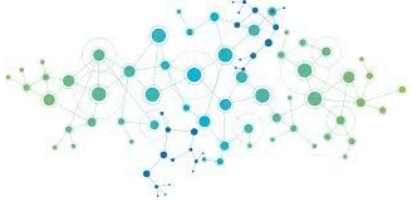


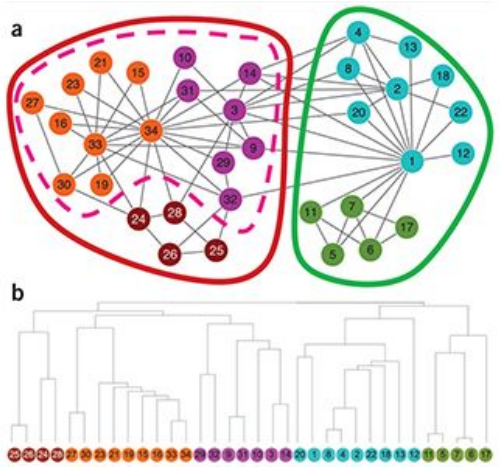
GNN - Introduction to Graph Neural Networks

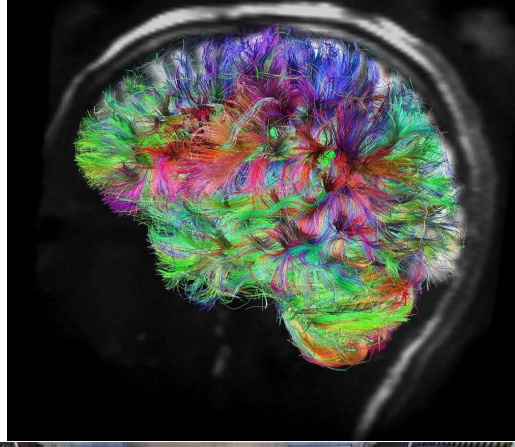
Prof. Patrick Terrematte

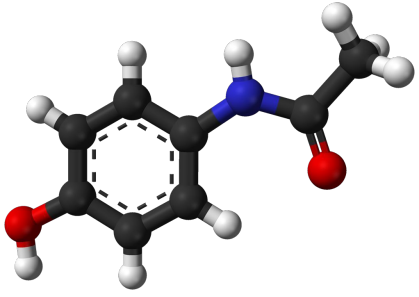
UFRN

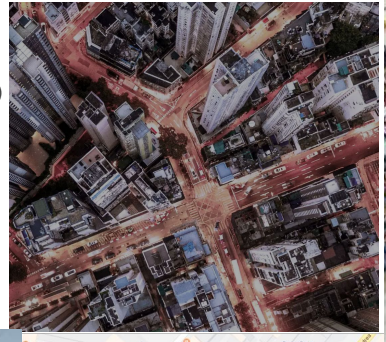
Instituto Metrópole Digital - IMD

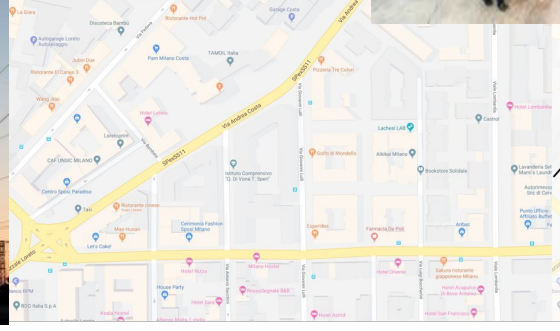
Everything is Connected!

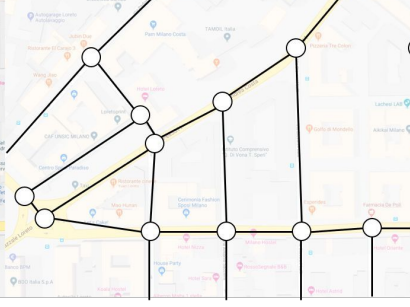






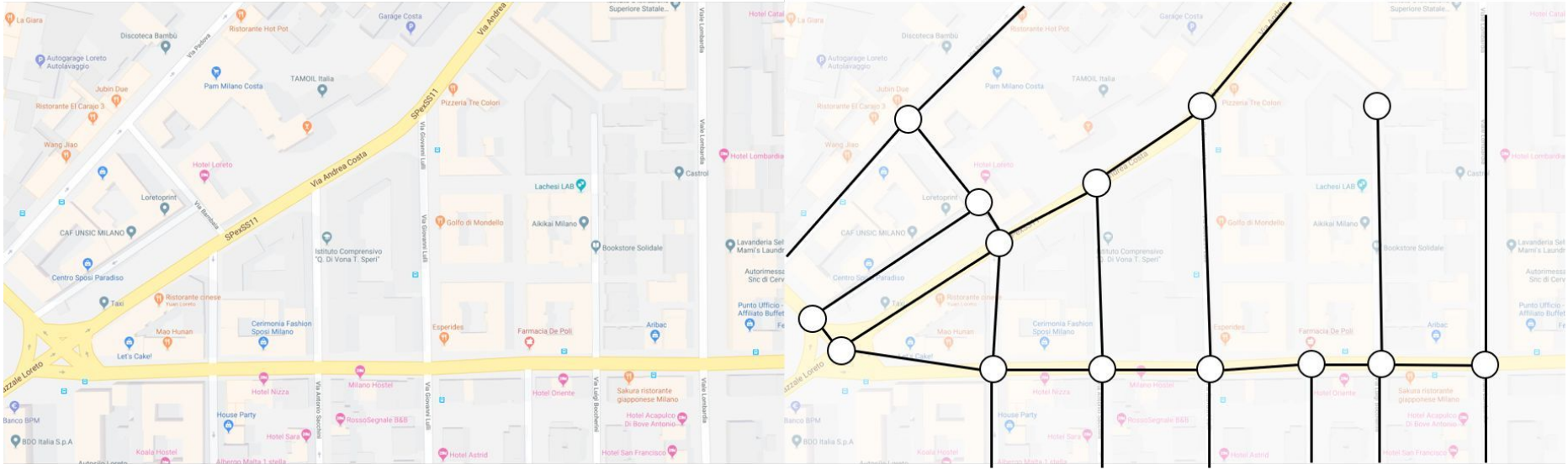






Traffic maps are graphs!

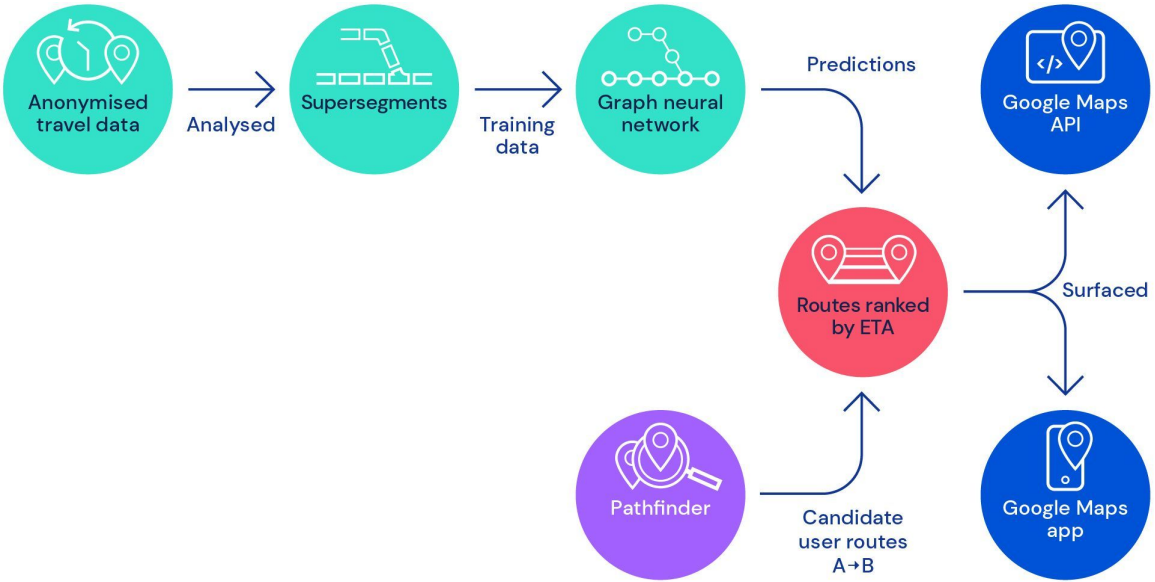
Transportation maps (e.g. the ones found on Google Maps) naturally modelled as graphs.

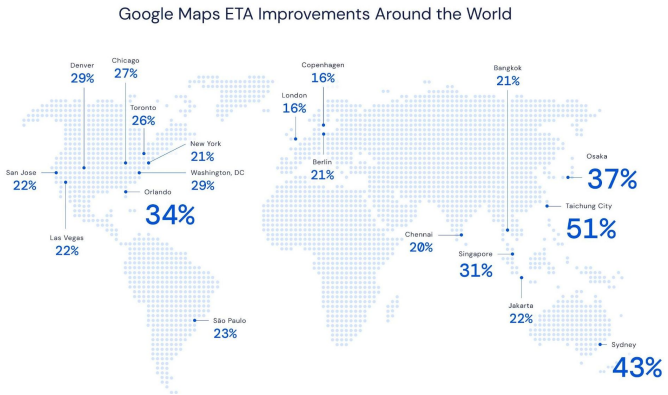


source: (Stokes et al., Cell'20)

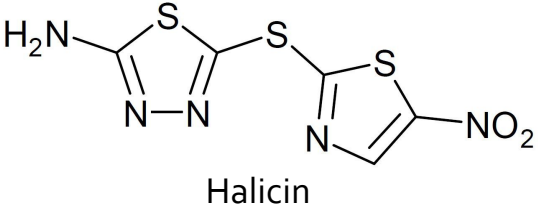
Applications in Computing

- Estimated Time of Arrival (ETA) Prediction
  - Given a start-point and end-point, what is the expected travel time?
  - Relevant node features: road length, current speeds, historical speeds
  - Use anonymised, crowd-sourced real-time / historical traffic data.





Graph Neural Networks for molecule classification

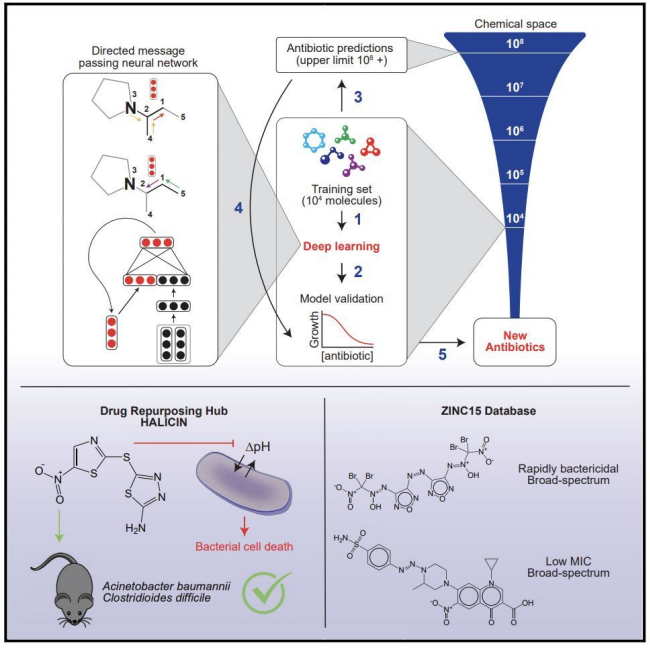


Article

Cell

A Deep Learning Approach to Antibiotic Discovery

Graphical Abstract



Authors

Jonathan M. Stokes, Kevin Yang, Kyle Swanson, ..., Tommi S. Jaakkola, Regina Barzilay, James J. Collins

Correspondence

regina@csail.mit.edu (R.B.), jimjc@mit.edu (J.J.C.)

In Brief

A trained deep neural network predicts antibiotic activity in molecules that are structurally different from known antibiotics, among which Halicin exhibits efficacy against broad-spectrum bacterial infections in mice.

source: (Stokes et al., Cell'20)

nature

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Powerful antibiotics discovered using AI

Machine learning spots molecules that work even against 'untreatable' strains of bacteria.

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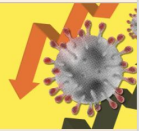

I intelligence

Robotics

'Death of the office' homeworking claims exaggerated

Anti-social robots harr increase social distanci

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AI discovers antibiotics to treat drug-resistant diseases

Machine learning uncovers potent new drug able to kill 35 powerful bacteria

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Scientists discover powerful antibiotic using AI

21 February 2020 Share

Applications in biology

- Proteomics
  - Protein interaction prediction
  - Protein function prediction
  - Protein structure prediction
- Drug development, discovery and polypharmacy
  - Drug–target prediction
  - Prediction of drug properties
  - DDI prediction
- Disease diagnosis
- Metabolic networks and GNNs
  - Metabolic Networks

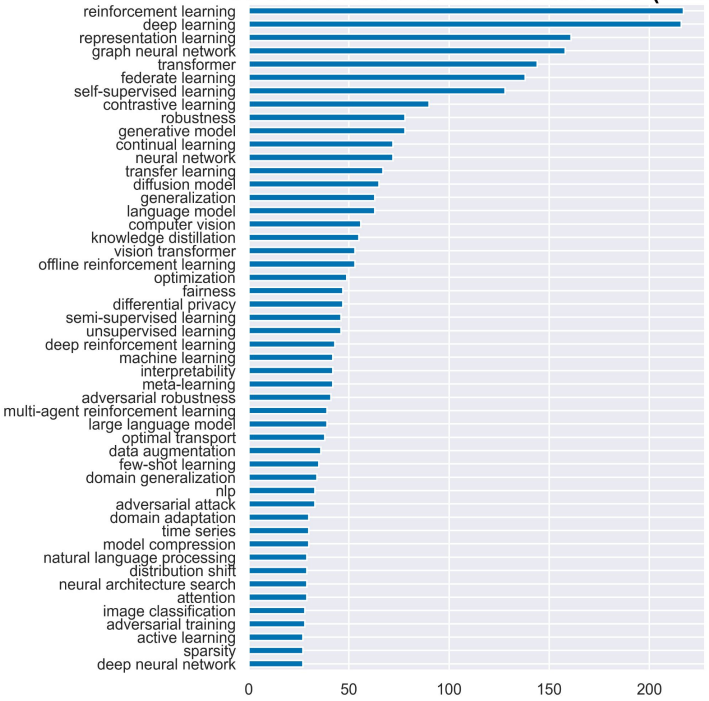
"Graph neural network"
Free text in full data

PUBLICATIONS	DATASETS	GRANTS	PATENTS	CLINICAL TRIALS	POLICY DOCUMENTS
81,155	511	411	15,293	3	13

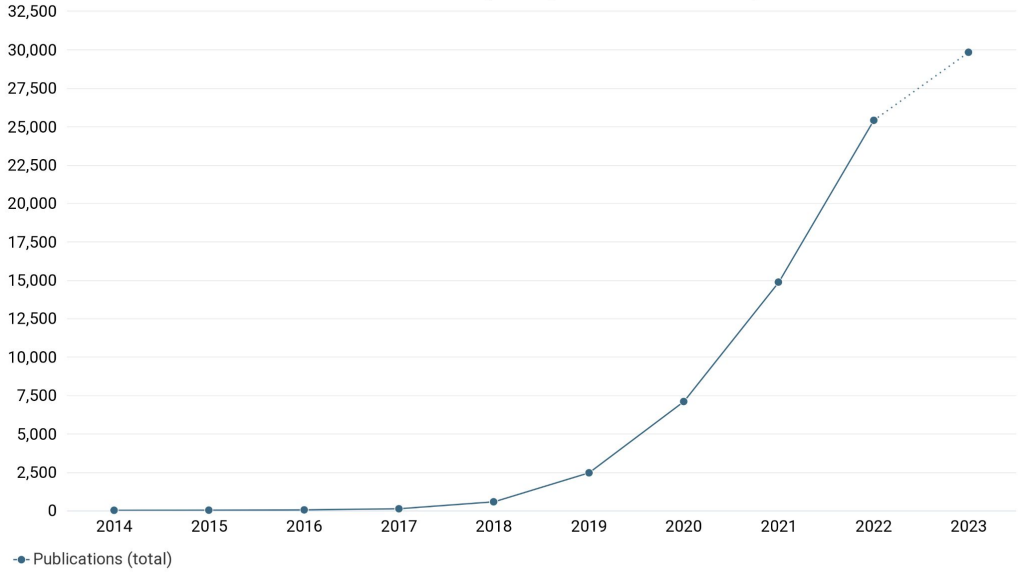
ICLR | 2023

Eleventh International Conference on Learning Representations

50 MOST APPEARED KEYWORDS (2023)

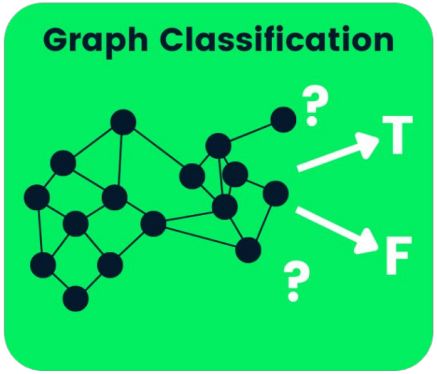


Publications in each year. (Criteria: see below)



Source:
https://app.dimensions.ai
Exported: November 13, 2023
Criteria: "Graph neural network" in full data.

Learning tasks on graphs



source: datacamp.com/portfolio/kingabzpro

Learning tasks on graphs

Biological network analysis with deep learning

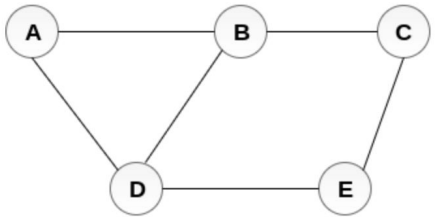
Giulia Muzio ✉, Leslie O'Bray ✉, Karsten Borgwardt ✉ Author Notes

Briefings in Bioinformatics, Volume 22, Issue 2, March 2021, Pages 1515–1530, https://doi.org/10.1093/bib/bbaa257

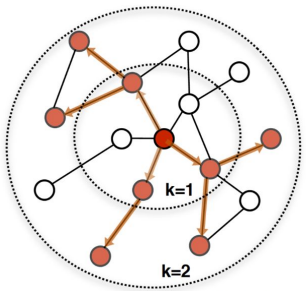
- Node Classification
  - classify the remaining unlabeled nodes in the network, e.g. protein function prediction in a PPI network. (semi-supervised learning)
- Link Prediction
  - known links in a graph are used to predict where additional links. (semi-supervised learning)
- Graph Embedding
  - finding a lower-dimensional, fixed-size vector representation of a graph (unsupervised learning)
- Graph Classification or Regression
  - graphs as its input, and then performs classification/regression for each individual graph (supervised learning problem)

Graphs

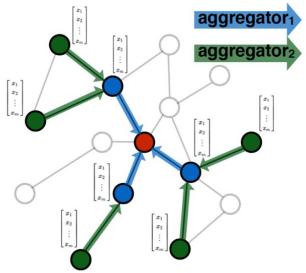
- arbitrary size
- complex topology
- non-euclidean objects
- no fix node ordering



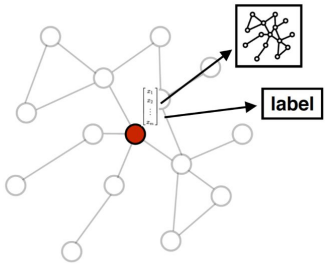
	A	B	C	D	E
A	0	1	0	1	0
B	1	0	1	1	0
C	0	1	0	0	1
D	1	1	0	0	1
E	0	0	1	1	0



1. Sample neighborhood

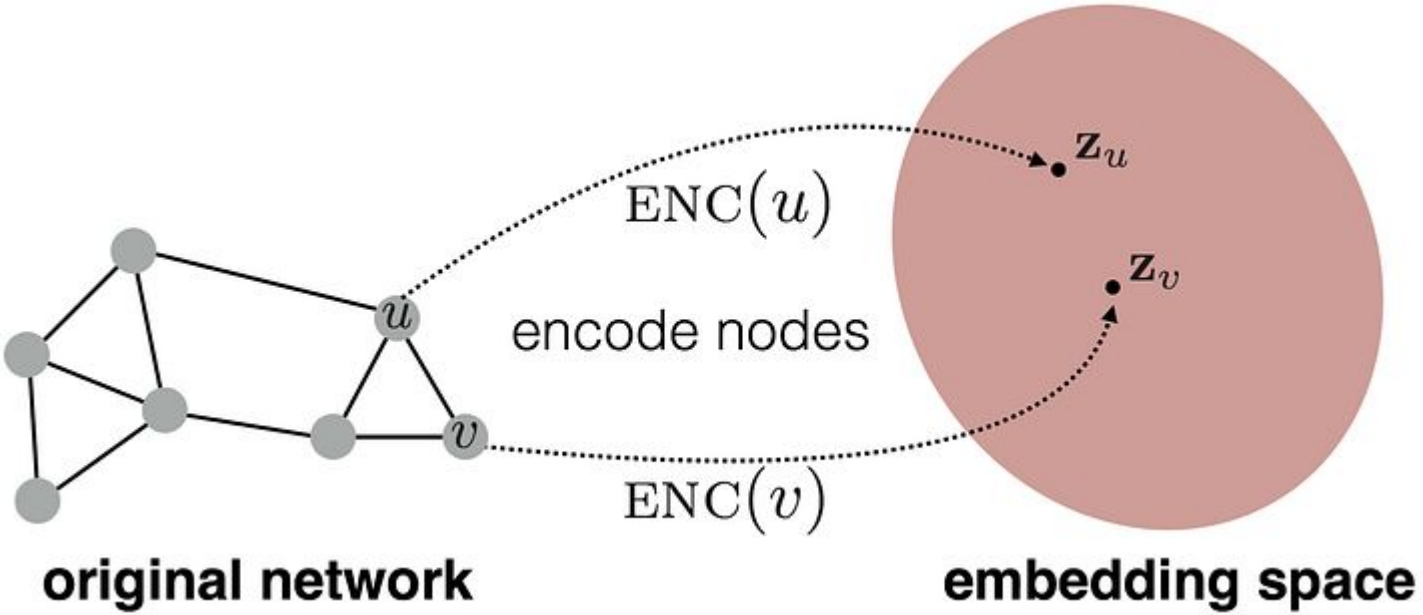


2. Aggregate feature information from neighbors

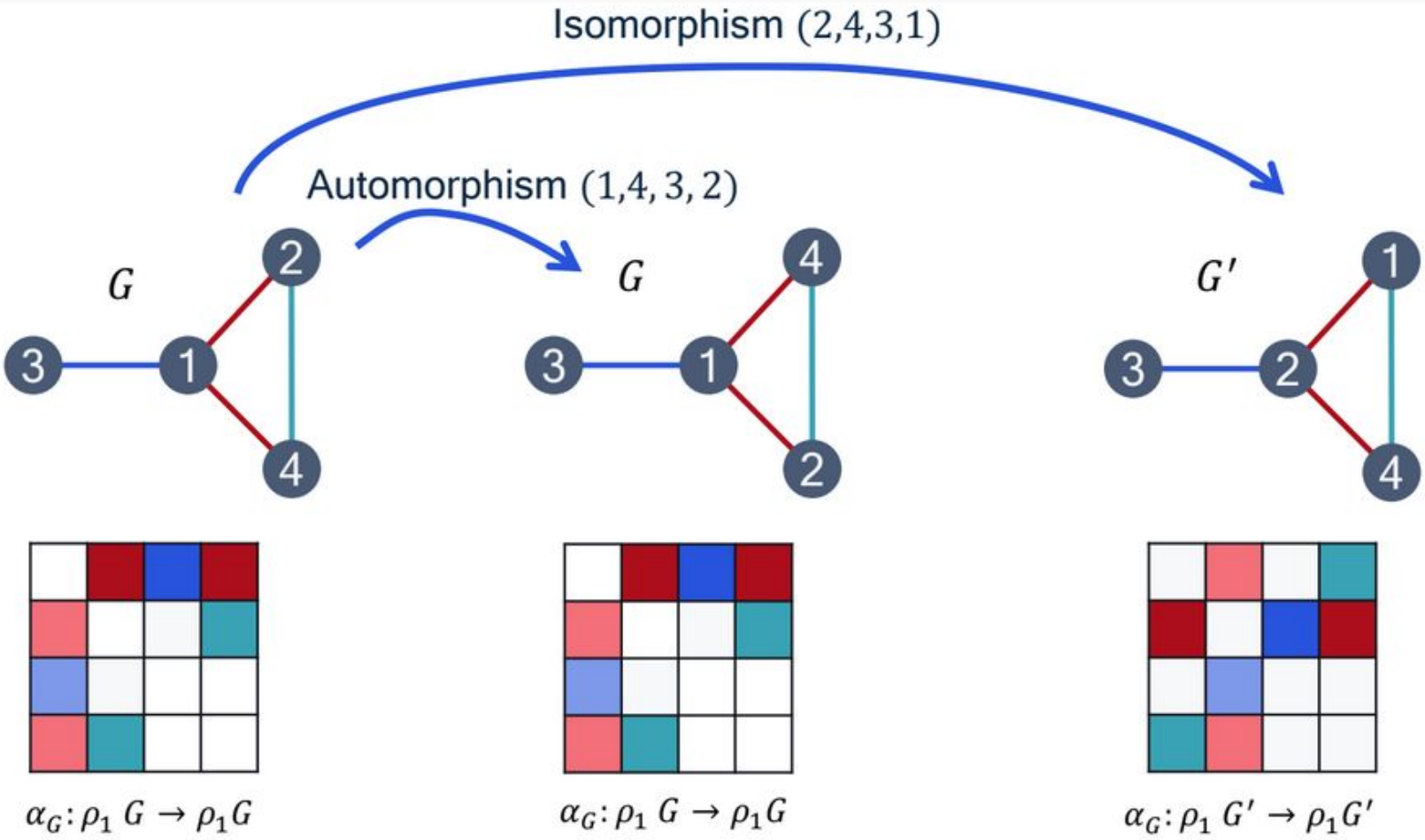


3. Predict graph context and label using aggregated information

source: snap.stanford.edu/graphsage



source: salmanfaroz.medium.com



Automorphisms give constraints, isomorphisms weight sharing

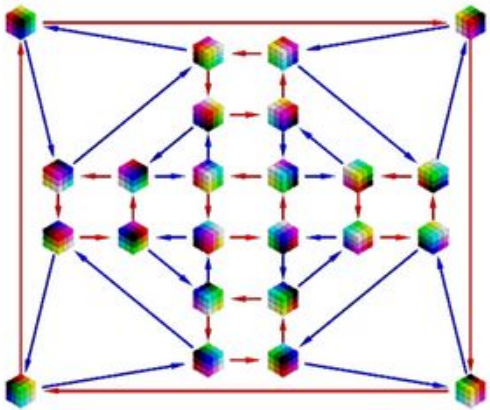
A group G is a set with a binary operation $G \times G \to G$ satisfying:

- **Identity**: there is a $e \in G$ such that $ge = eg = g$
- **Associativity**: $(gh)f = g(hf)$
- **Invertibility**: for all g, there is a g^{-1} such that $gg^{-1} = g^{-1}g = e$

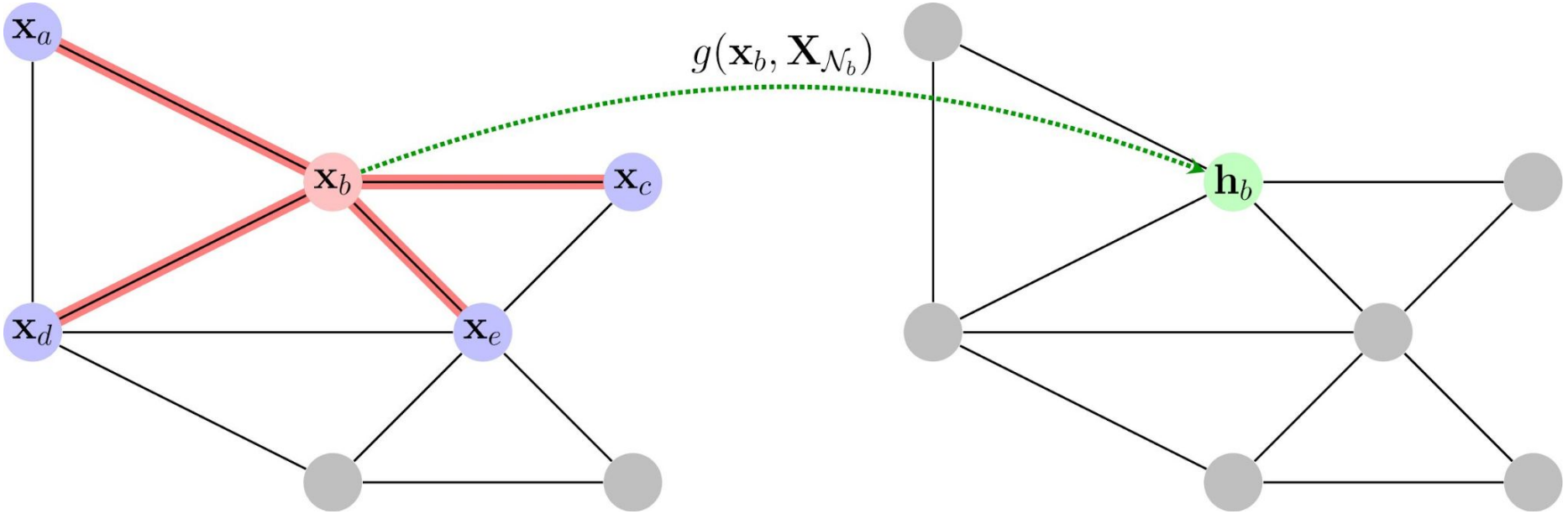
A group $\mathbf{B}G$ is a groupoid with a unique object $\star$.

$$\mathrm{Hom}_{\mathbf{B}G}(\star,\star) = G$$

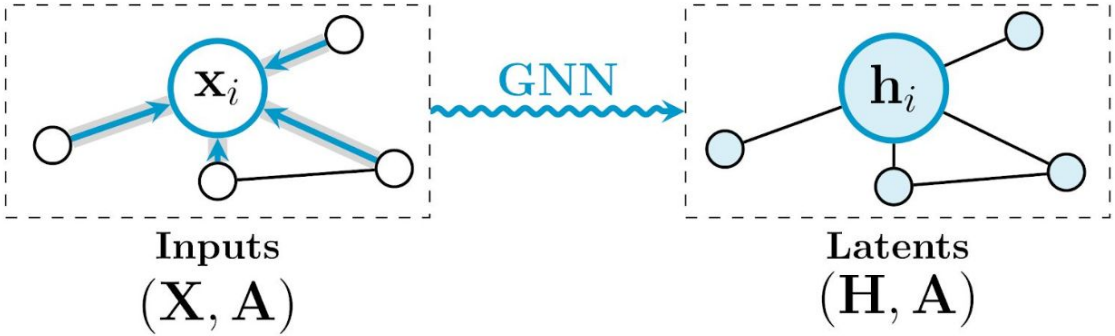
For any groupoid $\mathcal{G}$, object A, the automorphisms $f: A \to A \in \mathrm{Aut}_{\mathcal{G}}(A)$ form a group.



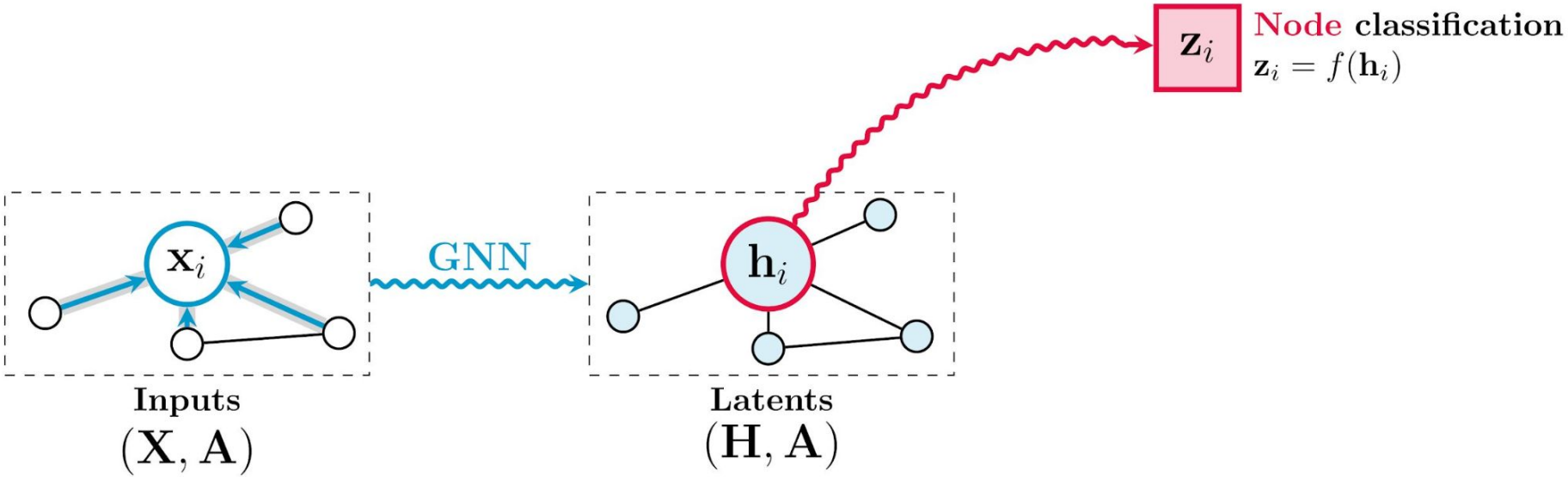
Rotational symmetries of the cube (group O_h)



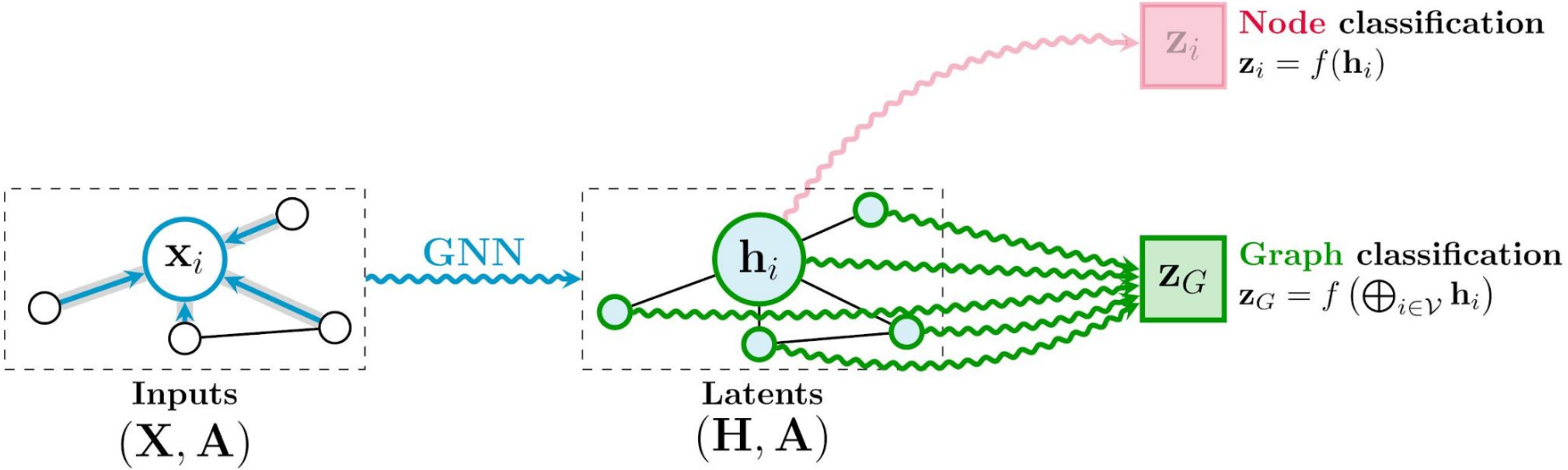
source: Petar Veličković, MLinPL2021



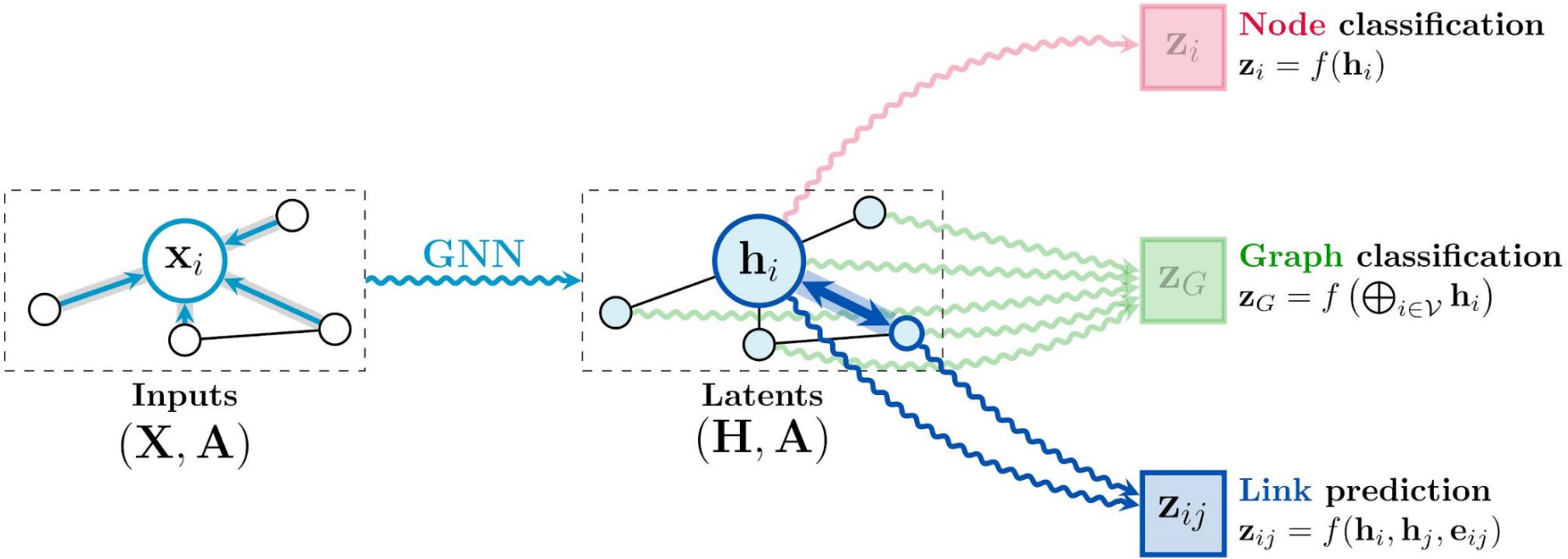
source: Petar Veličković, MLinPL2021



source: Petar Veličković, MLinPL2021

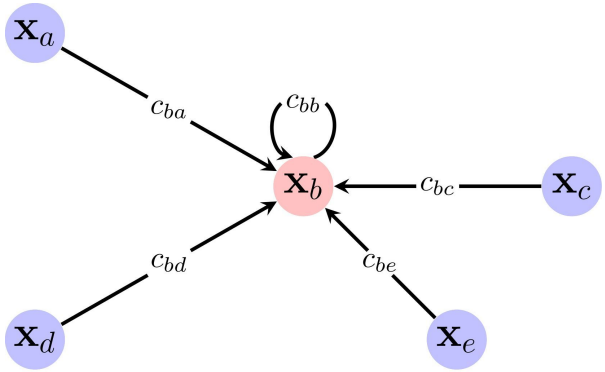


source: Petar Veličković, MLinPL2021

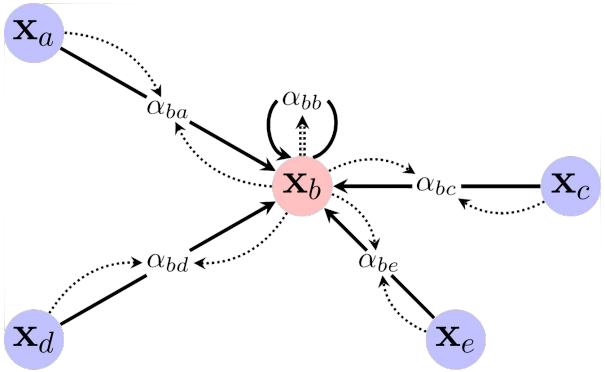


source: Petar Veličković, MLinPL2021

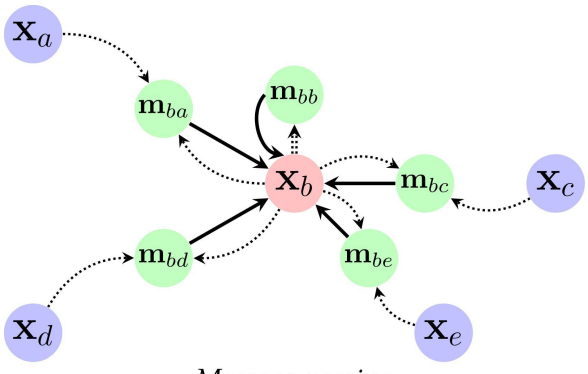
GNN layers



Convolutional



Attentional



Message-passing

$$\mathbf{h}_i = \phi\left(\mathbf{x}_i, \bigoplus_{j \in \mathcal{N}_i} c_{ij}\psi(\mathbf{x}_j)\right)$$

$$\mathbf{h}_i = \phi\left(\mathbf{x}_i, \bigoplus_{j \in \mathcal{N}_i} a(\mathbf{x}_i, \mathbf{x}_j)\psi(\mathbf{x}_j)\right)$$

$$\mathbf{h}_i = \phi\left(\mathbf{x}_i, \bigoplus_{j \in \mathcal{N}_i} \psi(\mathbf{x}_i, \mathbf{x}_j)\right)$$

source: Petar Veličković, MLinPL2021

k-layer GCN

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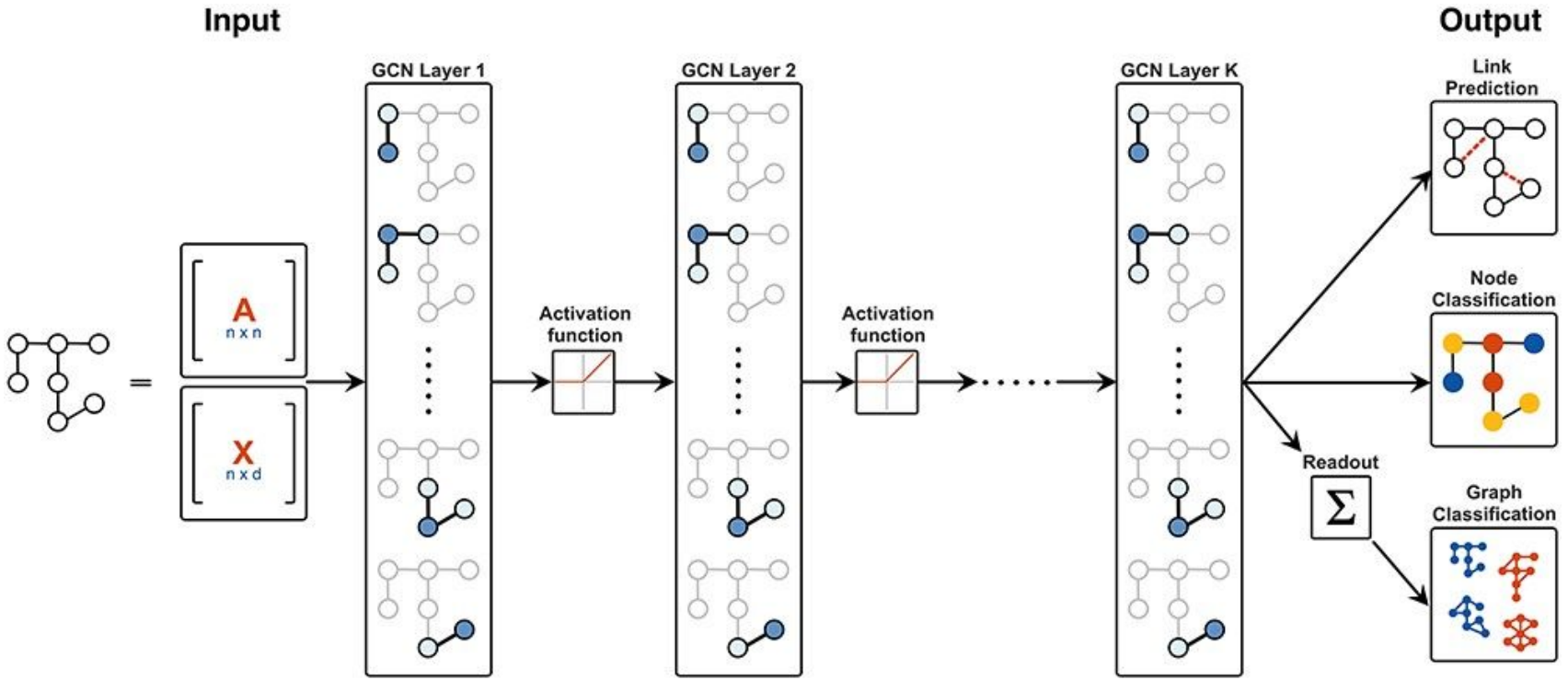
Giulia Muzio ✉, Leslie O'Bray ✉, Karsten Borgwardt ✉ Author Notes

Briefings in Bioinformatics, Volume 22, Issue 2, March 2021, Pages 1515–1530, https://doi.org/10.1093/bib/bbaa257



Frameworks

PyTorch geometric

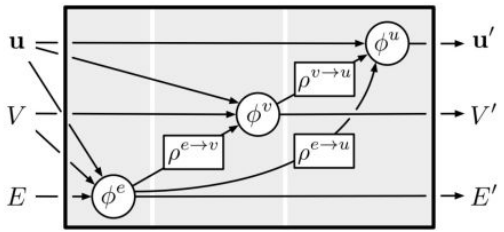
github.com/rusty1s/pytorch_geometric

Spektral

graphneural.network

DGL

dgl.ai



github.com/deepmind/graph_nets

https://pytorch-geometric.readthedocs.io/en/latest/get_started/colabs.html

Colab Notebooks and Video Tutorials

Official Examples

We have prepared a list of Colab notebooks that practically introduces you to the world of **Graph Neural Networks** with PyG:

1. Introduction: Hands-on Graph Neural Networks
2. Node Classification with Graph Neural Networks
3. Graph Classification with Graph Neural Networks
4. Scaling Graph Neural Networks
5. Point Cloud Classification with Graph Neural Networks
6. Explaining GNN Model Predictions using Captum
7. Customizing Aggregations within Message Passing
8. Node Classification Instrumented with Weights&Biases
9. Graph Classification Instrumented with Weights&Biases
10. Link Prediction on MovieLens
11. Link Regression on MovieLens

All Colab notebooks are released under the MIT license.

A Comprehensive Introduction to Graph Neural Networks (GNNs)

https://colab.research.google.com/drive/1Lu-e6xL1jrEAB7epe5nH3YZcbxaWYf1g?usp=sharing

Final lesson:

Let’s Run!

Dive into Graph Neural Network and Network Analysis

- "Deep Learning" by Goodfellow, Bengio and Courville
  - https://www.deeplearningbook.org/
- Will Hamilton's, GRL Textbook (esp. Chapter 7)
  - https://www.cs.mcgill.ca/~wlh/grl_book/
- Petar Veličković
  - https://petar-v.com
- Network Science by Albert-László Barabási
  - http://networksciencebook.com/
- The Atlas for the Aspiring Network Scientist, 2021
  - https://www.networkatlas.eu/index.htm
- Complex Network Analysis in Python, 2018
  - https://pragprog.com/titles/dzcnapy/complex-network-analysis-in-python/

Categories for AI

Home Program

https://cats.for.ai/

A group G is a set with a binary operation $G \times G \to G$ satisfying:

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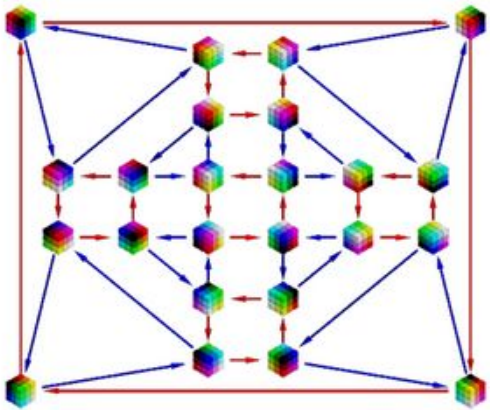

Rotational symmetries of the cube (group O_h)

Prof. Dr. Patrick Terrematte

patrick.terrematte@ufrn.br

Discord patrickterrematte