SAISON 23/24

Formation

# Introduction au Deep Learning

Séquence n°10

"Travailler avec des données structurées : Graph Neural Network (GNN)"

FIDLE

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# Introduction au Deep Learning

https://fidle.cnrs.fr

Powered by CNRS CRIC,
and UGA DGDSI of Grenoble, thanks !

- Course materials (pdf)
- Practical work environment
- Corrected notebooks
- Videos (YouTube)

docker

(*) Procedure via Docket or pip
Remember to get the latest version !

FIDLE

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# Introduction au Deep Learning

Questions and answers :

https://fidle.cnrs.fr/q2a

**Accompanied by:**
IA Support (dream) Team of IDRIS

**Directed by:**
Agathe, Baptiste et Yanis - UGA/DAPI
Léo, Kamel, Thibaut - IDRIS

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# Introduction au Deep Learning

FIDLE https://fidle.cnrs.fr/listeinfo

Fidle information list

New !

Agoria http://fidle.cnrs.fr/agoria

AI exchange list

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# Introduction au Deep Learning

https://listes.services.cnrs.fr/wws/info/devlog

List of ESR* « Software developers » group

https://listes.math.cnrs.fr/wws/info/calcul

List of ESR* « Calcul » group

(*) ESR is Enseignement Supérieur et Recherche, french universities and public academic research organizations

Abonnez-vous !

https ://fidle.cnrs.fr/youtube
https://www.youtube.com/@CNRS-FIDLE

Panoram'IA

Le magazine de actualité en IA

Vendredi 16 février, 10h00

http://www.idris.fr/panoramia.html
https://www.youtube.com/@IDRISCNRS

Envoyez-nous des photos « cartes postales ! »

Hakone, Japon
From : Pauline K.

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SAISON 23/24

## Bases, Concepts et Enjeux

1. **History and Fundamental Concepts**
2. New ! **Data, models and representation's hell** Data and models
3. New ! **Demonstration Illustration** LLM / Text to Image
4. **AI, Law, Society and Ethics**

## L'IA comme un outil,

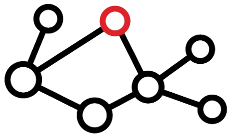
5. New ! **Mathematics, gradients everywhere !**
6. New ! **Learning methodology**
7. **Convolutional models** CNN
8. **Sparse (text) and sequences data** Embedding, RNN
9. **«Attention is All You Need»** Transformers
10. **Graph Neural Network** GNN
11. **Autoencoder networks** AE
12. **Variational Antoencoder** VAE
13. **Generative Adversarial Networks** GAN
14. **Diffusion Model** Text to image
15. **Deep Reinforcement Learning** RL
16. **Physics-Informed Neural Networks** PINNS

## Acteur de l'IA

17. **Learning faster and cheaper,** Eco-Friendly
18. **Jean-Zay** GPU acceleration
19. New ! **New models** VLM, SM, Multimodal, ...
20. New ! **Case Study** Experience feedback

# Roadmap

10



**Graph Neural Network**

GNN

## 1 Graphs are everywhere

- Complex data structures
- Basics of graph theory

## 2 Learning on Graphs

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

## 3 A few examples

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

# Roadmap

10

**Graph Neural Network**

GNN

1 **Graphs are everywhere**

- Complex data structures
- Basics of graph theory

2 **Learning on Graphs**

- Graph embedding
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- Tasks on graph learning

3 **A few examples**

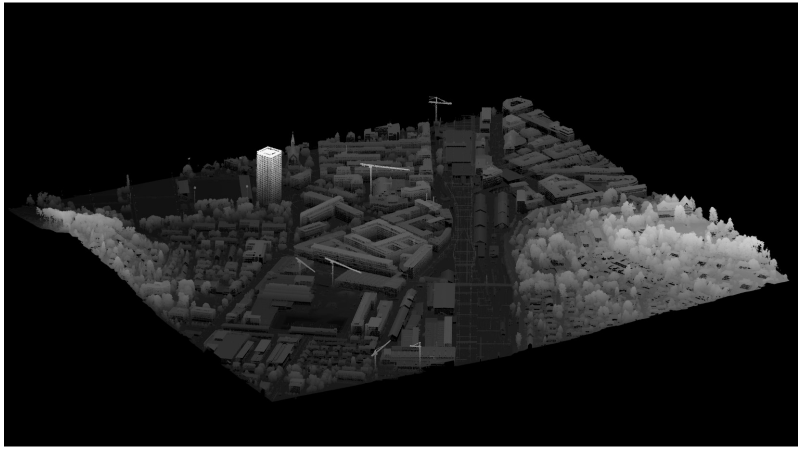
- Taxonomy of methods
- Graph convolution
- Message passing
- Graph Transformer

# Highly ordered data

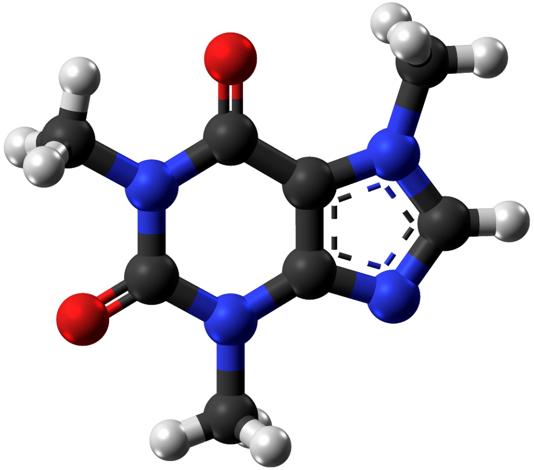
Rebirth of Deep learning was thanks to pictures, text and speech recognition


# Data structures: Data is not always euclidean

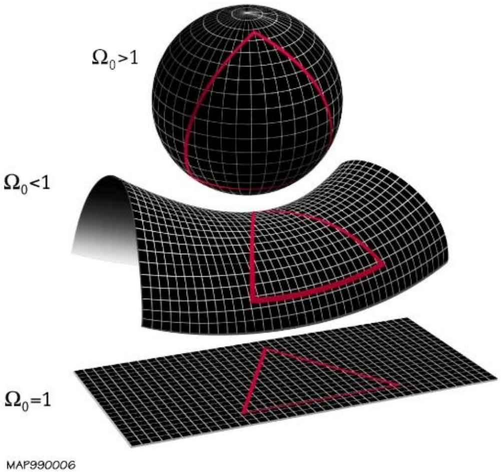
**LIDAR**



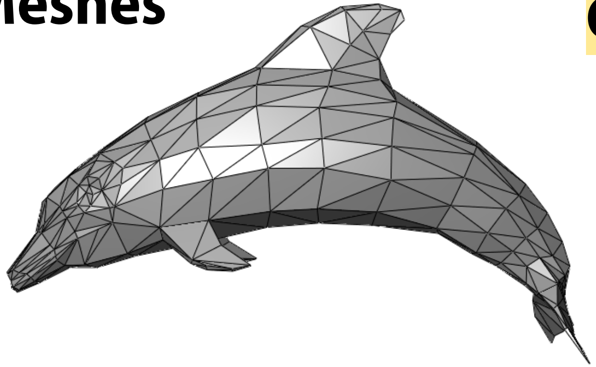
**Molecules**



**Complex geometries**



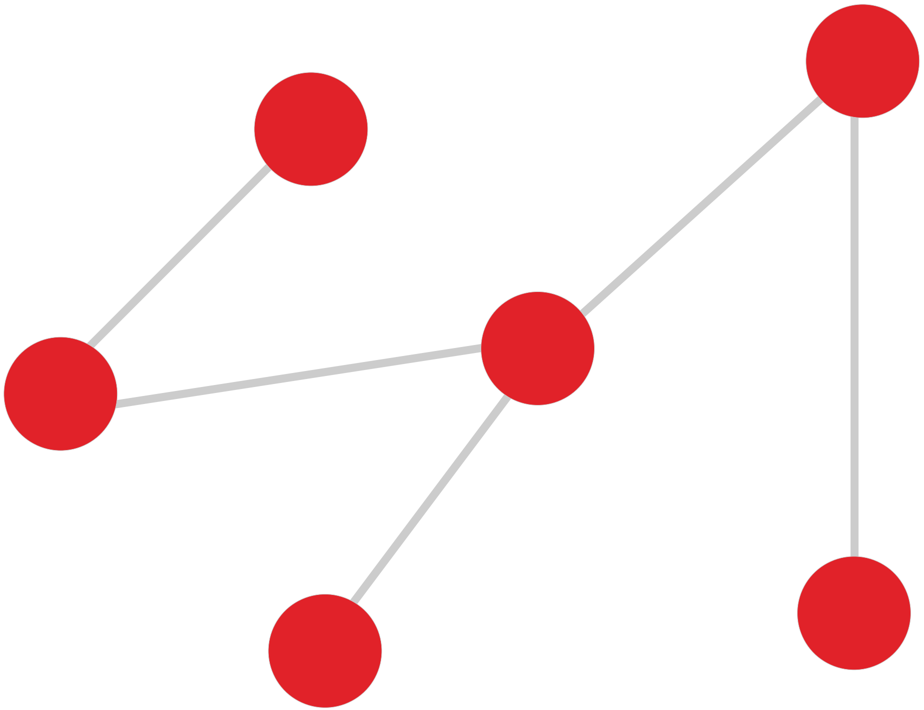

**Meshes**



**Geometric deep learning**


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

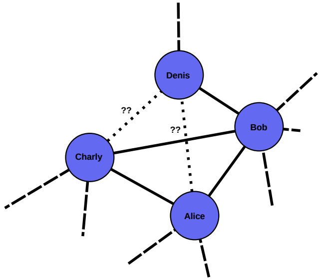
# Graphs are everywhere



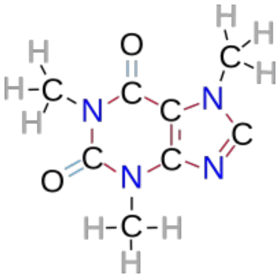
Data as a set of interconnected entities

# Graphs are everywhere

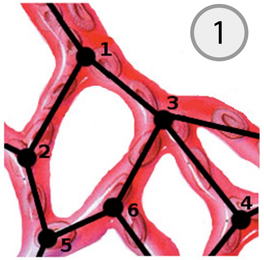
## Social networks




## Molecules

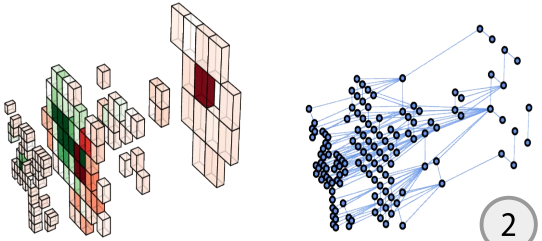


## Capillary networks



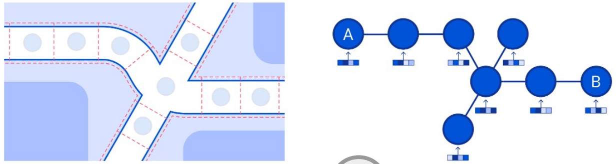

1

## Particle physics



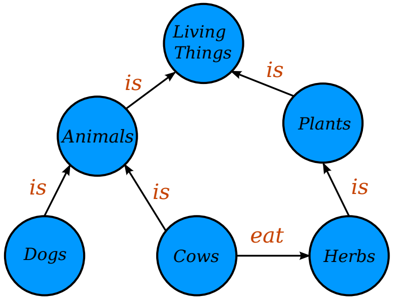
2

## Directions recommendation




3

## Knowledge graphs



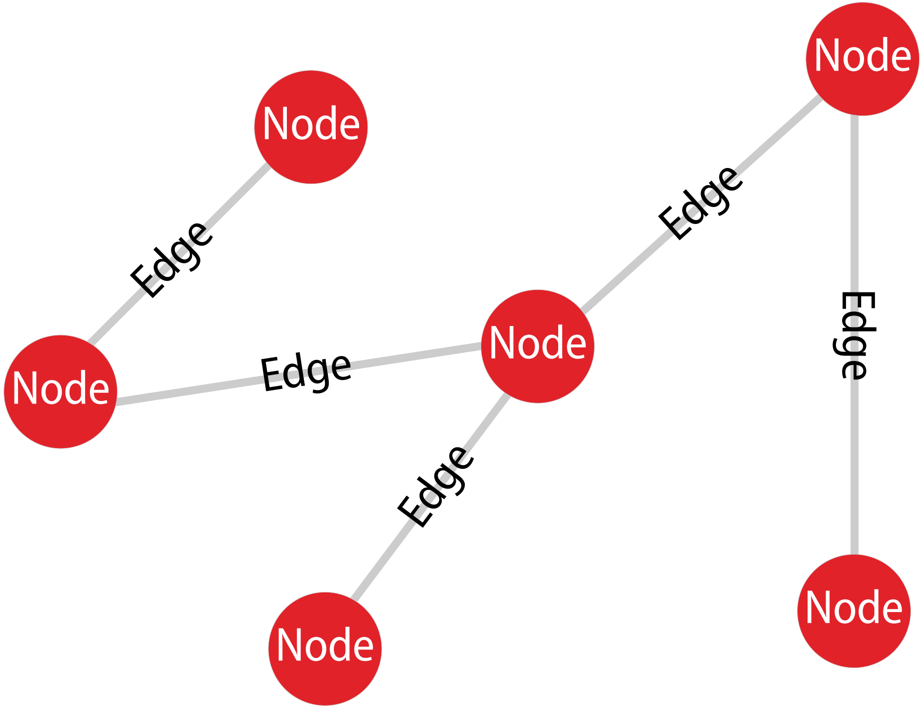

Many other fields

- 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

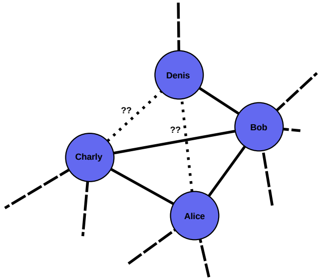
## Graph



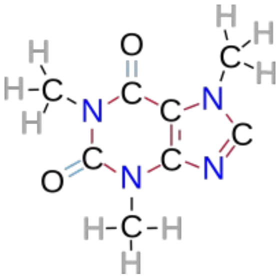
# Node/vertex

# Some example of nodes

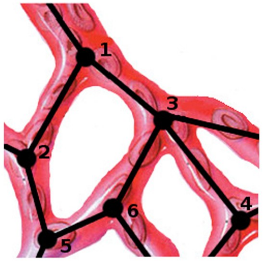
## Persons



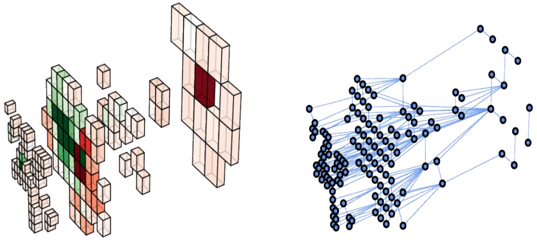

## Atoms



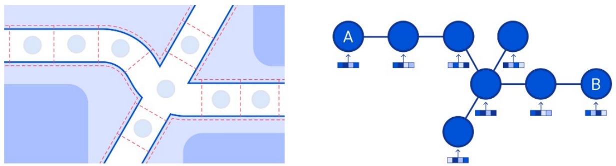
## Intersections



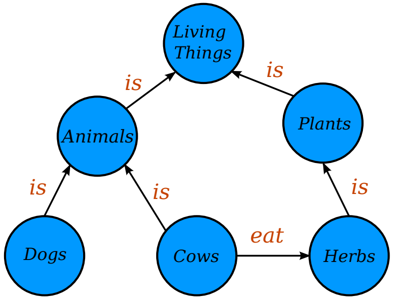

## Particles



## Road sections




## Concepts



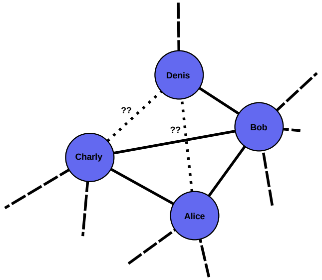

Many other fields

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

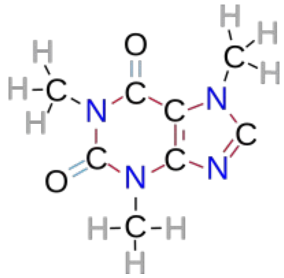
# Edge

## Some example of edges

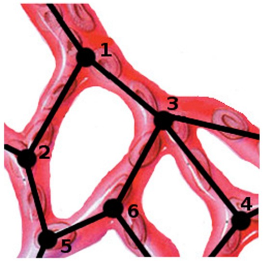
### Relationship



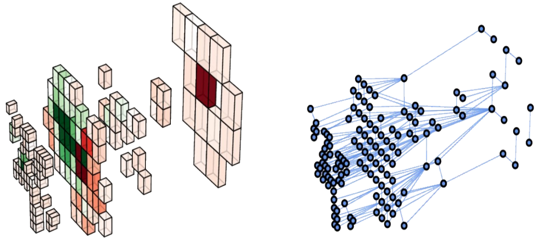

### Type of bond



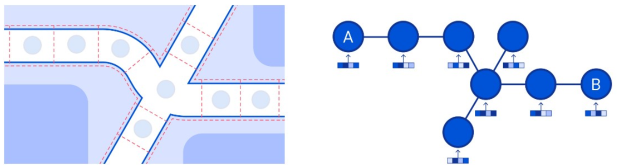
### Vessel



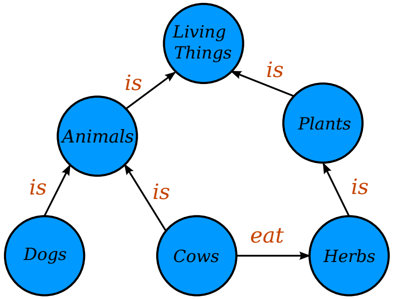

### Decayed to



### Time




### Statement



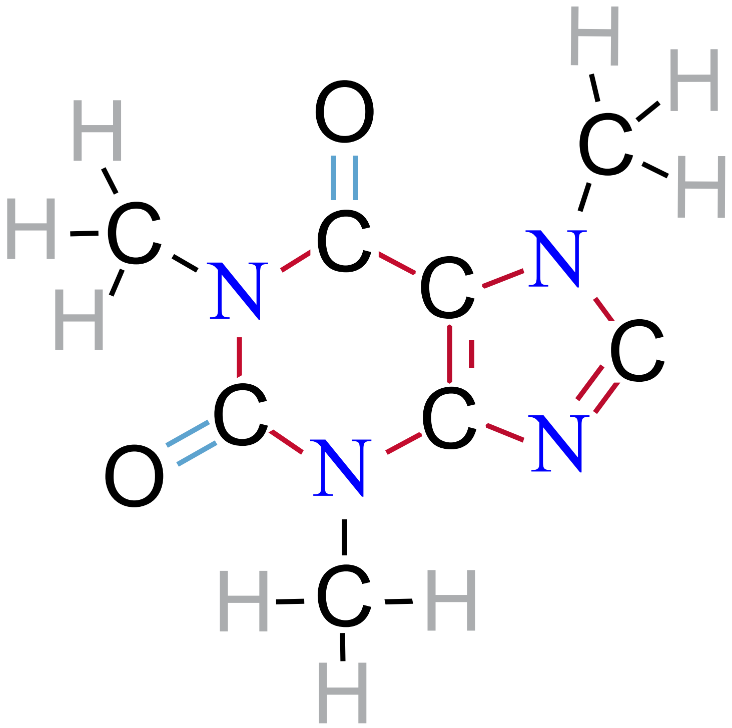

Many other fields

- 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**

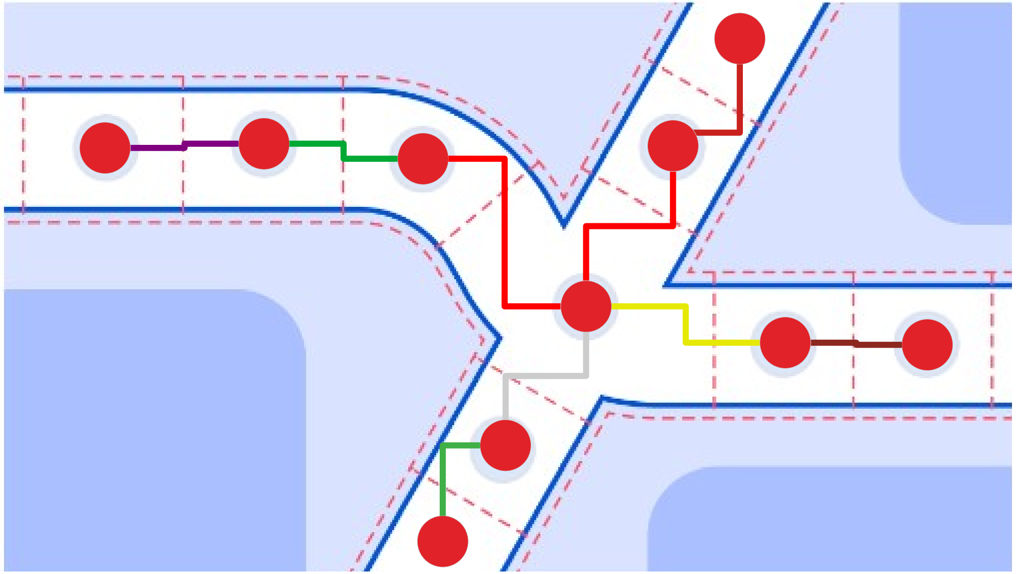
Undirected graphs



Directed graphs

# 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, ...

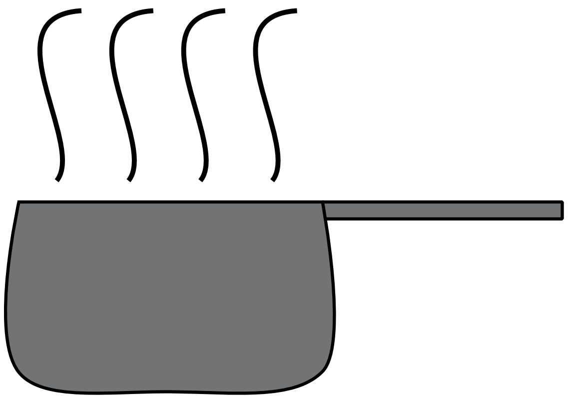
# Formal definition

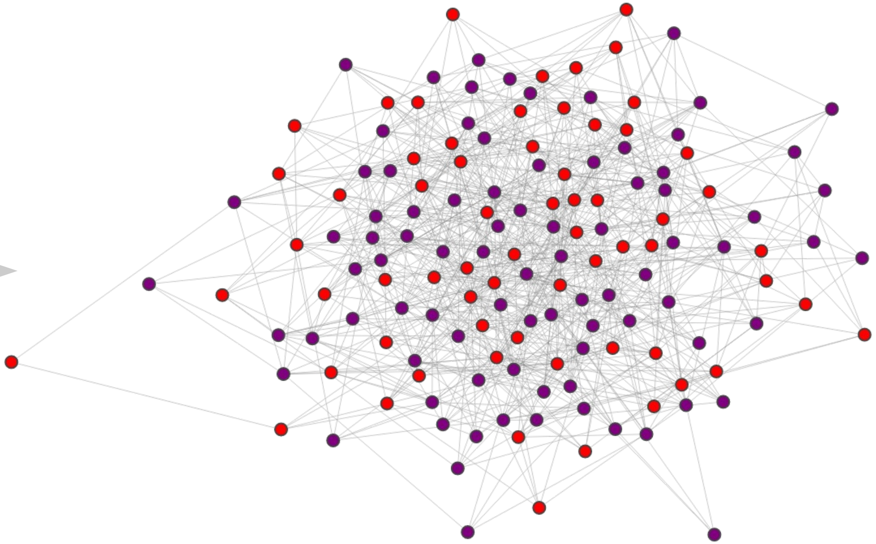
## G = (V, E): a set of nodes and edges

**Features**

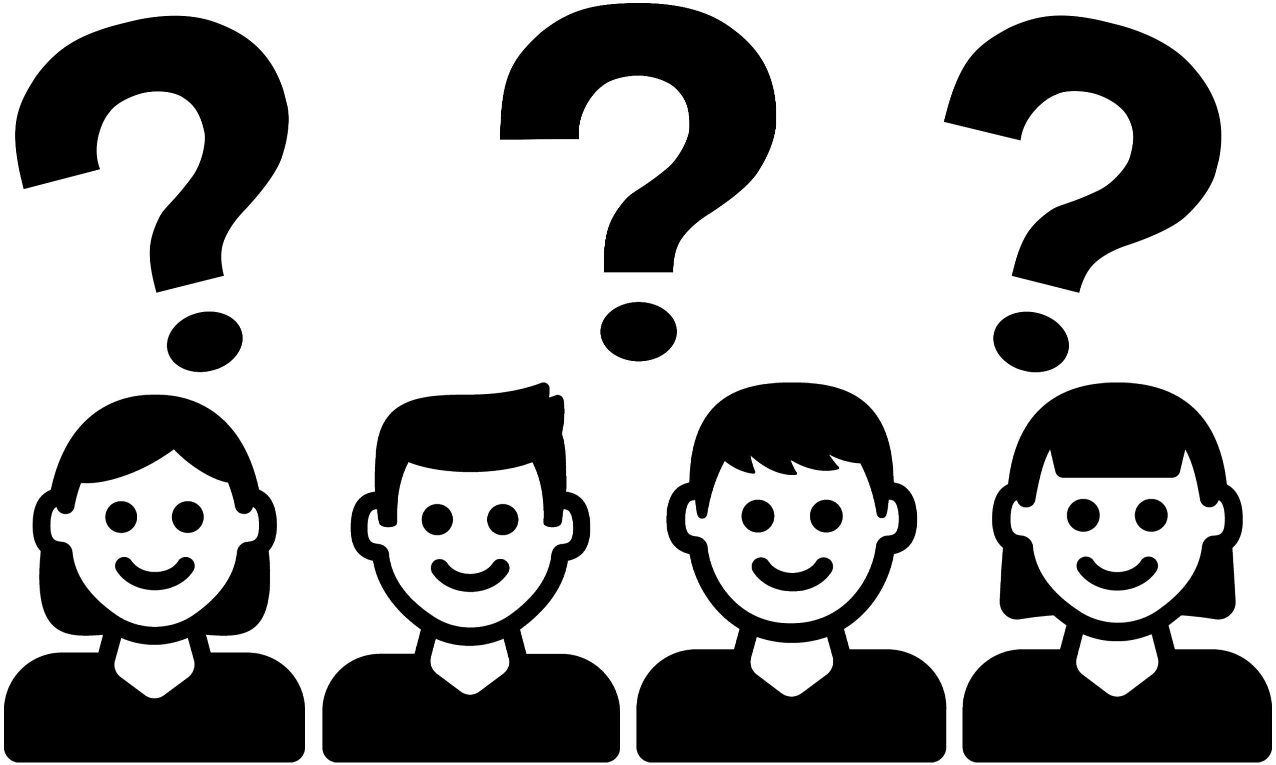
$\{y_i^V\}$ $\{y_i^E\}$ $\{y_i^G\}$

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

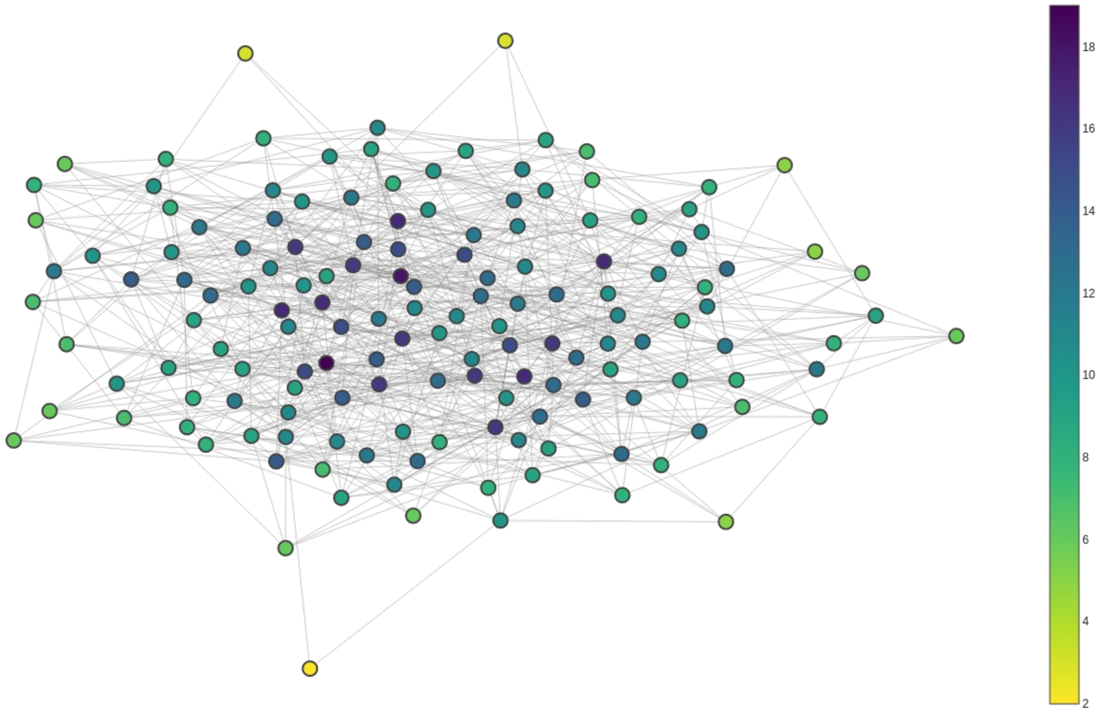




# Question break



# Graph: Complexity



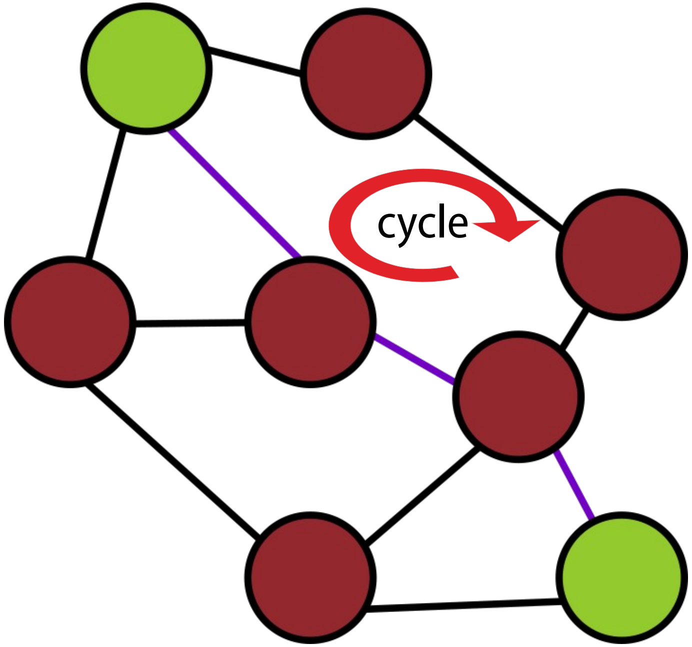

Number of neighbors

- 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
- ...

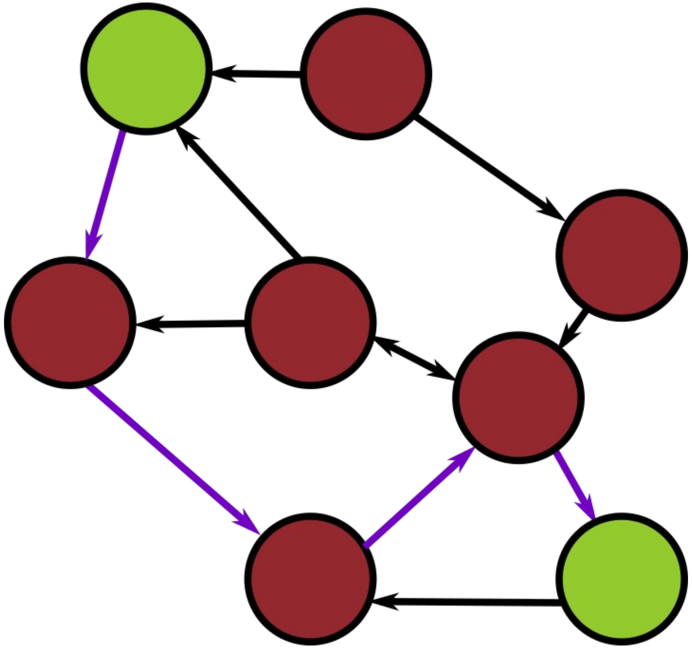
# Graph: Paths

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

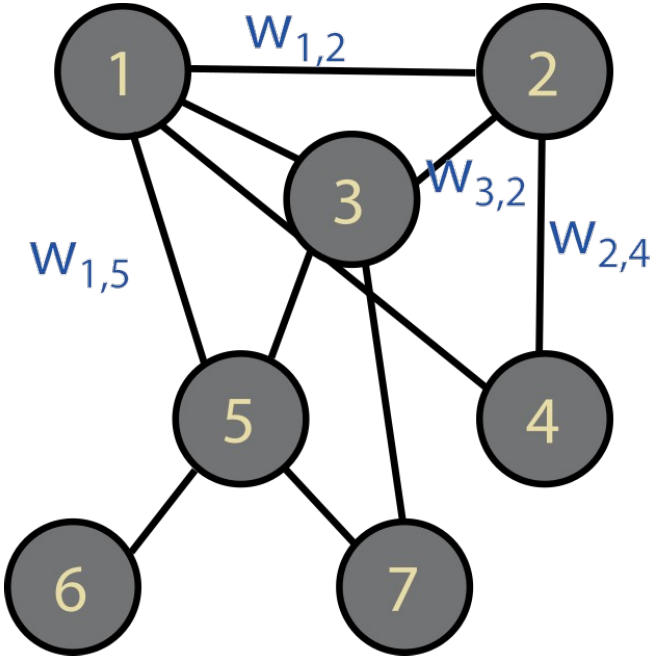
Undirected graph




Directed graph



# Graph: Node proximity and centrality



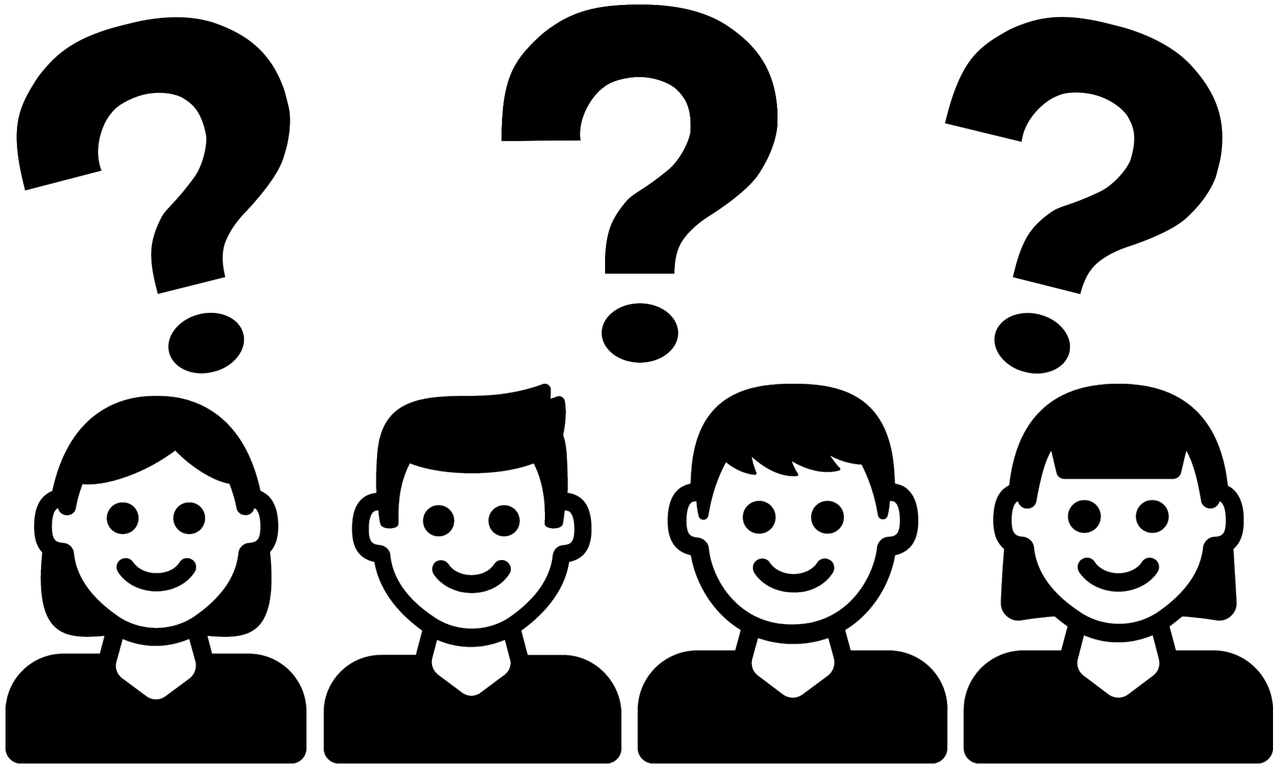

**Node centrality**

Measure how many paths goes through the node

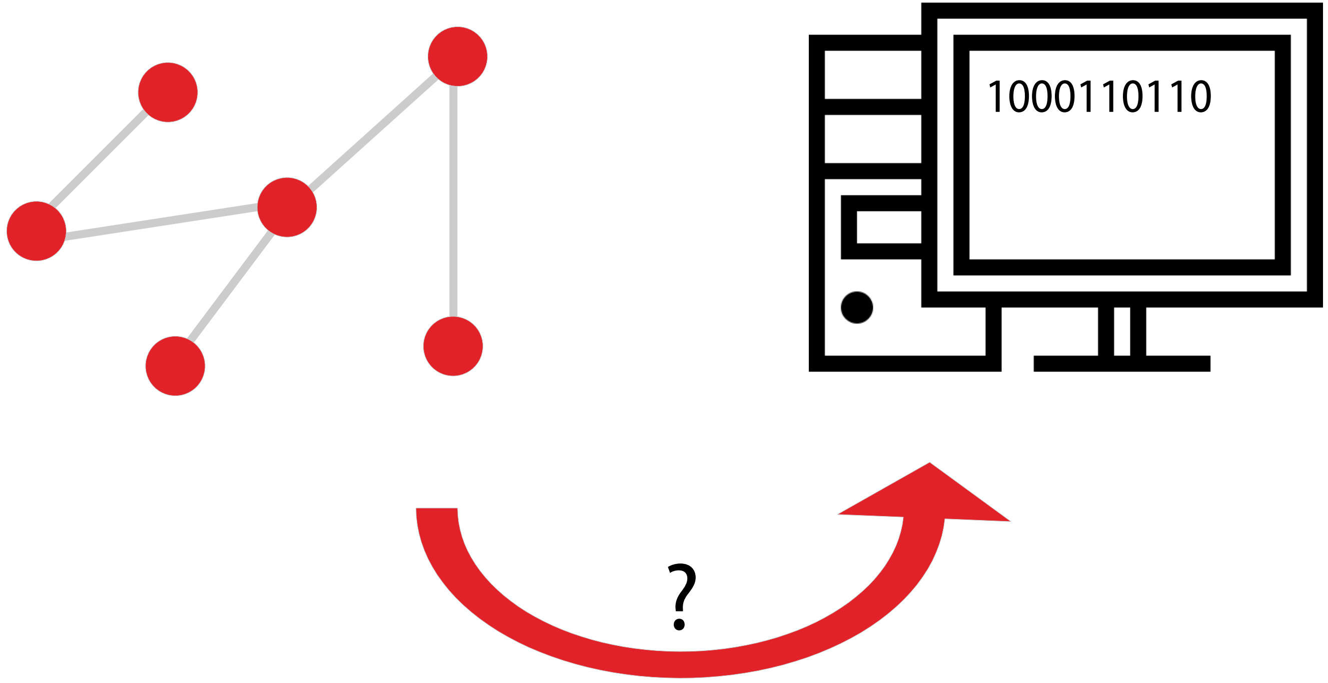
**Node proximity**

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

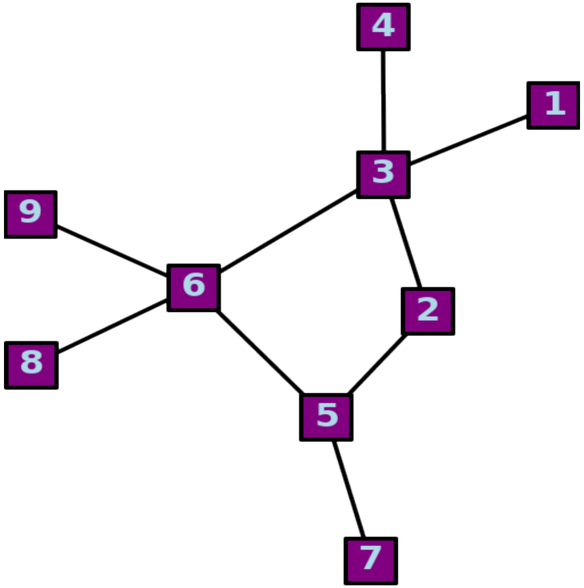
# Question break



# Graph representation



# Graph representation

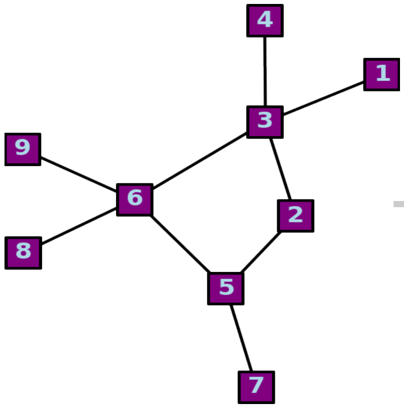


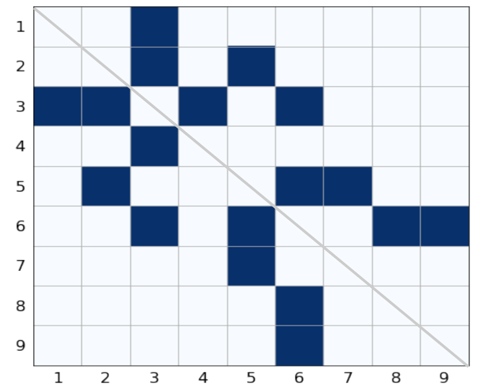

**Random numbering of nodes**

# Graph representation

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

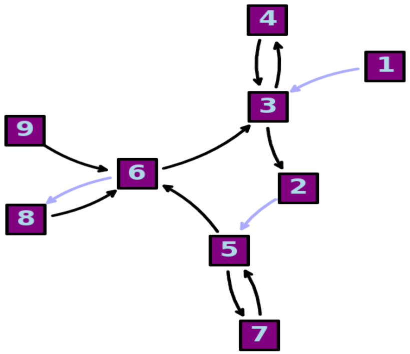
**Undirected**

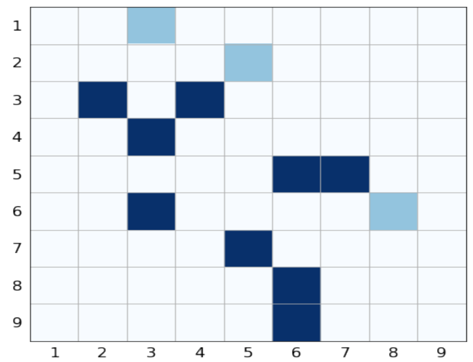



**Symmetric**

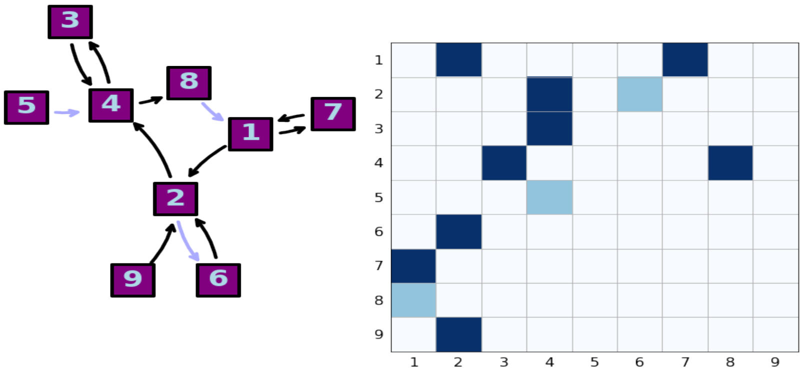
**Directed**



# Graph representation

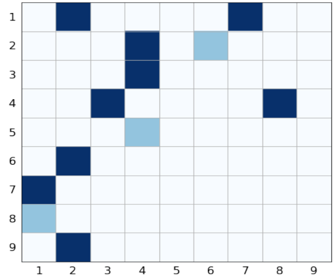
## Adjacency list




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




Adjacency list: [[5, 4],
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[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]

- 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

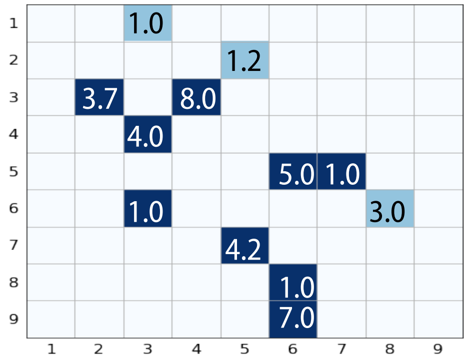


https://www.geeksforgeeks.org/comparison-between-adjacency-list-and-adjacency-matrix-representation-of-graph/

# 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.

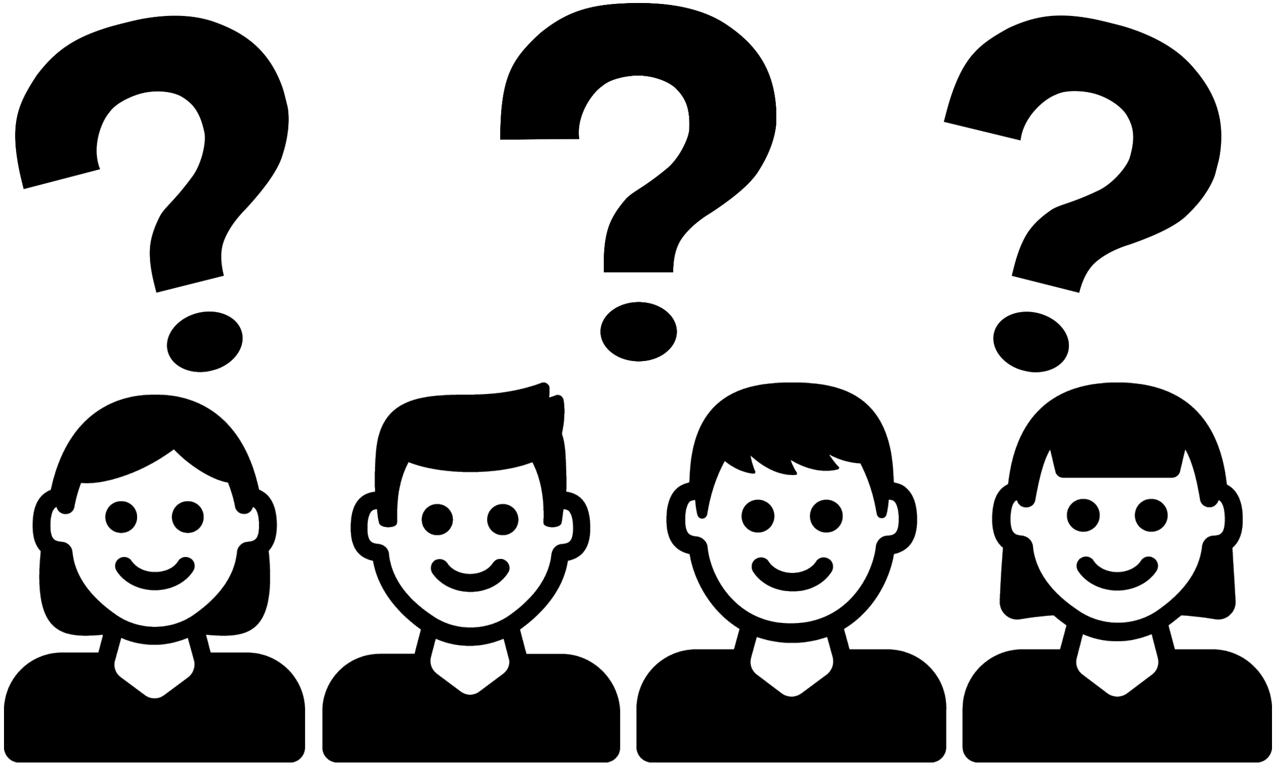
Nodes: [4.1, 4.2, 6.4, 1.0, 1.0, 5.0, 1.7,
3.0, 5.0]

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

1 **Graphs are everywhere**

- Complex data structures
- Basics of graph theory

2 **Learning on Graphs**

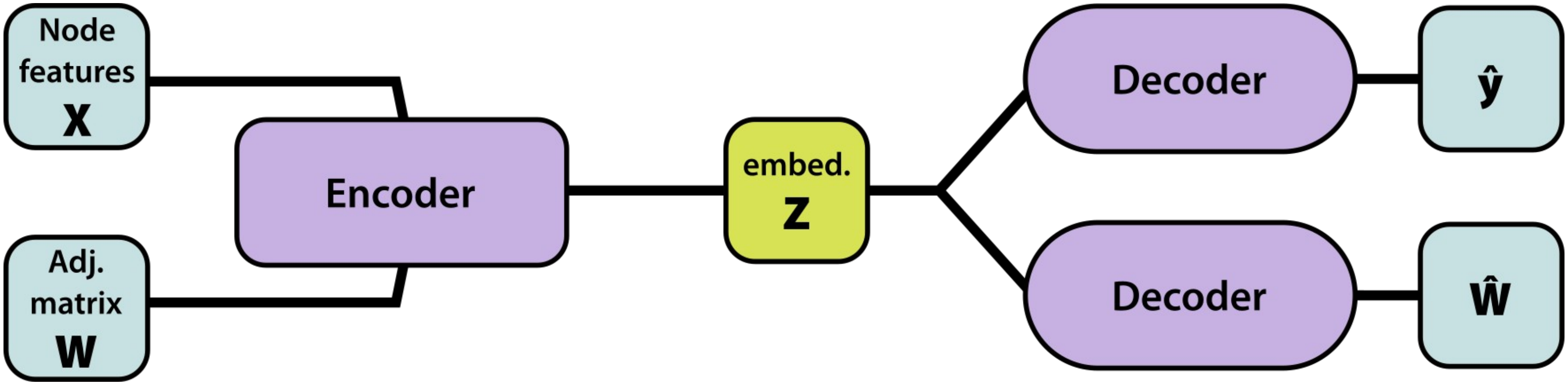
- Graph embedding
- Transductive and inductive learning
- Tasks on graph learning

3 **A few examples**

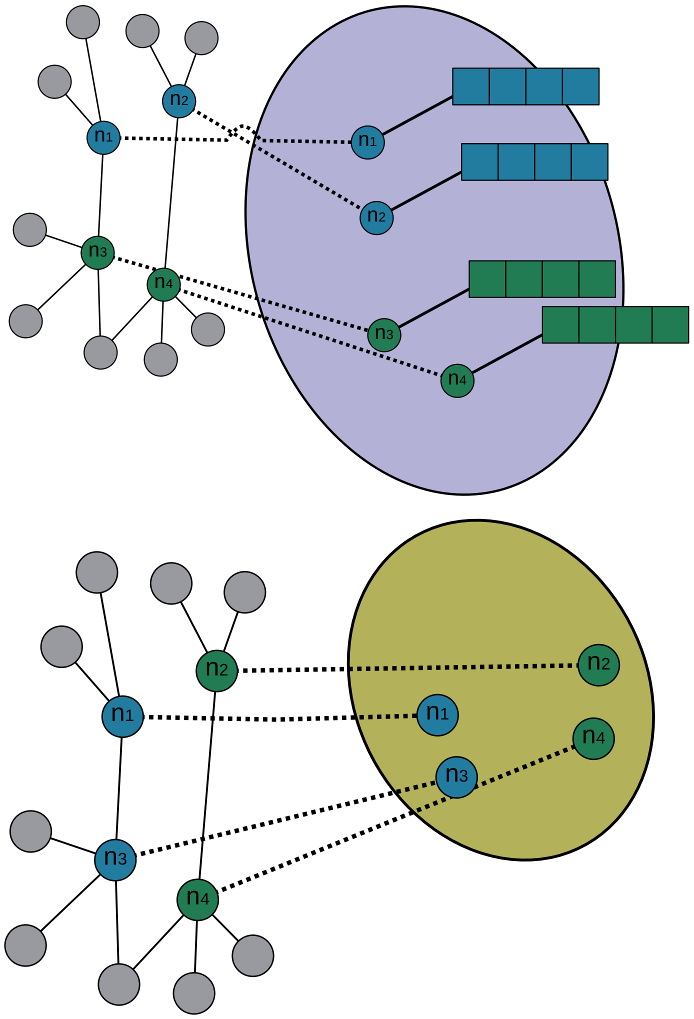
- Taxonomy of methods
- Graph convolution
- Message passing
- Graph Transformer

# Graph embedding

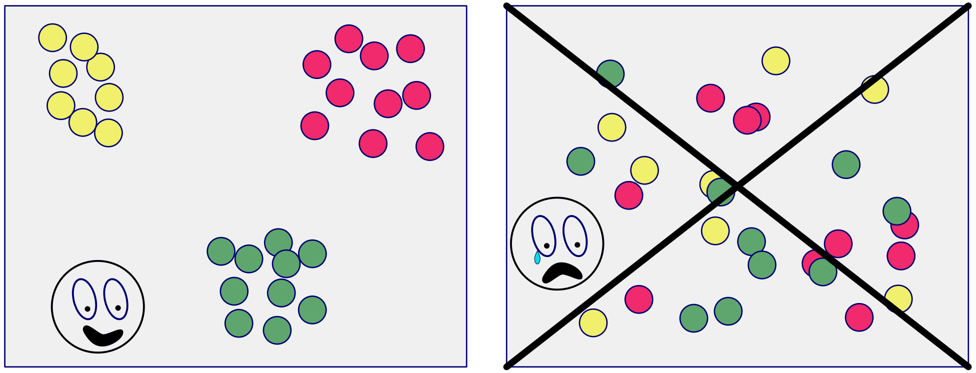
- We need to find a representation of the graph that is processable



# 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.**

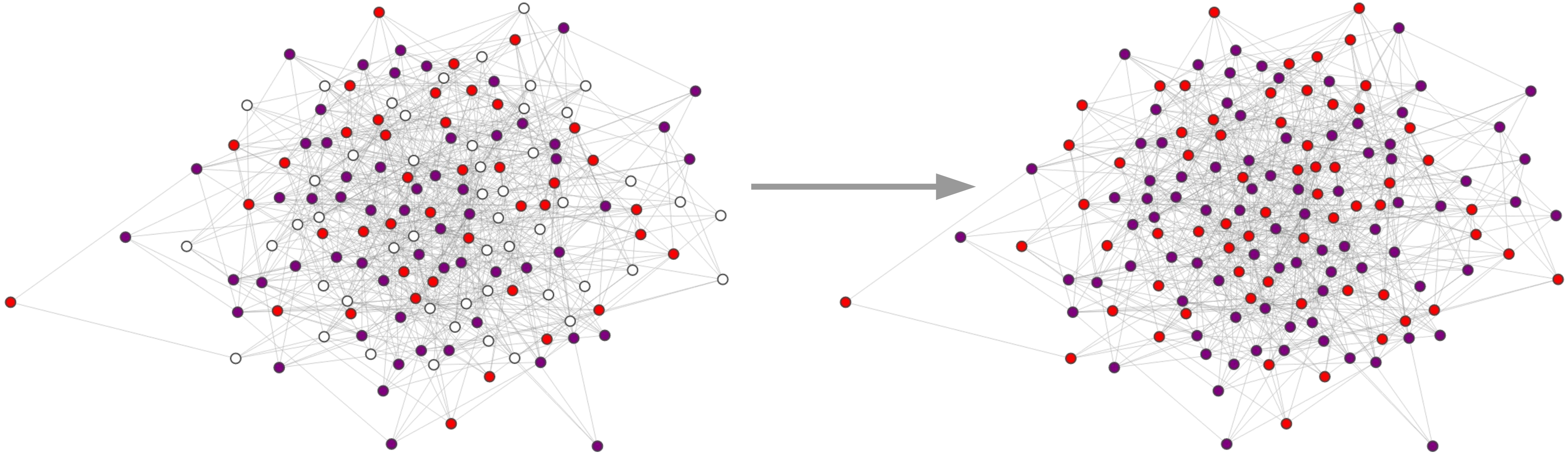


# Transductive learning

The model has access to the complete graph

It is not possible to add new nodes

Node labeling

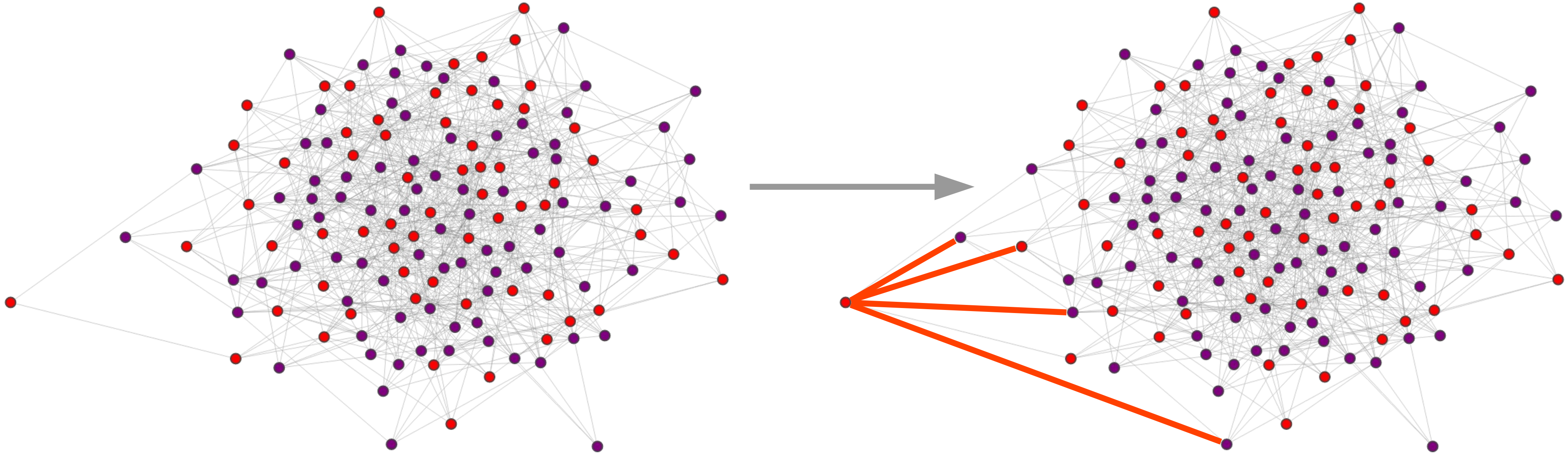


# Transductive learning

The model has access to the complete graph

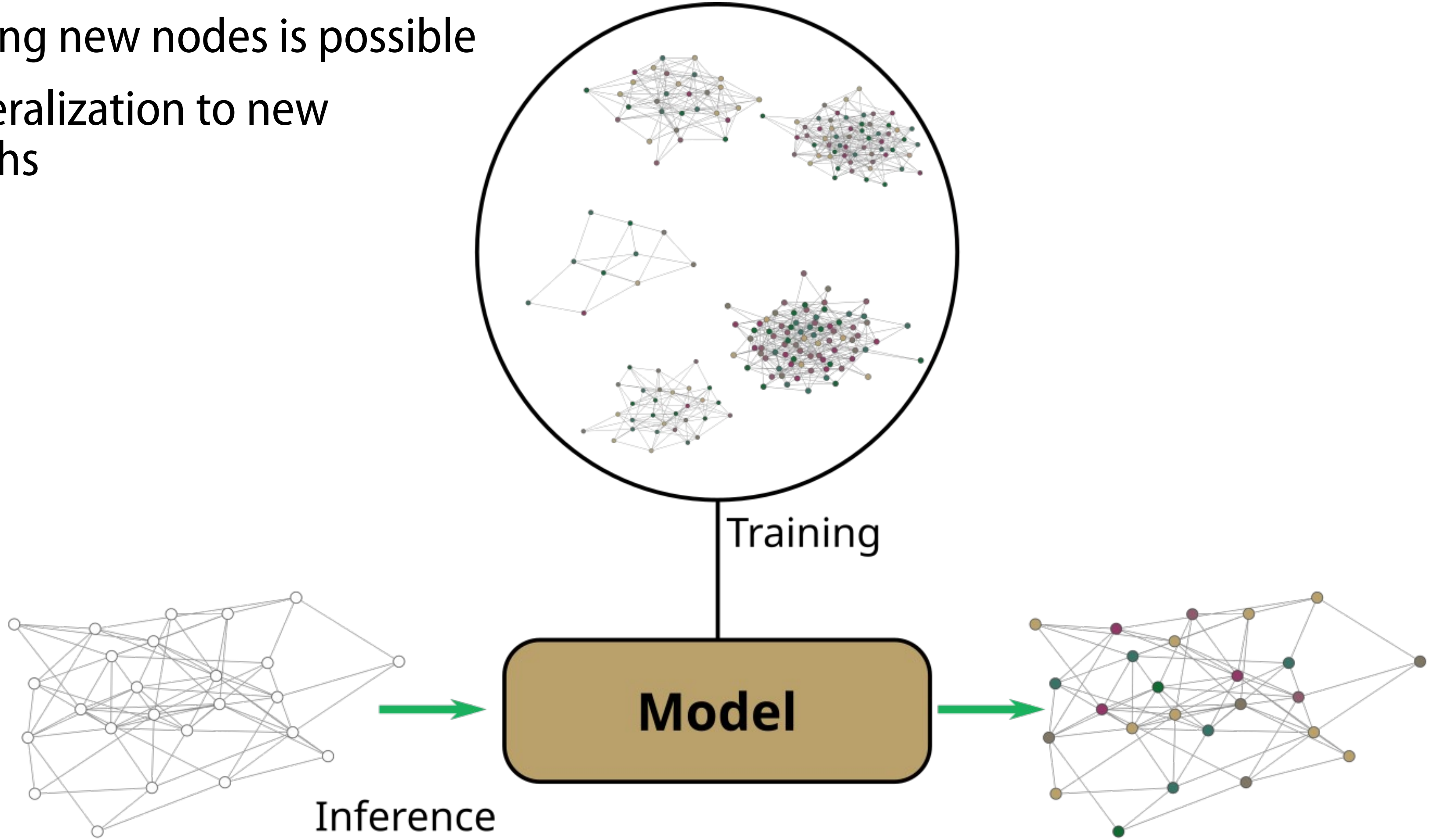
It is not possible to add new nodes

Find new edges



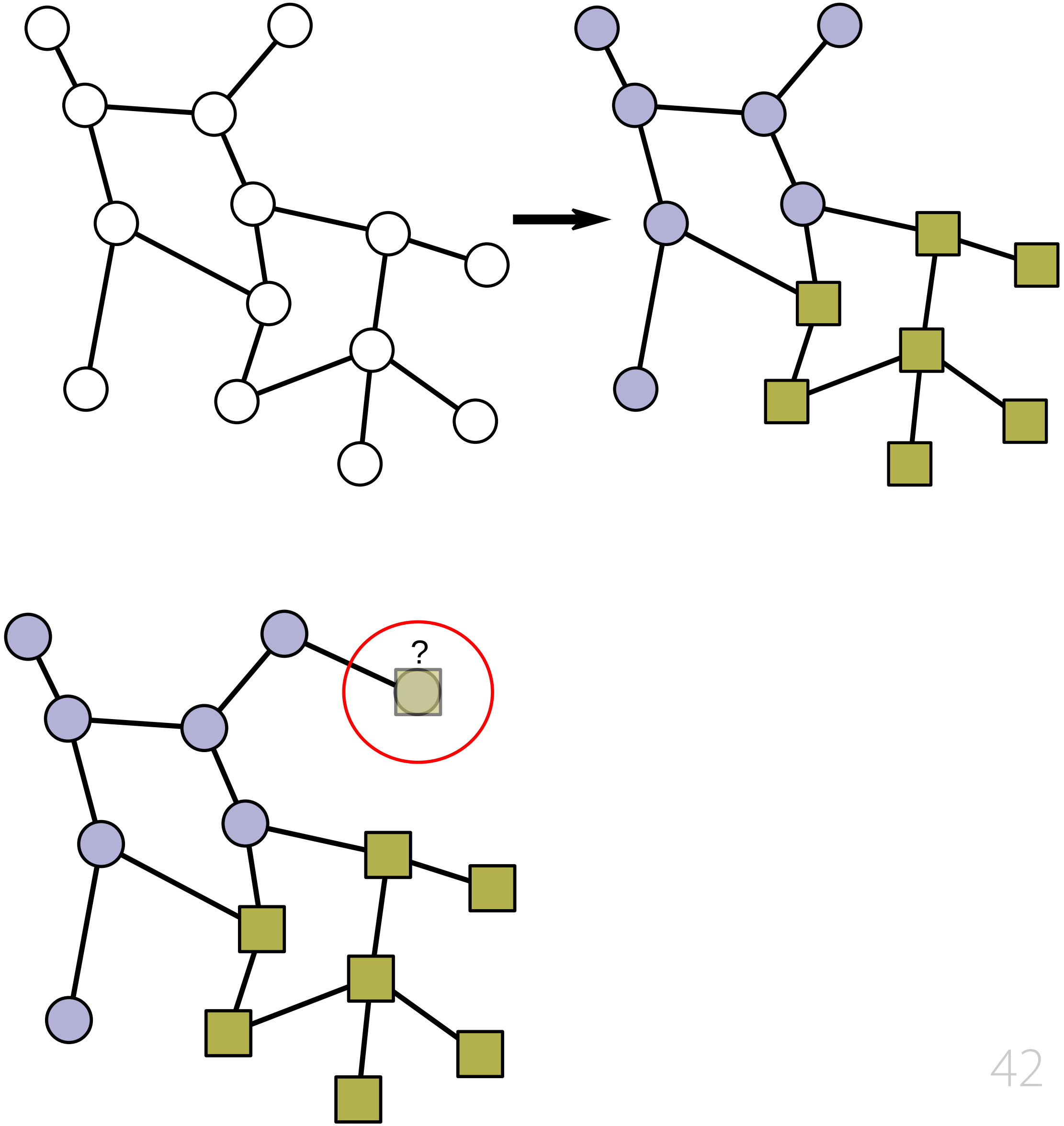
# Inductive learning

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



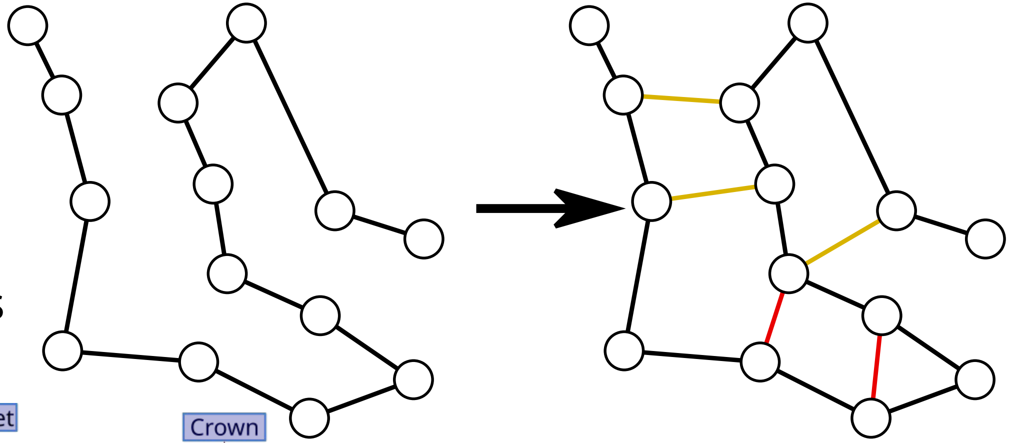
# Tasks on nodes

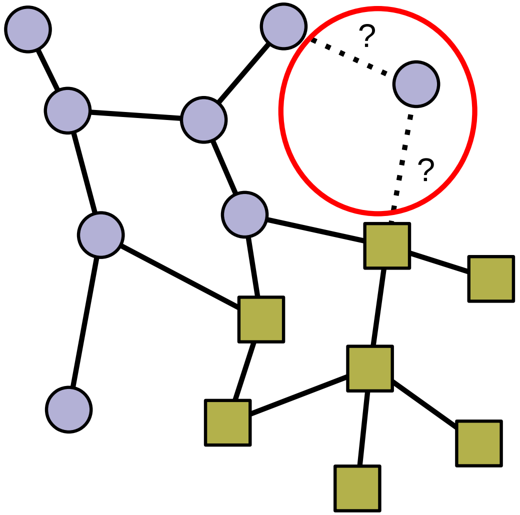
- Labeling nodes in a graph (clustering)
  - Find topic of a research paper (CORA, etc)
  - Find bots in a social network
  - …
- Labeling new nodes
- Perform regression

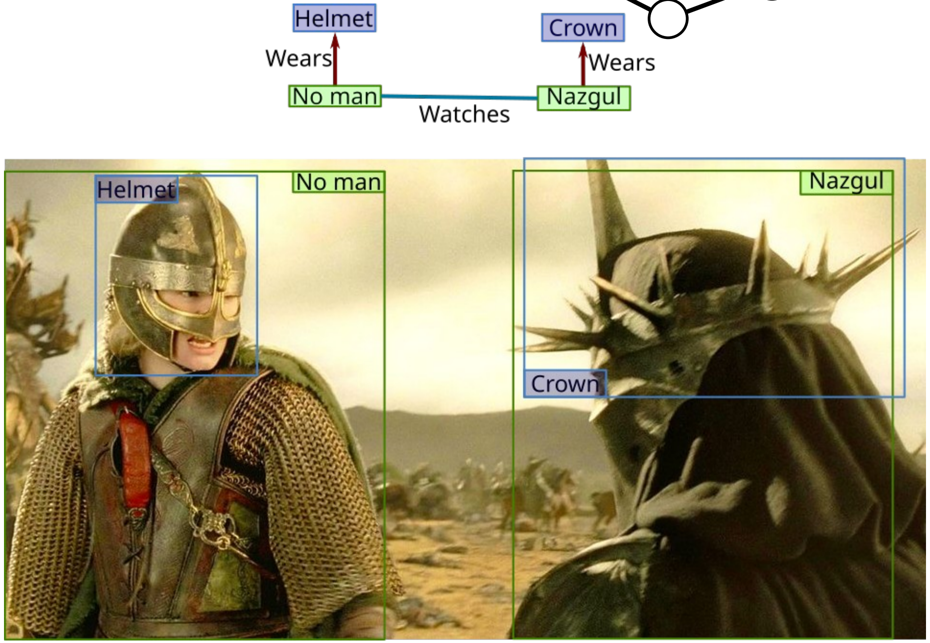


# Tasks on edges

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



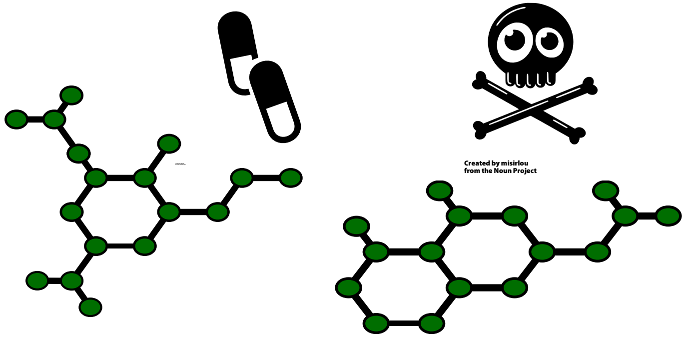


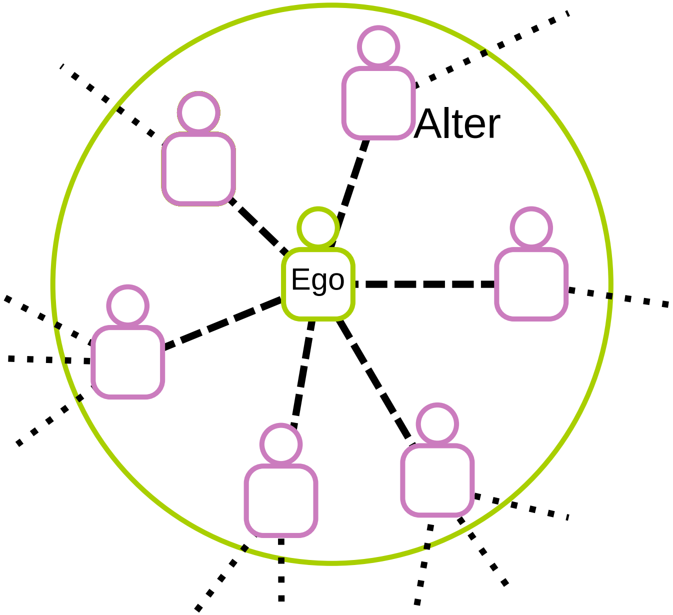




G. Zhu et al., "Scene Graph Generation: A Comprehensive Survey." arXiv, Jun. 22, 2022. doi: 10.48550/arXiv.2201.00443.

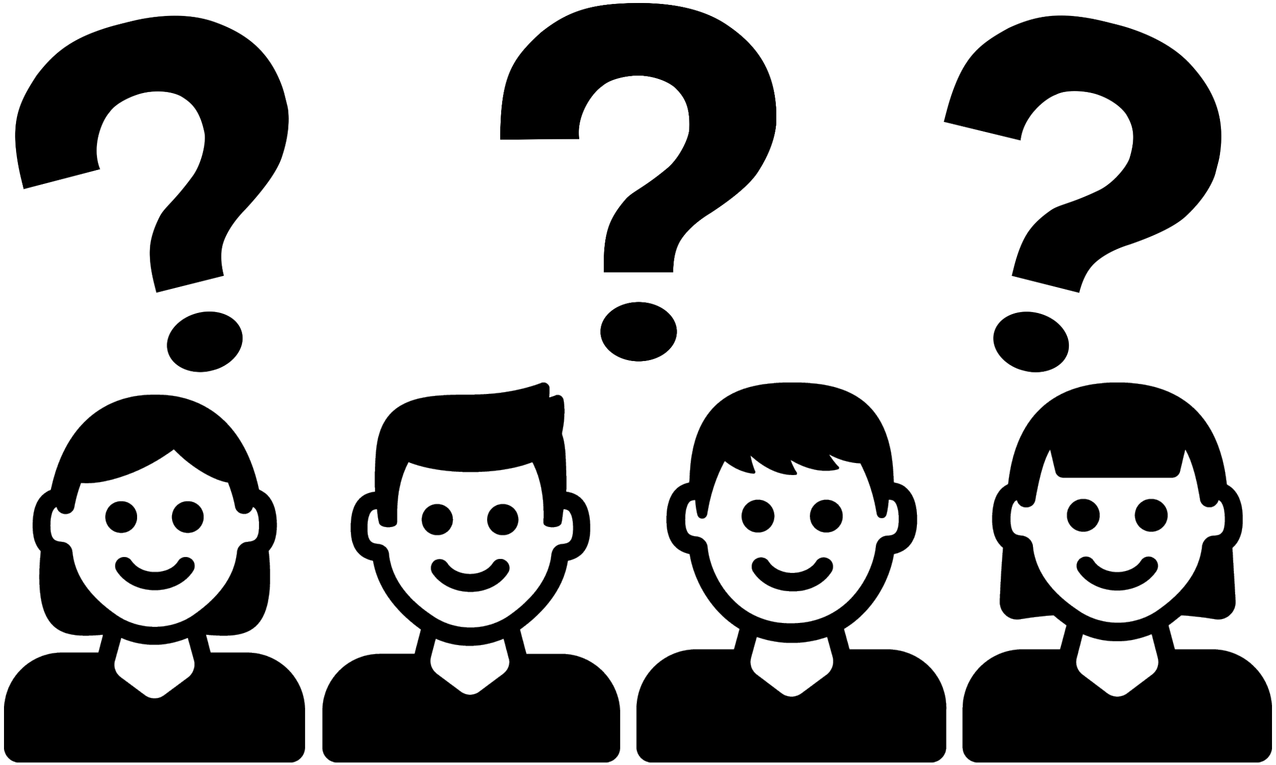
# Tasks on graphs

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



# Question break



# Roadmap

10

**Graph Neural Network**

GNN

1 **Graphs are everywhere**

- Complex data structures
- Basics of graph theory

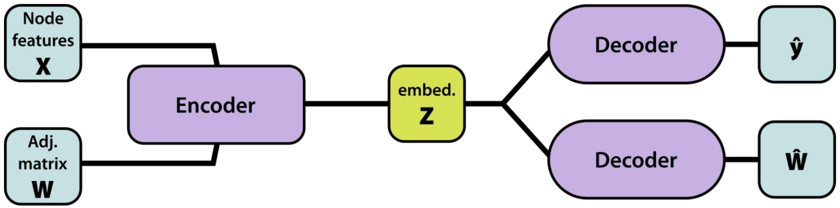
2 **Learning on Graphs**

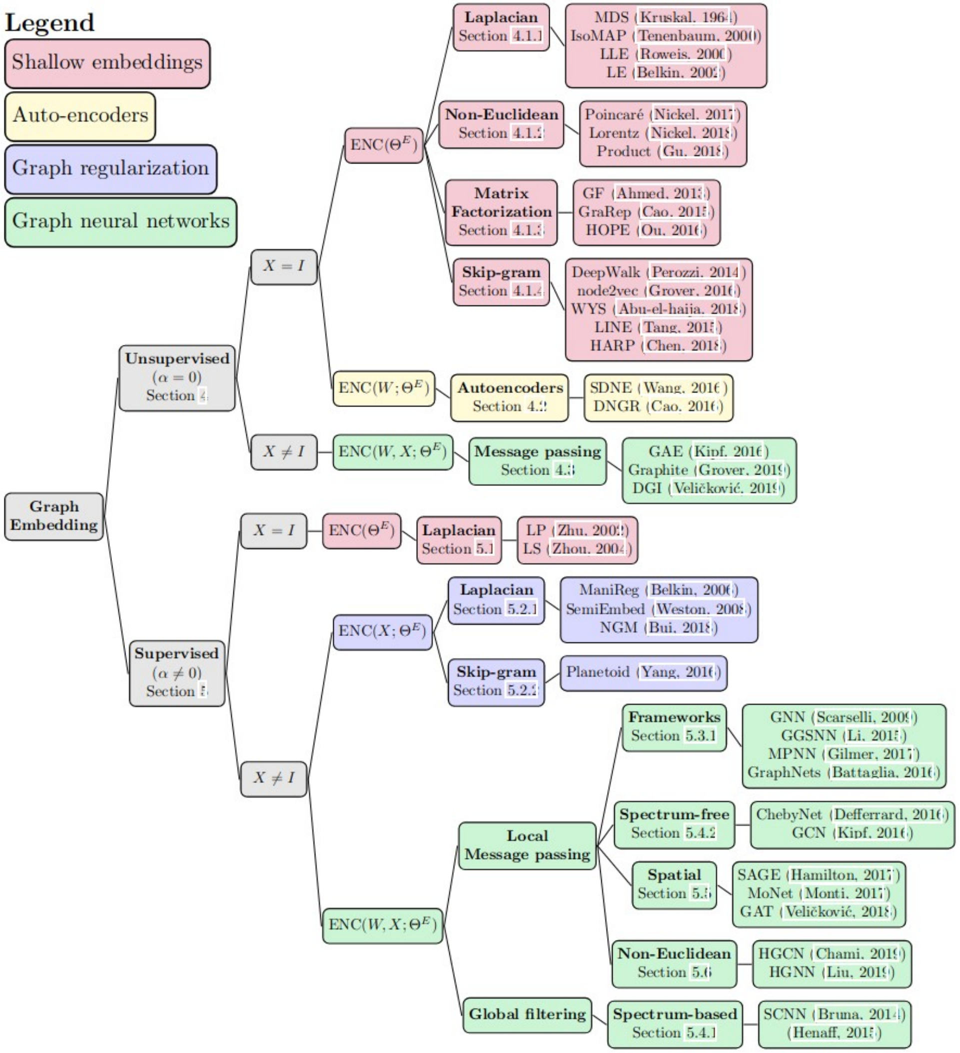
- Graph embedding
- Transductive and inductive learning
- Tasks on graph learning

3 **A few examples**

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

# Taxonomy of methods

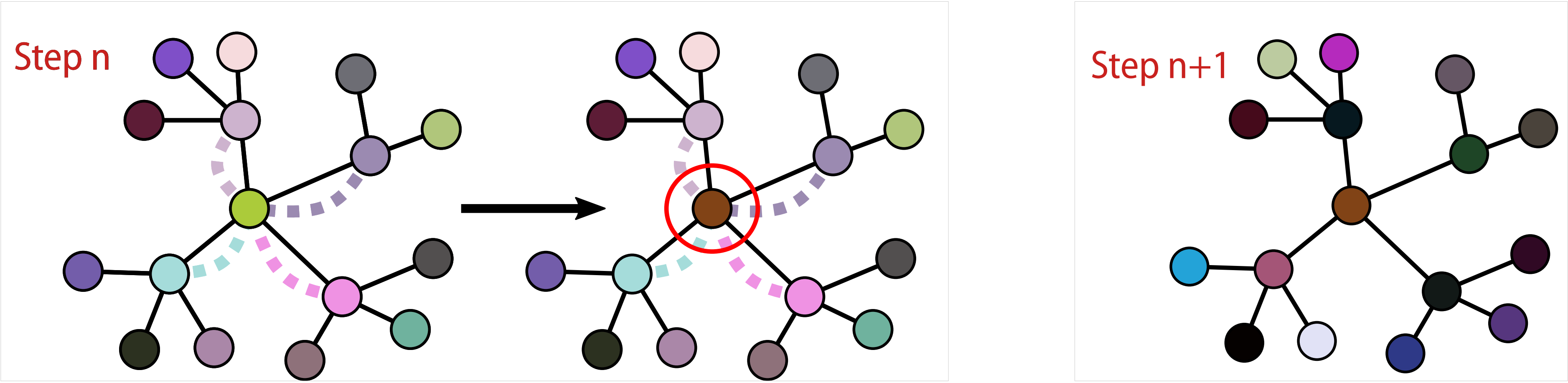



I. Chami, S. Abu-El-Haija, and B. Perozzi,
"Machine Learning on Graphs: A Model and Comprehensive Taxonomy".

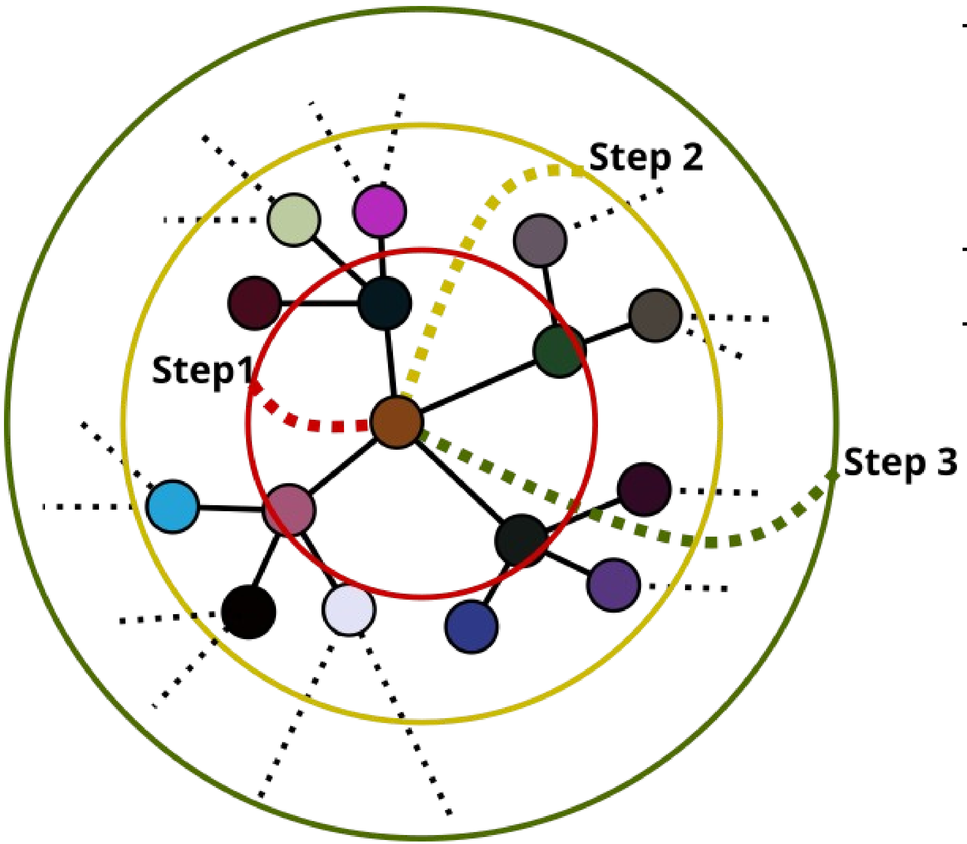
# Graph convolution

- 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.

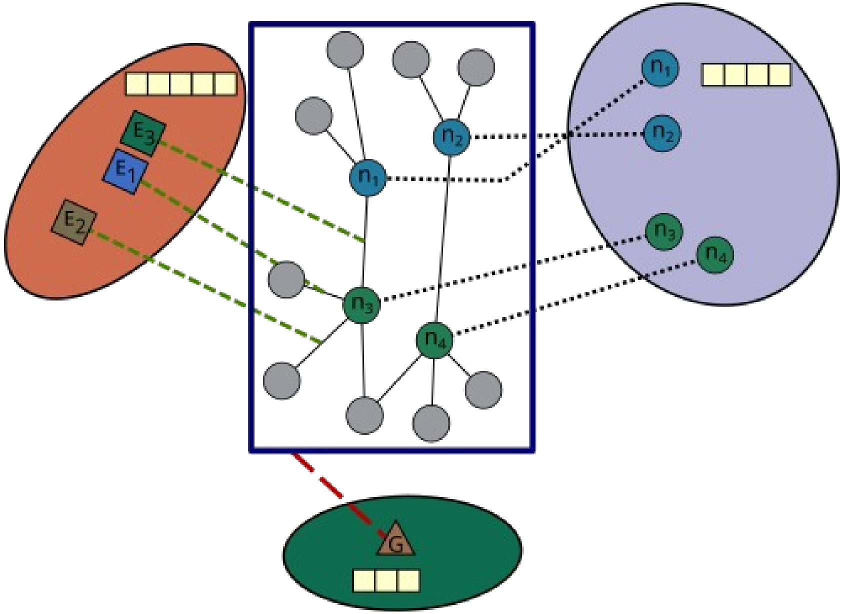
# Graph convolution

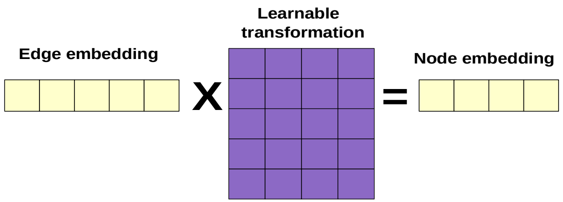


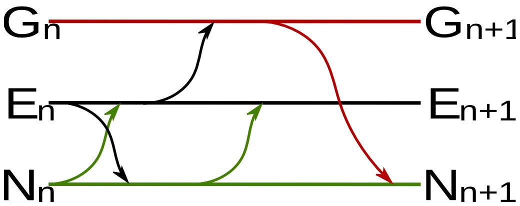

- Several steps are needed to retrieve information for distant nodes.
- For large graphs → a **cutoff**
- It is possible to use a **virtual node** connected to all other nodes. But in practice this becomes quickly intractable.

# Message passing

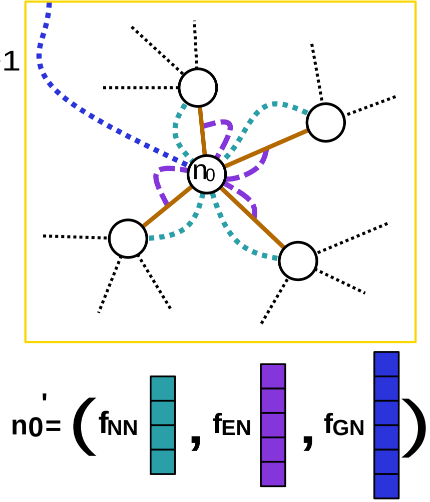
- We have embeddings for each part of the graph (possibly different vector sizes).
- Each part can learn from the others via a transformation.



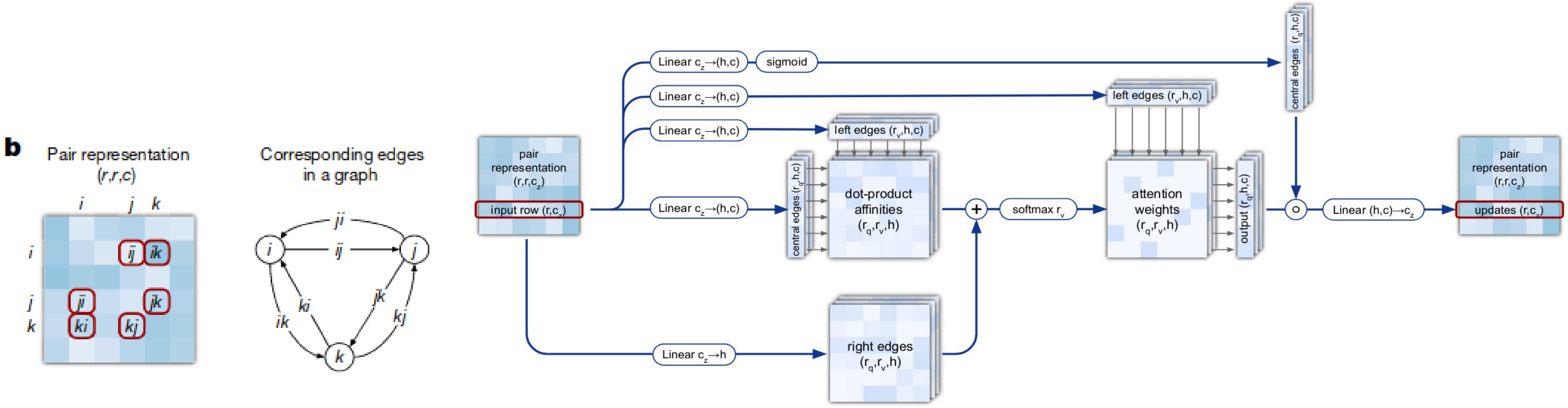




- Information is aggregated to form a message that the node/edge will send to others.



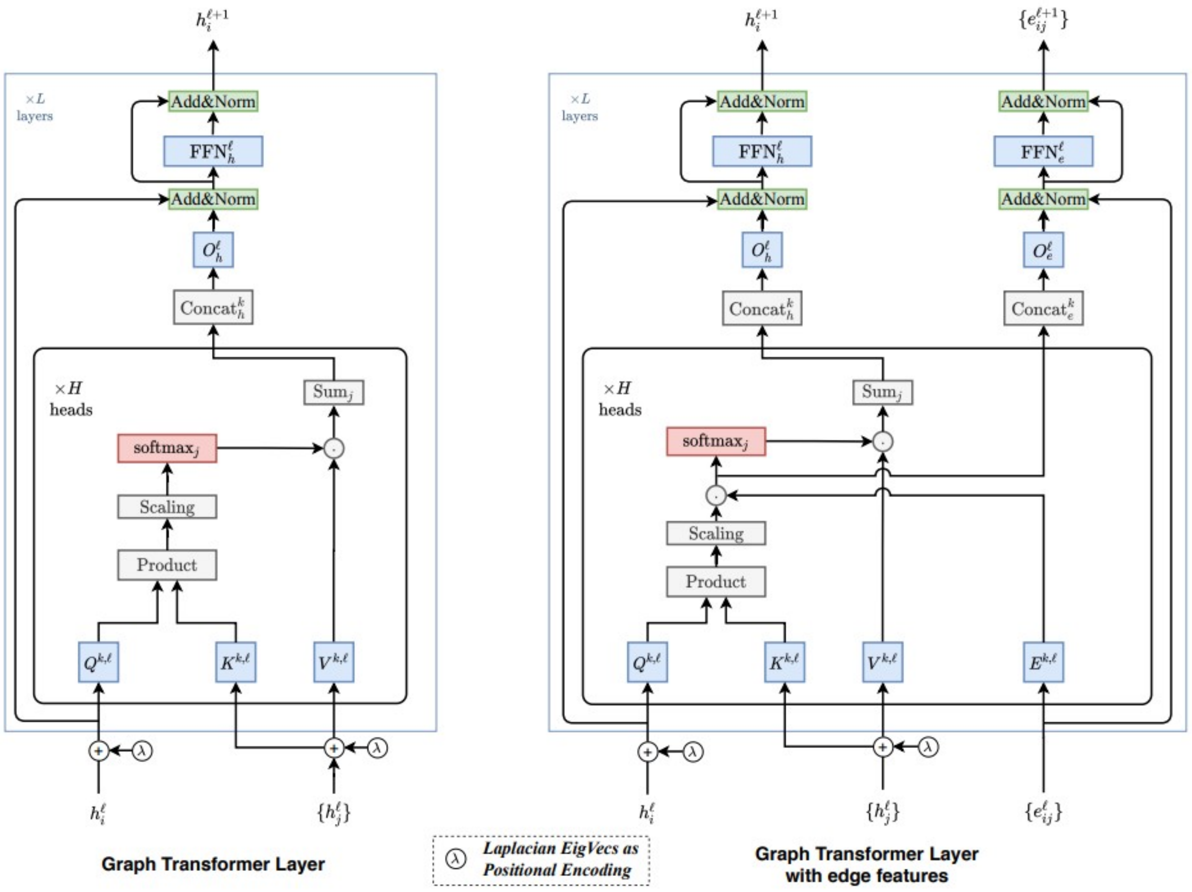
# Alphafold transformer




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

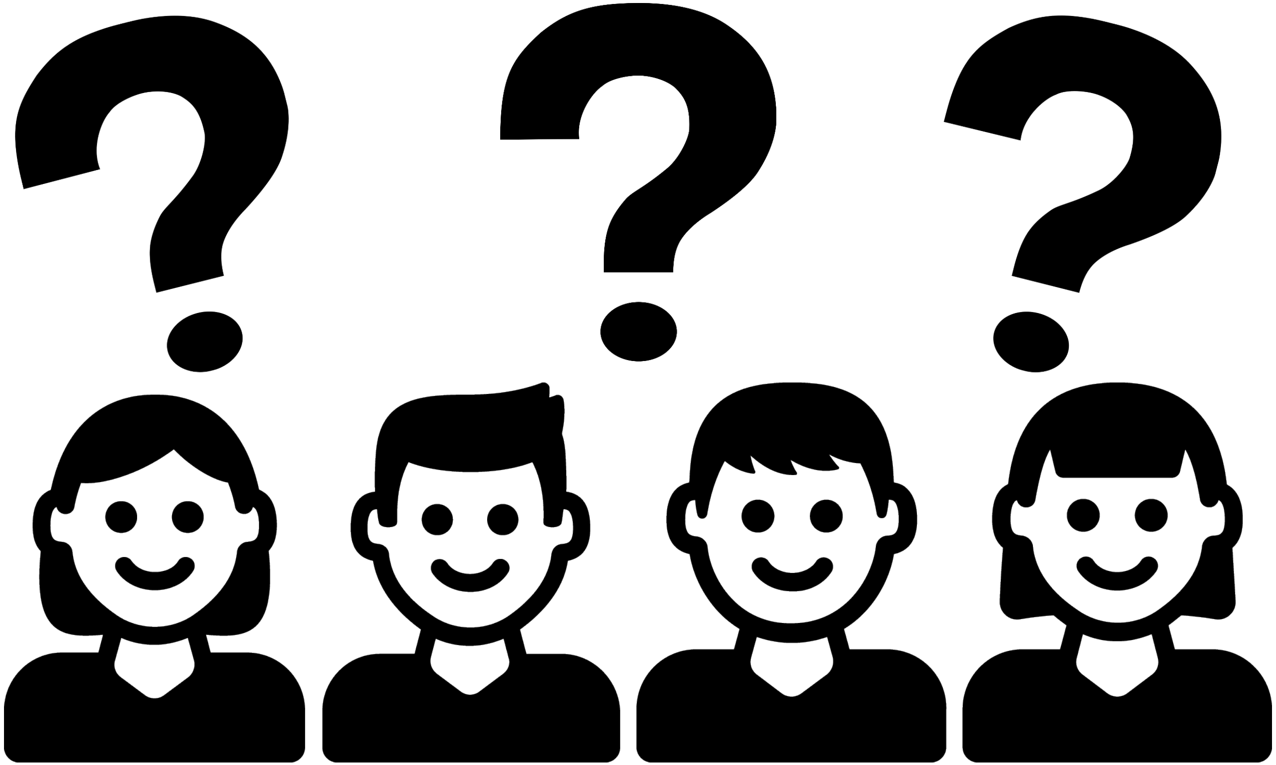
J. Jumper et al., Highly accurate protein structure prediction with AlphaFold, Nature, vol. 596, no. 7873, Art. no. 7873, Aug. 2021, doi: 10.1038/s41586-021-03819-2.

# 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

# References

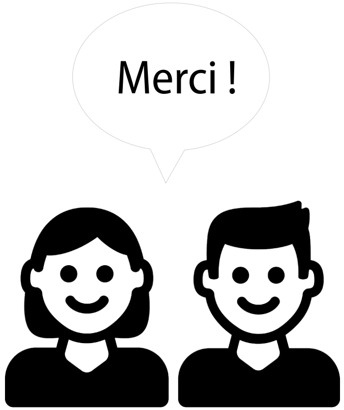
- Books
  - Deep Learning on Graphs (Jiliang Tang and Yao Ma)
  - Introduction to Graph Neural Networks (Introduction to Graph Neural Networks)
- Websites
  - https://distill.pub/2021/gnn-intro/
  - https://neptune.ai/blog/graph-neural-network-and-some-of-gnn-applications
  - https://venturebeat.com/2021/10/13/what-are-graph-neural-networks-gnn/
  - https://theaisummer.com/graph-convolutional-networks/
  - https://towardsdatascience.com/node-embeddings-for-beginners-554ab1625d98
- Articles


- **Chami, S. Abu-El-Haija, and B. Perozzi, "Machine Learning on Graphs: A Model and Comprehensive Taxonomy".**
- Zhou, Jie, et al. "Graph neural networks: A review of methods and applications." AI Open 1 (2020): 57-81.
- Scarselli, Franco, et al. "The graph neural network model." IEEE transactions on neural networks 20.1 (2008): 61-80.
- Kipf, Thomas N., and Max Welling. "Semi-supervised classification with graph convolutional networks." arXiv preprint arXiv:1609.02907 (2016).
- Perozzi, Bryan, Rami Al-Rfou, and Steven Skiena. "Deepwalk: Online learning of social representations." Proceedings of the 20th ACM SIGKDD international conference on Knowledge discovery and data mining. 2014.
- Shlomi, Jonathan, Peter Battaglia, and Jean-Roch Vlimant. "Graph neural networks in particle physics." Machine Learning: Science and Technology 2.2 (2020): 021001.
- Duong, Chi Thang, et al. "On node features for graph neural networks." arXiv preprint arXiv:1911.08795 (2019).
- Dwivedi, Bresson "A Generalization of Transformer Networks to Graphs" 2020, https://arxiv.org/abs/2012.09699
- G. Zhu et al., "Scene Graph Generation: A Comprehensive Survey." arXiv, Jun. 22, 2022. doi: 10.48550/arXiv.2201.00443

# Message Passing Graph Convolution Network binary classification

**Objective :**
We want to classify if a molecule is active as an anti-HIV drug.

**Dataset :**
OGB-molHIV
41000 molecules
https://ogb.stanford.edu/docs/graphprop/#ogbg-mol


Merci !

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Jeudi
07
Mars
à 14h00

**Next, on Fidle :**

L'IA comme un outil

11

**Autoencoder networks**
AE

Réalisation, technique et mise en scène :
Agathe, Baptiste et Yanis - UGA/DAPI
Thibaut, Kamel, Léo - IDRIS

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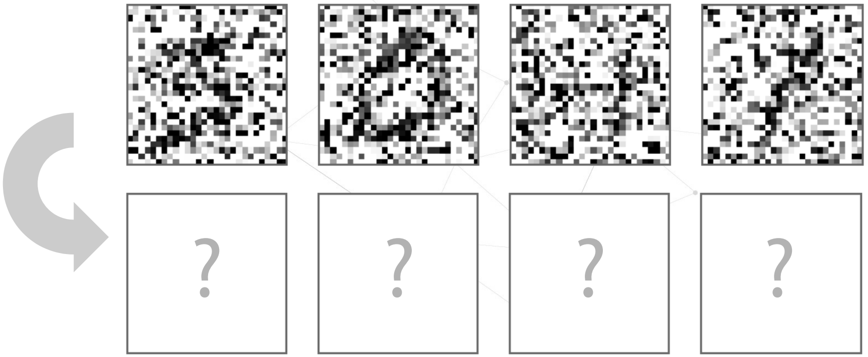


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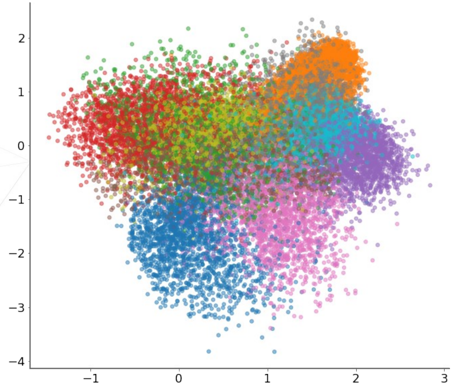


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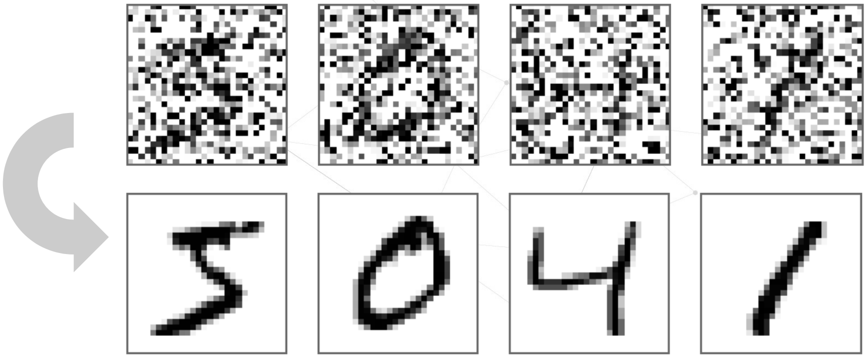

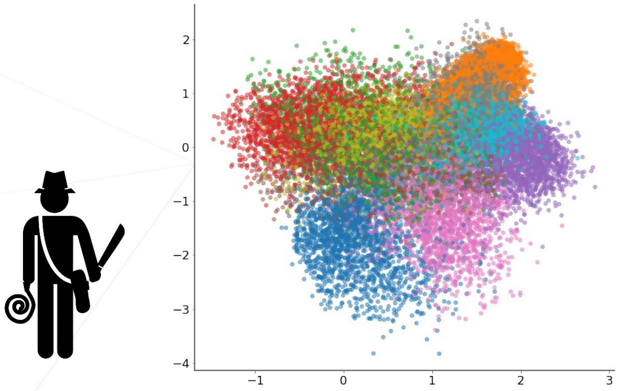


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