

9.2 **Learning on Graphs**

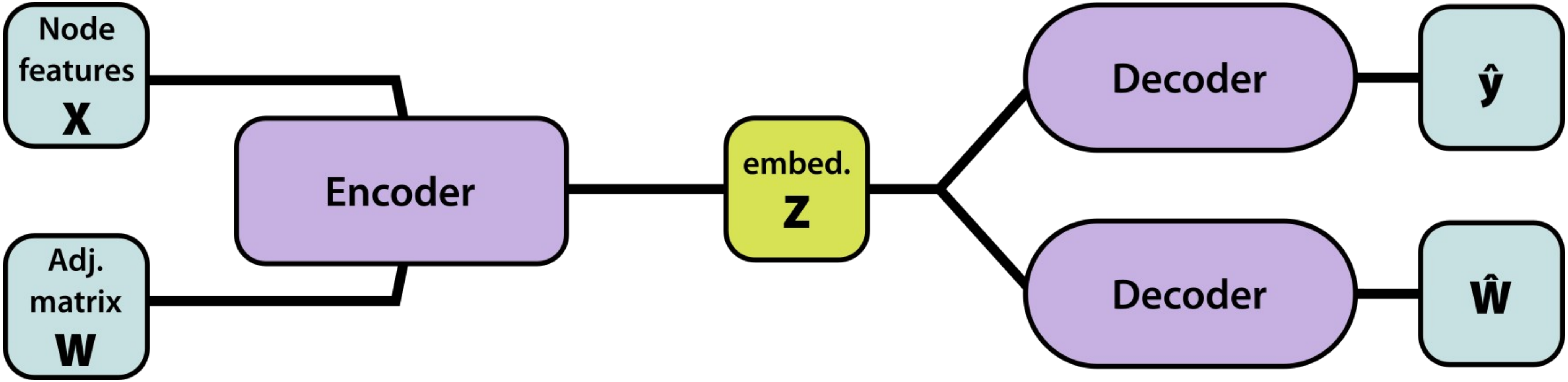
- Graph embedding
- Transductive and inductive learning
- Tasks on graph learning

9.3 **A few examples**

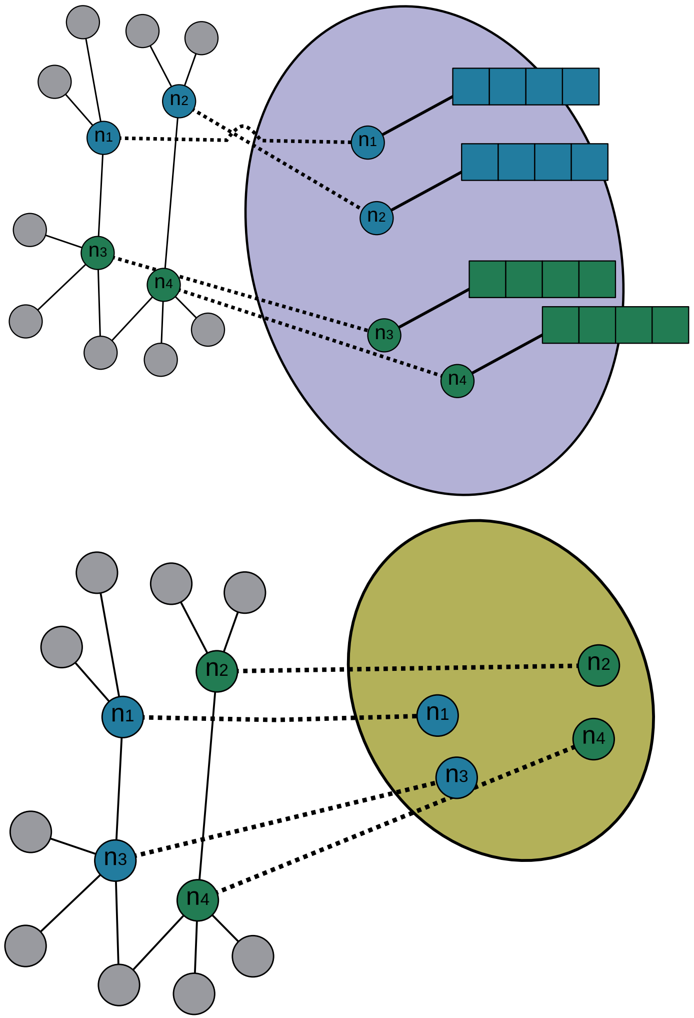
- Taxonomy of methods
- Graph convolution
- Message passing
- Graph Transformer

Graph embedding

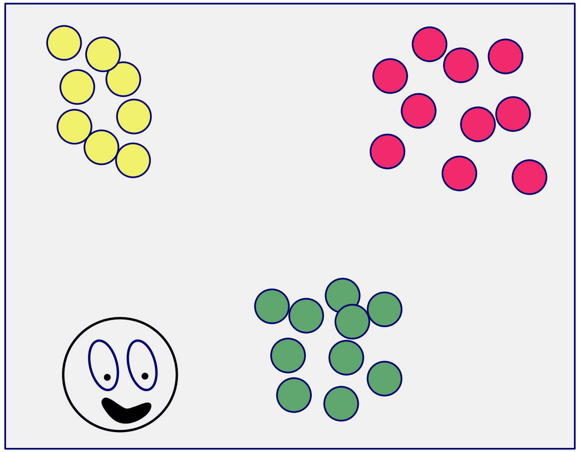
- We need to find a representation of the graph that is processable

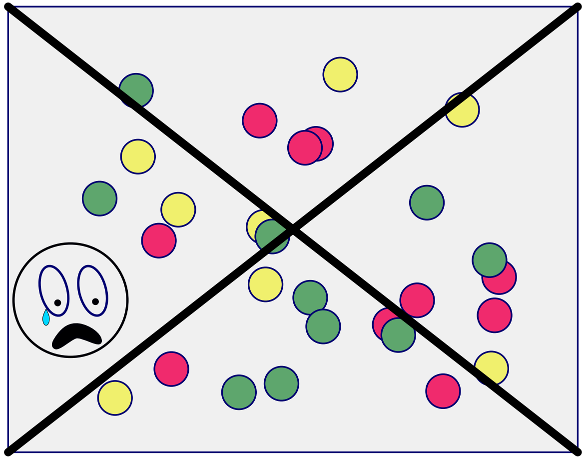


Graph embedding



- Features stored in nodes/edges/graphs are not easily processed.
- We transform the features into a vector in the latent space (**Dimension is a hyperparameter**).
- The embedding has to be suited for the task → **Learnable.**



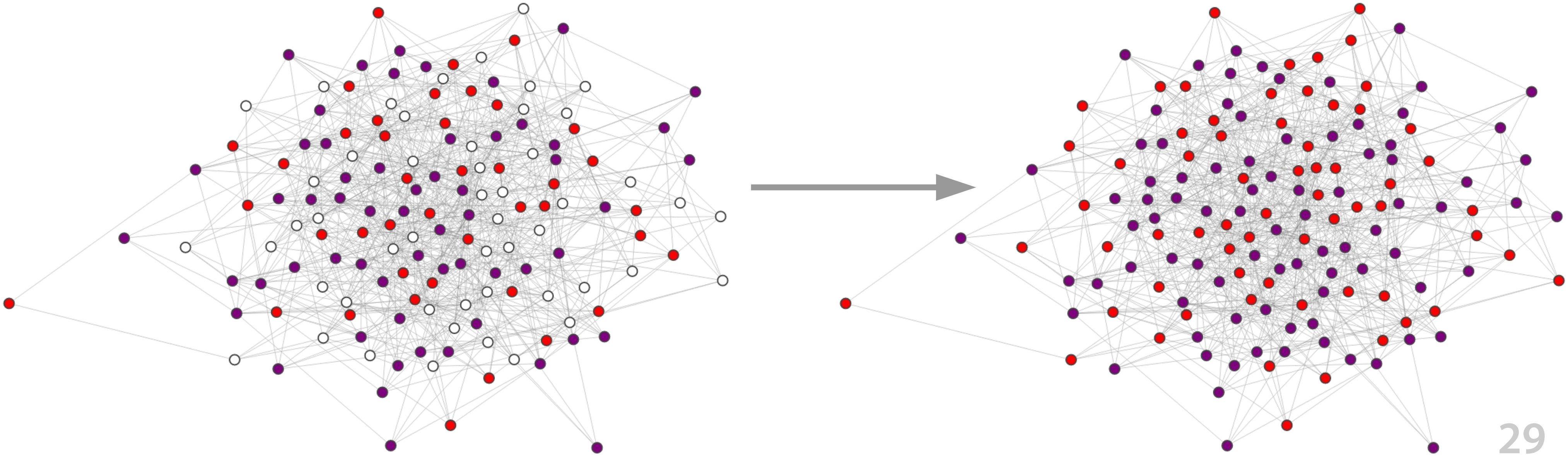


Transductive learning

The model has access to the complete graph

It is not possible to add new nodes

Node labeling

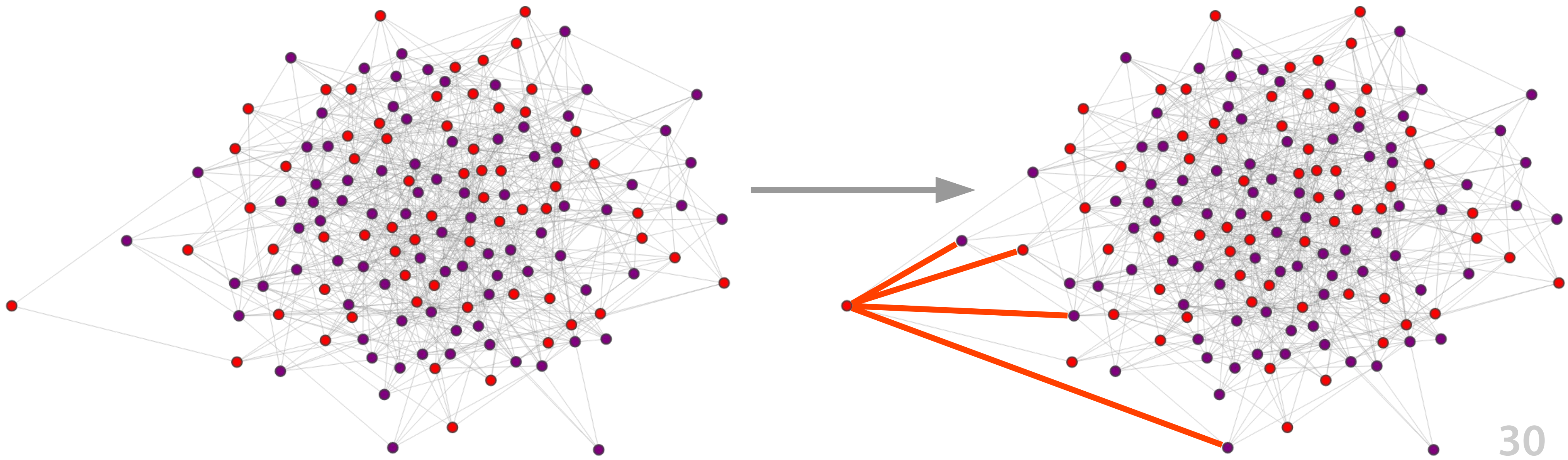


Transductive learning

The model has access to the complete graph

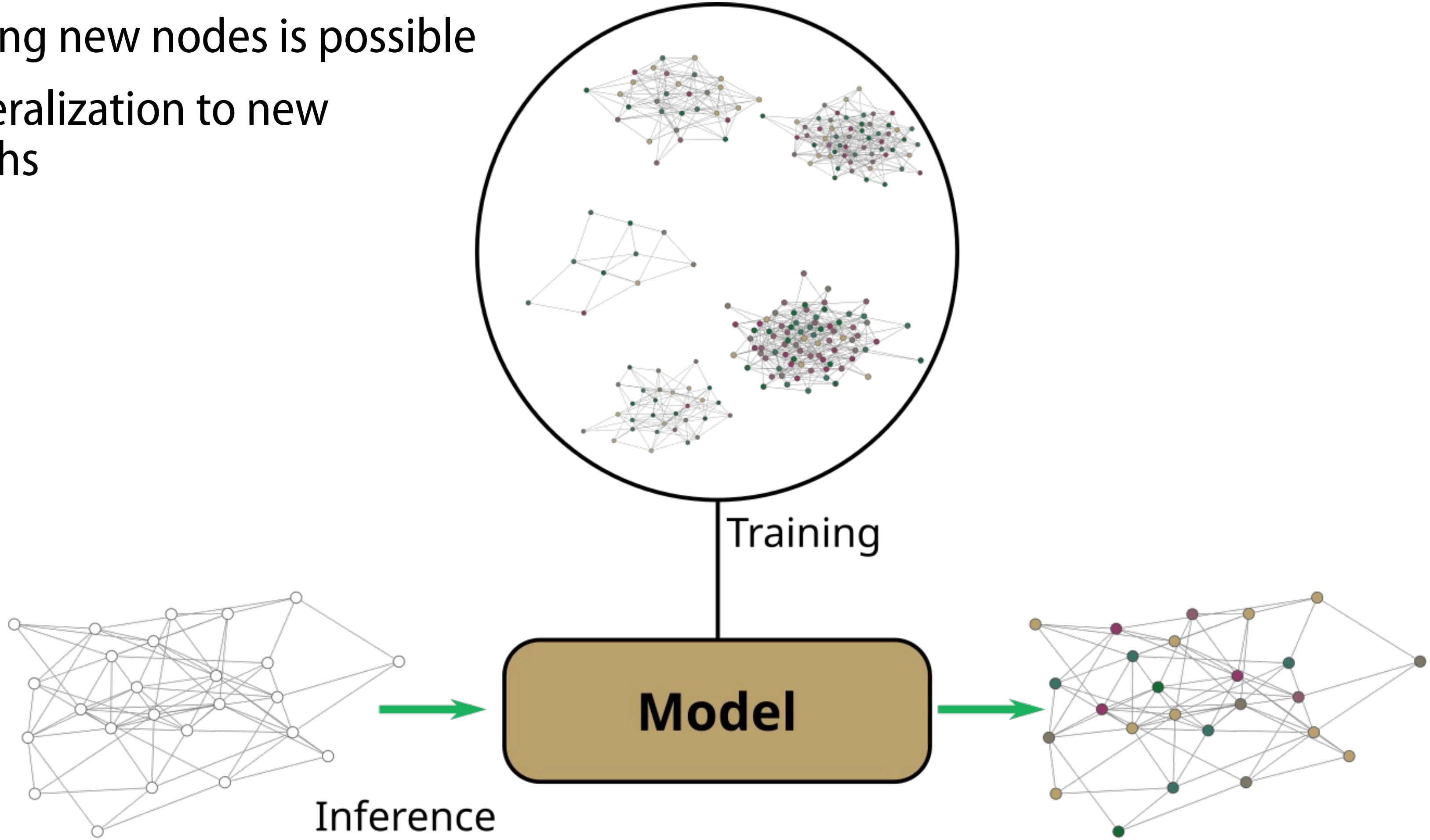
It is not possible to add new nodes

Find new edges



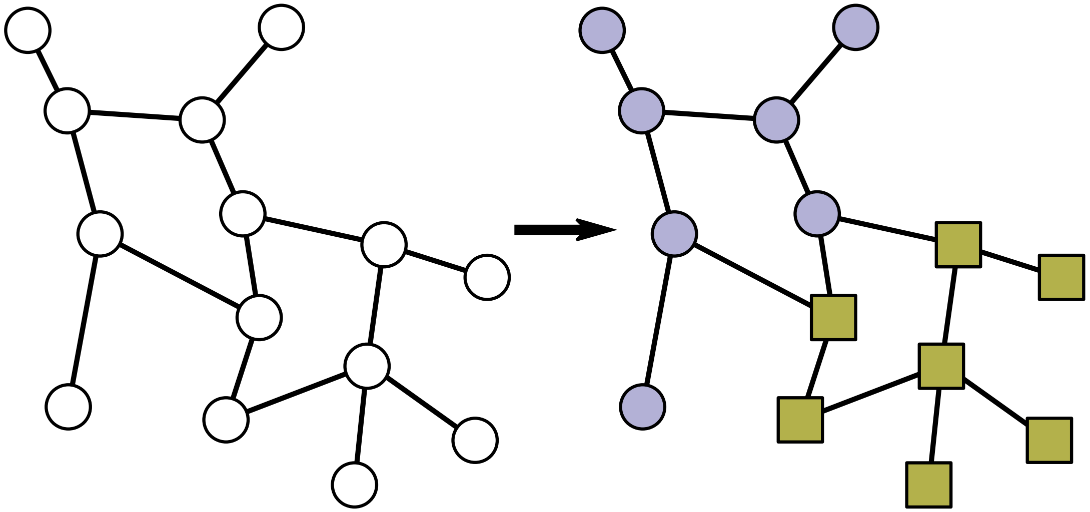
Inductive learning

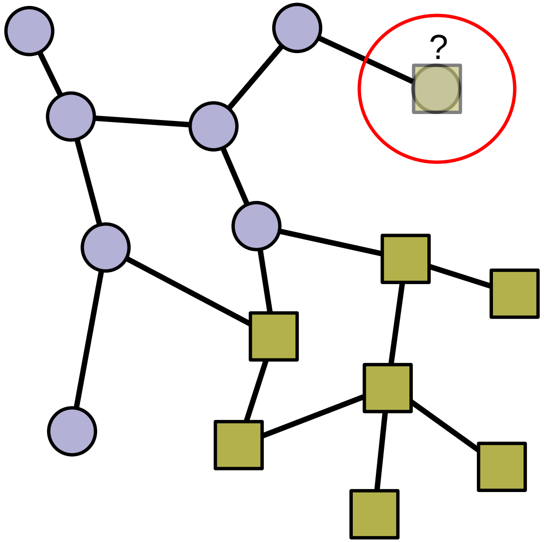
- The model has access only to a part of the graph (train set)
- Adding new nodes is possible
- Generalization to new graphs



Tasks on nodes

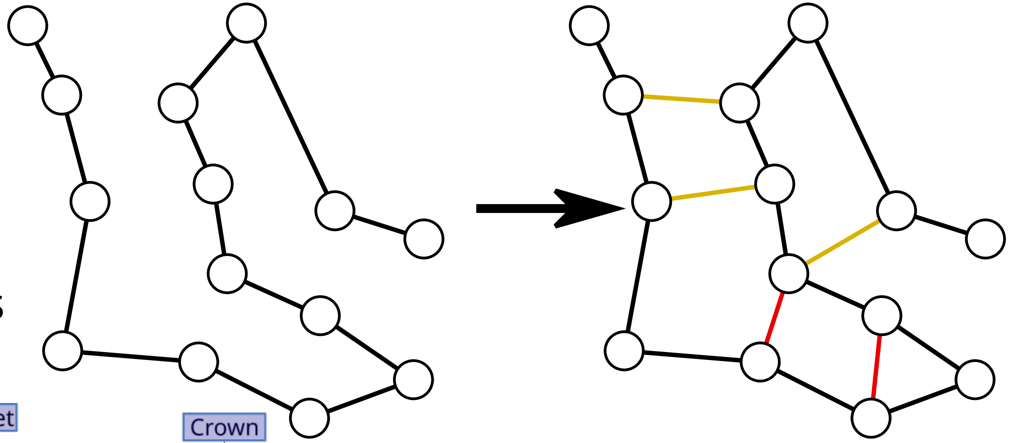
- Labeling nodes in a graph (clustering)
  - Find topic of a research paper (CORA, etc)
  - Find bots in a social network
  - …
- Labeling new nodes
- Perform regression

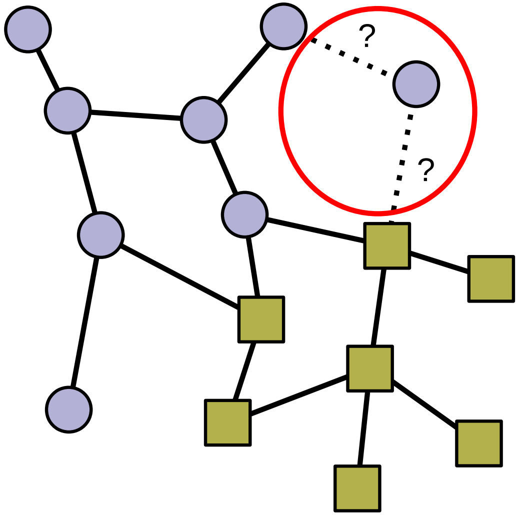


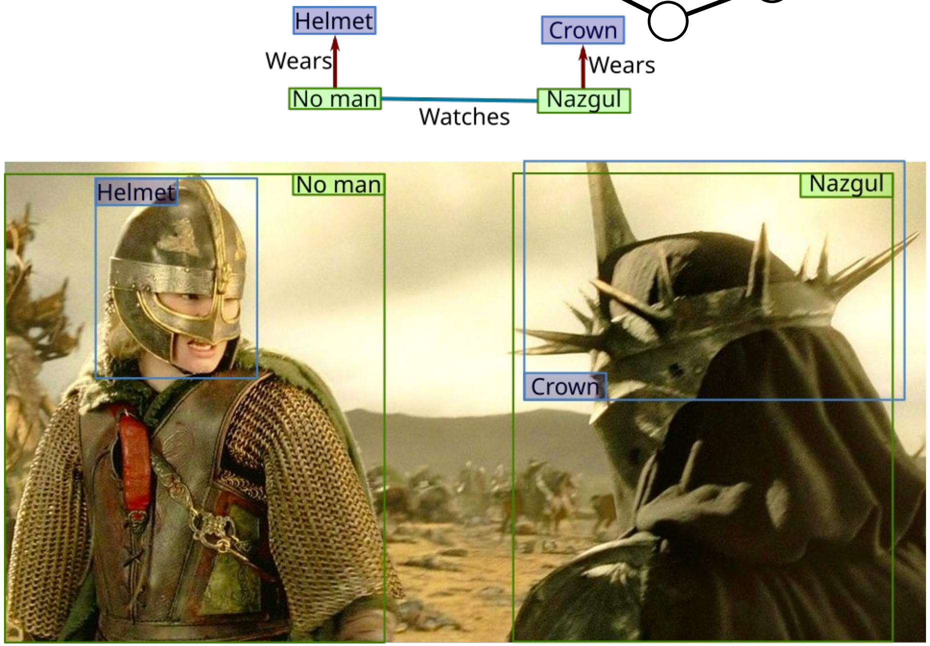


Tasks on edges

- Find relationships
  - Contact map of aminoacids (Alphafold)
  - Contact suggestion (social network)
  - ETA for directions (regression)
  - Relationships between segments in pictures
  - ...



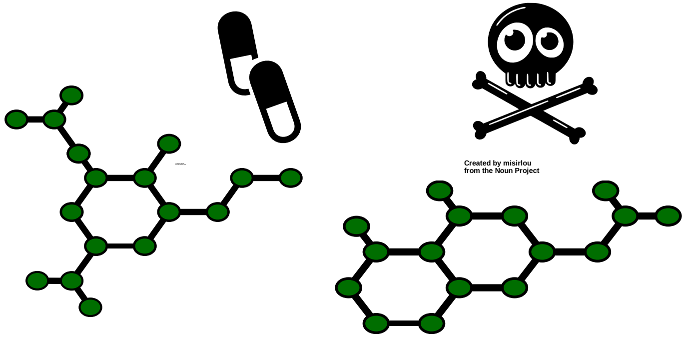


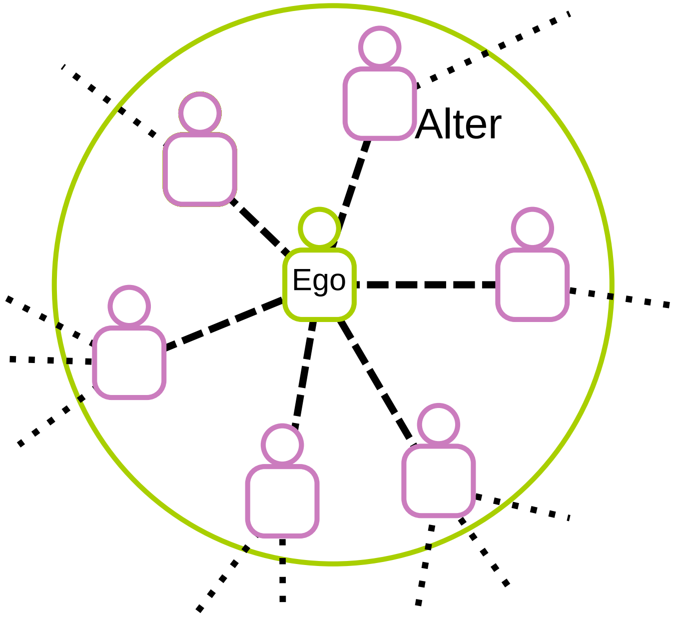


G. Zhu et al., "Scene Graph Generation: A Comprehensive Survey." arXiv, Jun. 22, 2022. doi: 10.48550/arXiv.2201.00443.

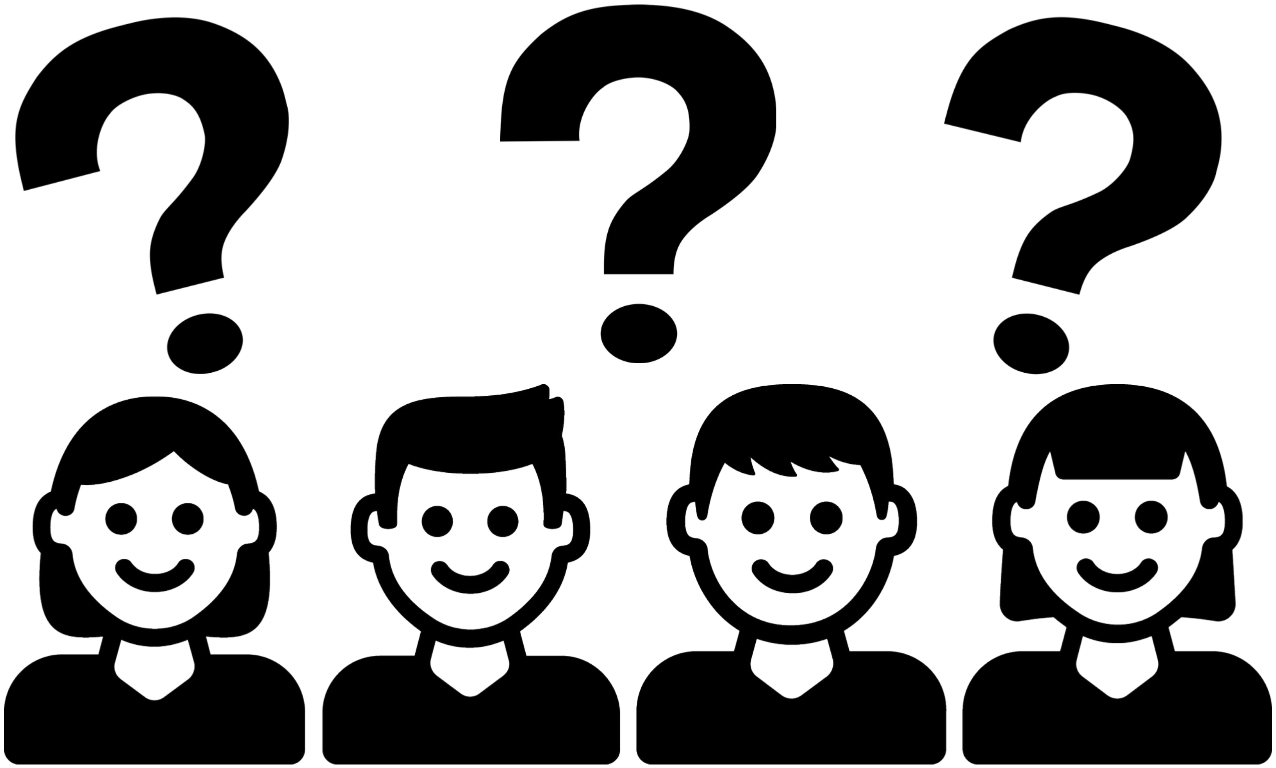
Tasks on graphs

- Predict properties of graphs
  - Chemical properties (solubility, carcinogenic, possible drug)
  - Classification of the research field in an ego network
  - ...

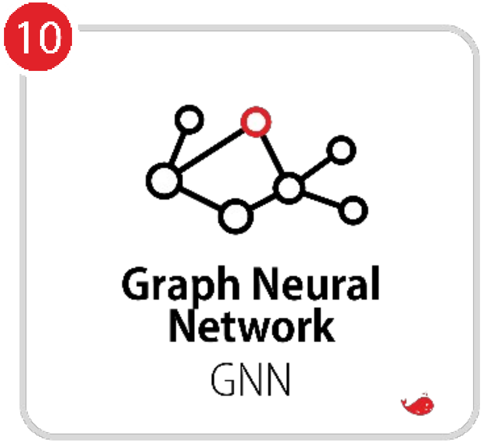




Question break



Roadmap



9.1 Graphs are everywhere

- Complex data structures
- Basics of graph theory

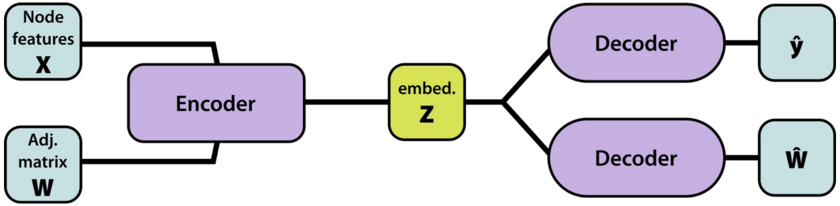
9.2 Learning on Graphs

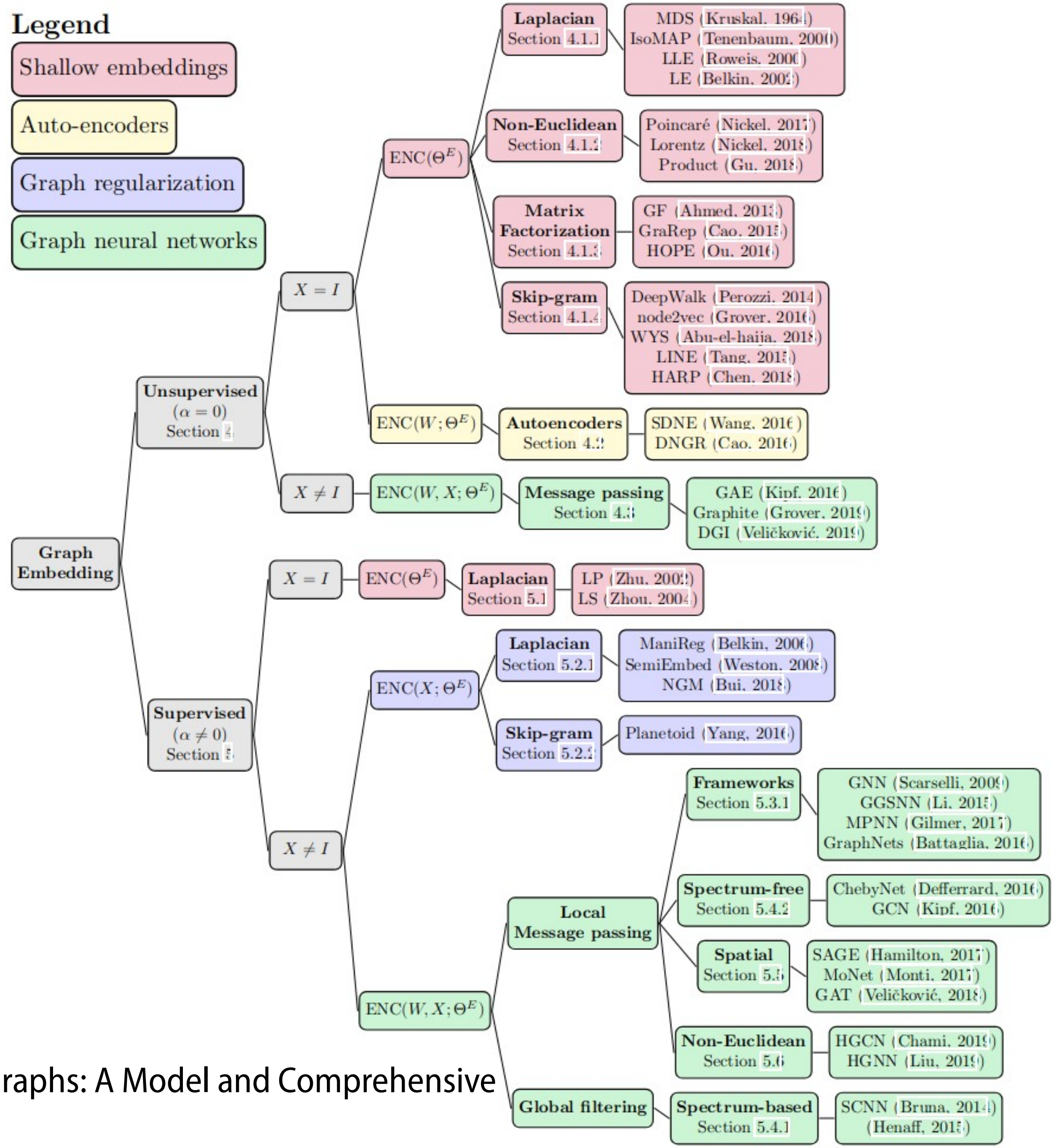
- Graph embedding
- Transductive and inductive learning
- Tasks on graph learning

9.3 A few examples

- Taxonomy of methods
- Graph convolution
- Message passing
- Graph Transformer

Taxonomy of methods

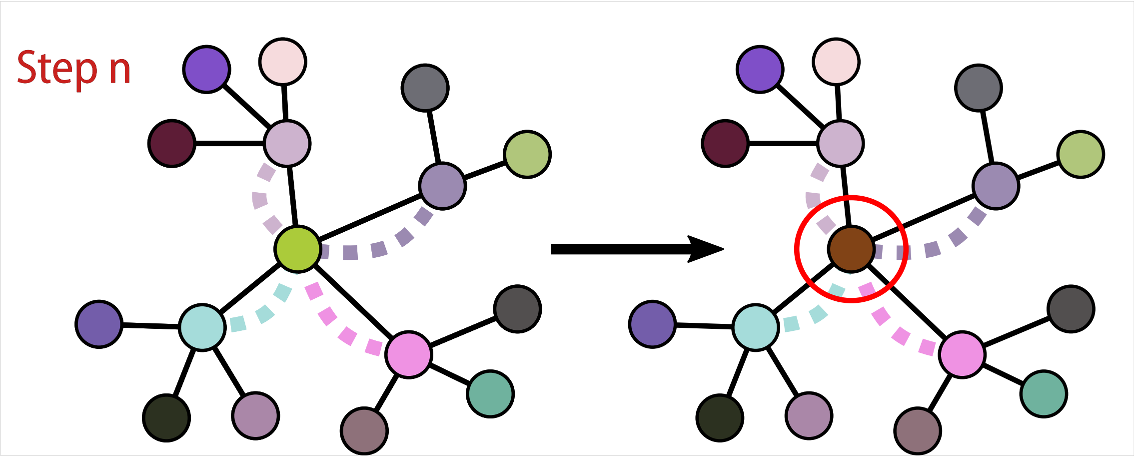


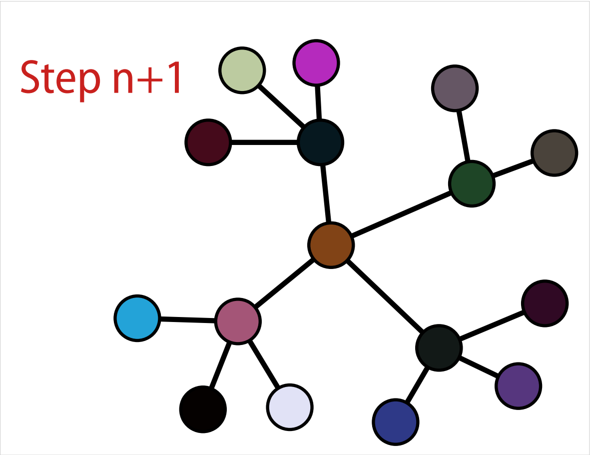


I. Chami, S. Abu-El-Haija, and B. Perozzi, “Machine Learning on Graphs: A Model and Comprehensive Taxonomy”.

Graph convolution

→ Just like for images we can learn from neighborhood with a convolution.

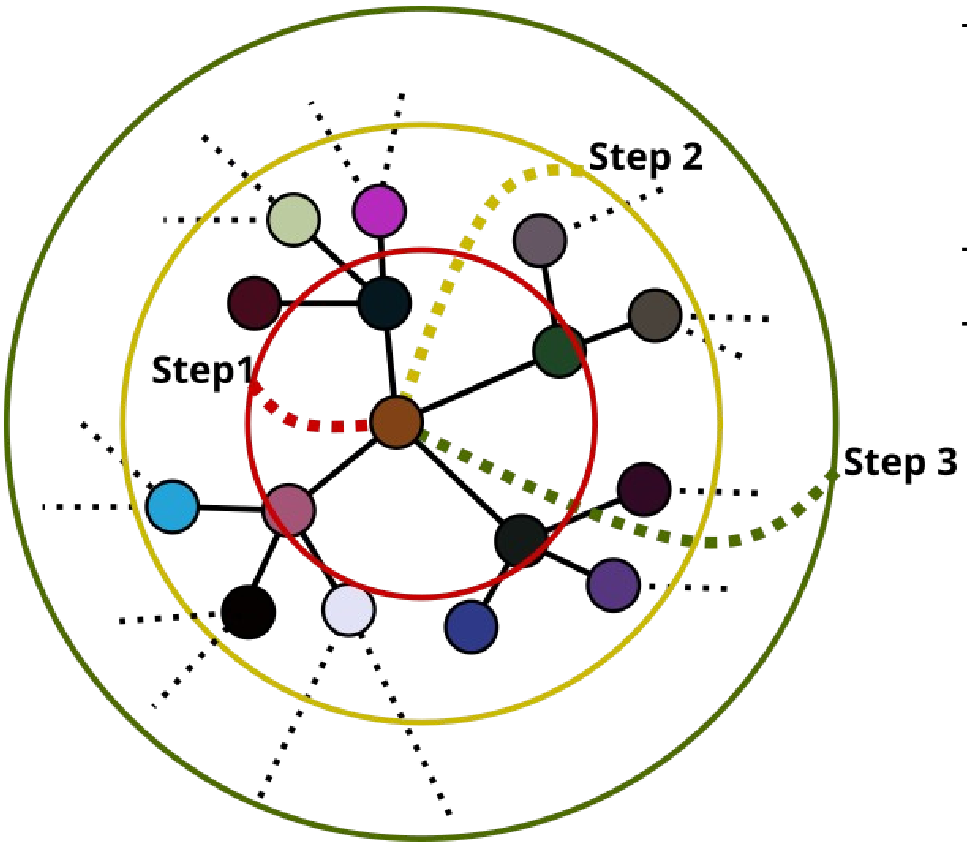




→ A bit more complex since the number of neighbors is unlikely to be constant.

→ We want the operator to be permutation invariant.

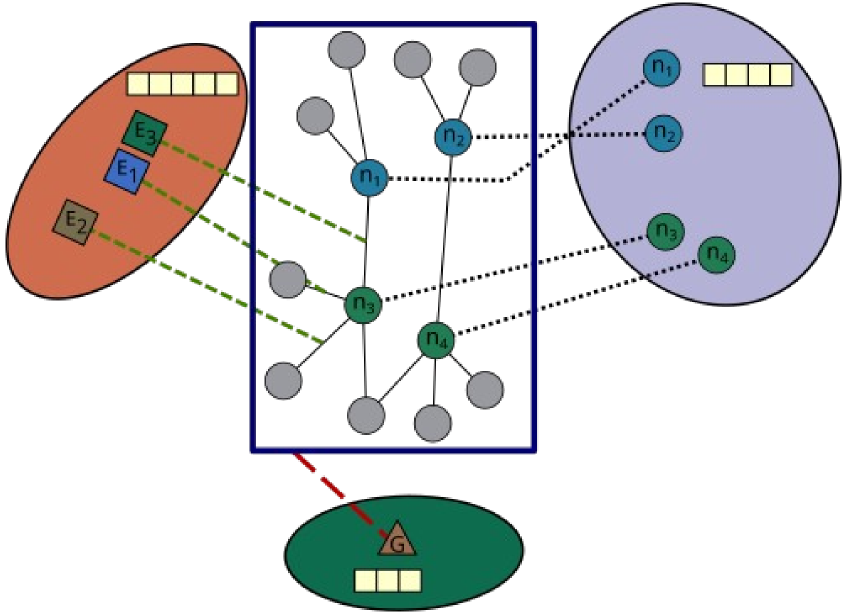
Graph convolution

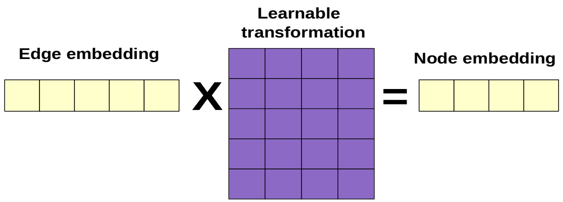


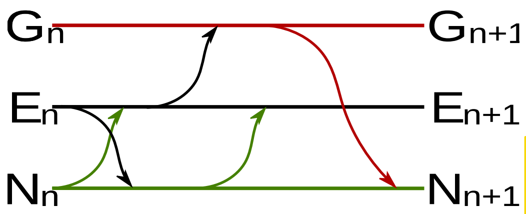
- Several steps are needed to retrieve information for distant nodes.
- For large graphs → a **cutoff**
- It is possible to use a **virtual node** connected to all other nodes. But in practice this becomes quickly intractable.

Message passing

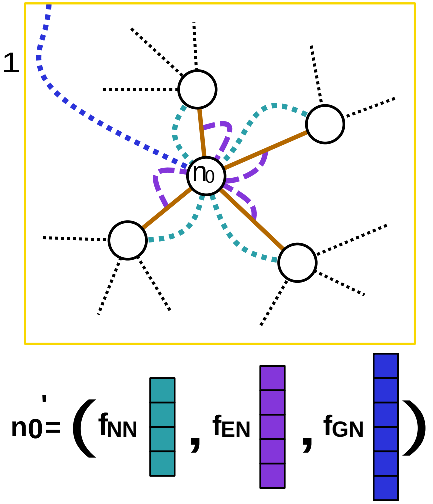
- We have embeddings for each part of the graph (possibly different vector sizes).
- Each part can learn from the others via a transformation.



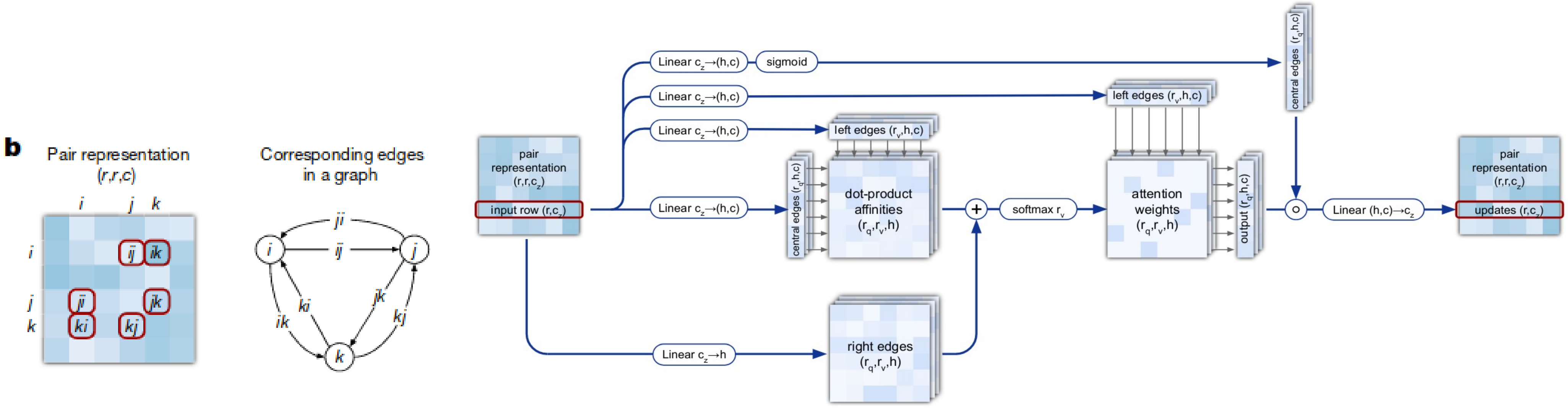




- Information is aggregated to form a message that the node/edge will send to others.



Alphafold transformer

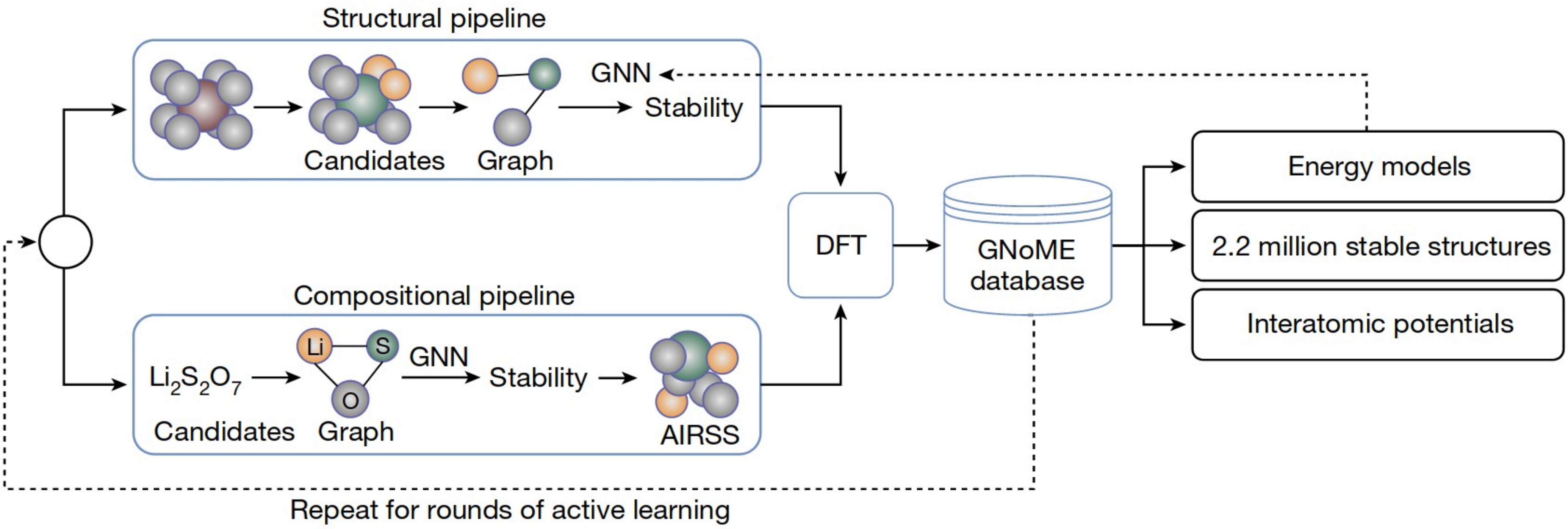


Supplementary Figure 7 | Triangular self-attention around starting node. Dimensions: r: residues, c: channels, h: heads

J. Jumper et al., Highly accurate protein structure prediction with AlphaFold, Nature, vol. 596, no. 7873, Art. no. 7873, Aug. 2021, doi: 10.1038/s41586-021-03819-2.

GNoME

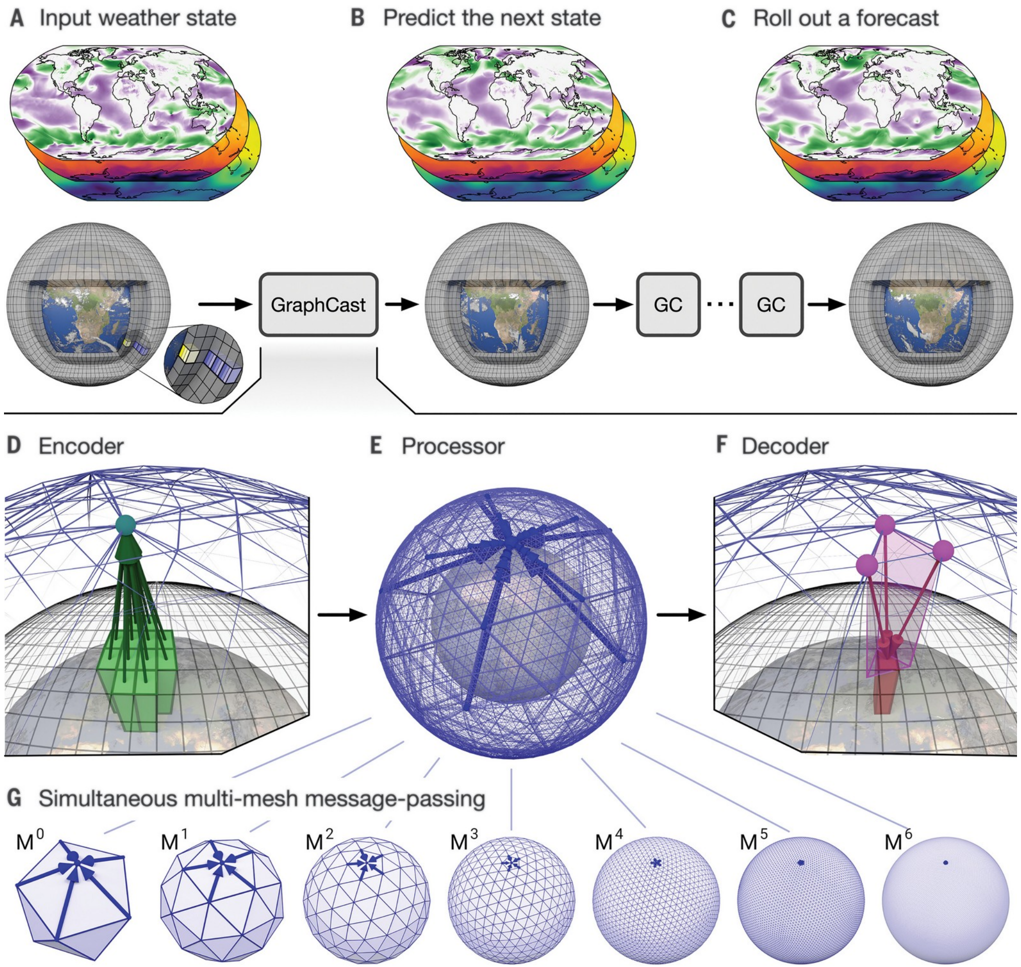
Generation of novel crystal structures



Merchant, A., Batzner, S., Schoenholz, S.S. et al. Scaling deep learning for materials discovery. Nature 624, 80–85 (2023). https://doi.org/10.1038/s41586-023-06735-9

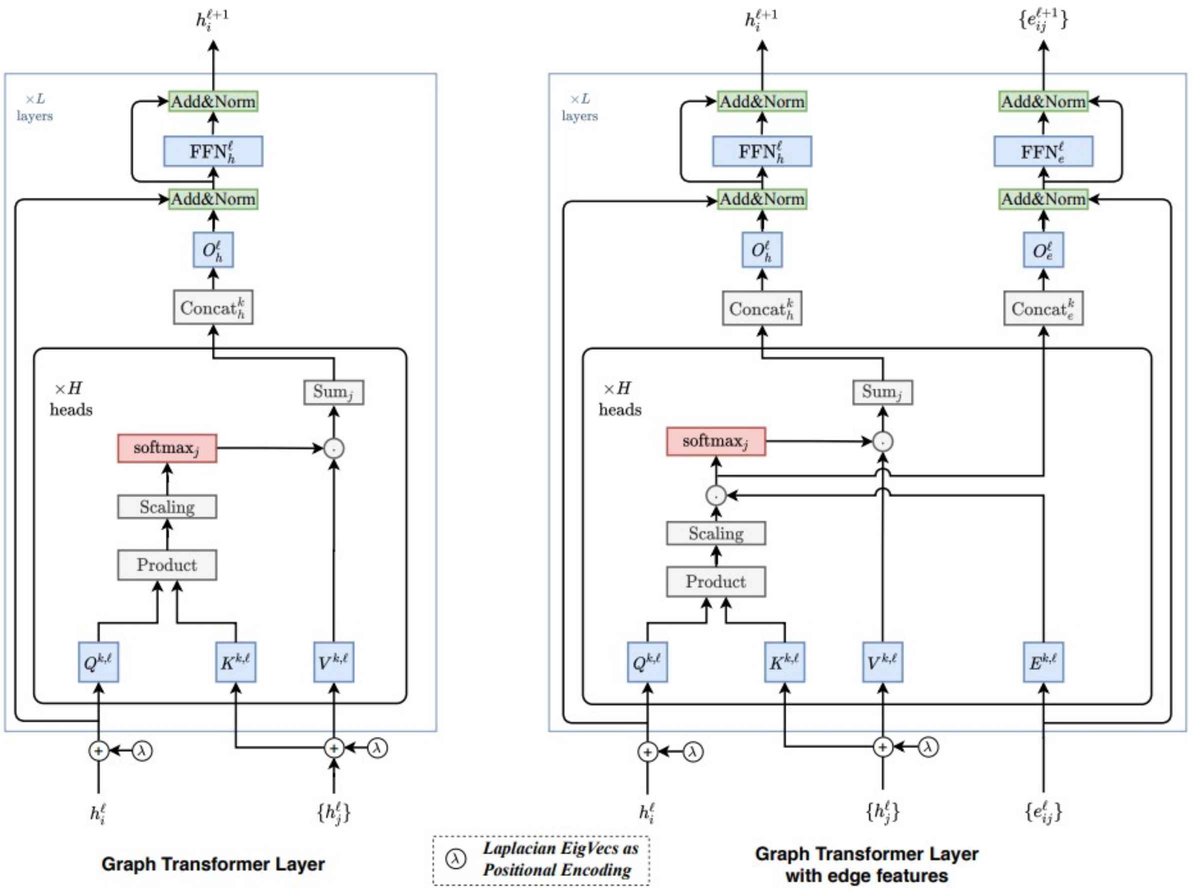
GraphCast

Prediction of the weather with temporal graphs



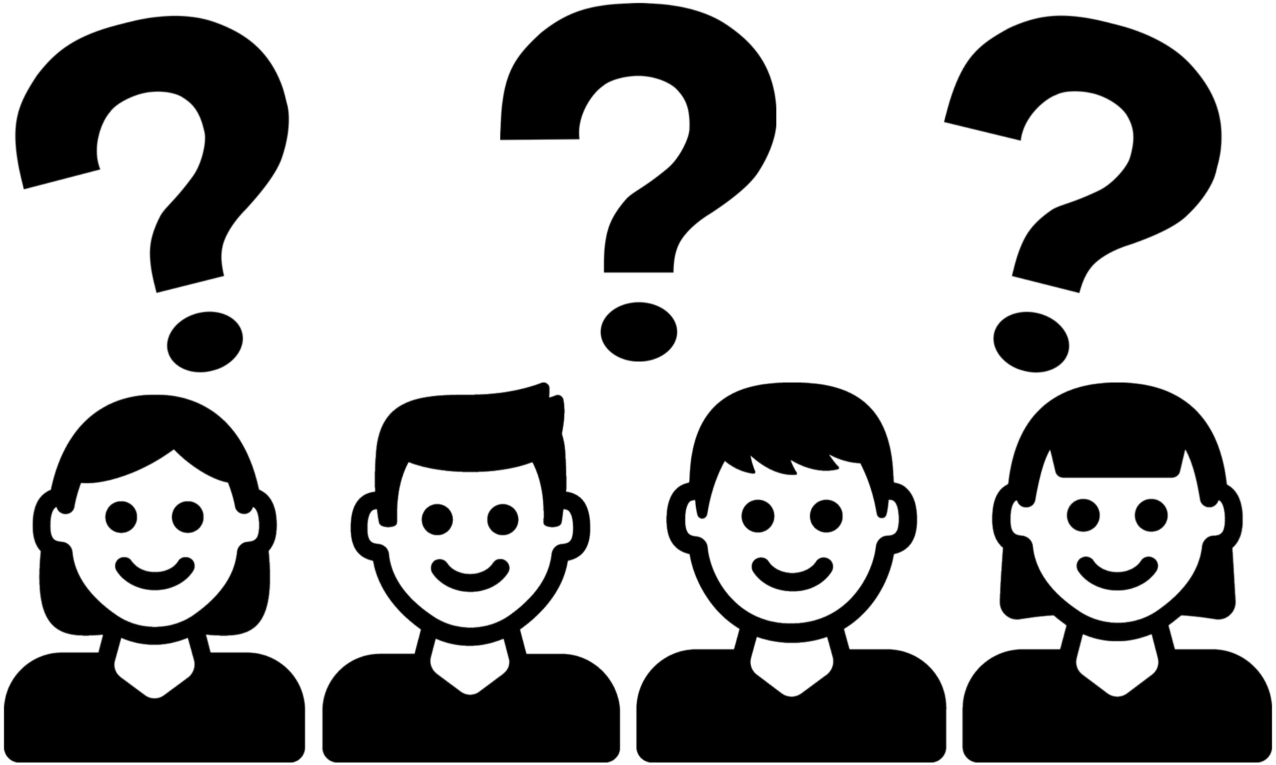
Remi Lam et al. Learning skillful medium-range global weather forecasting.Science382,1416-1421(2023).DOI:10.1126/science.adi2336

Graph Transformer Network



Dwivedi, Bresson A Generalization of Transformer Networks to Graphs 2020, https://arxiv.org/abs/2012.09699

Question break



Resources

Libraries

- → Pytorch Geometric
- → Deep Graph Library
- → Graph Nets
- → Spektral
- → ...

- → https://logconference.org/
- → https://ogb.stanford.edu/

Tutorials

- → https://antoniolonga.github.io/Pytorch_geometric_tutorials/
- → https://docs.dgl.ai/tutorials/blitz

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- Books
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  - https://venturebeat.com/2021/10/13/what-are-graph-neural-networks-gnn/
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- Articles

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