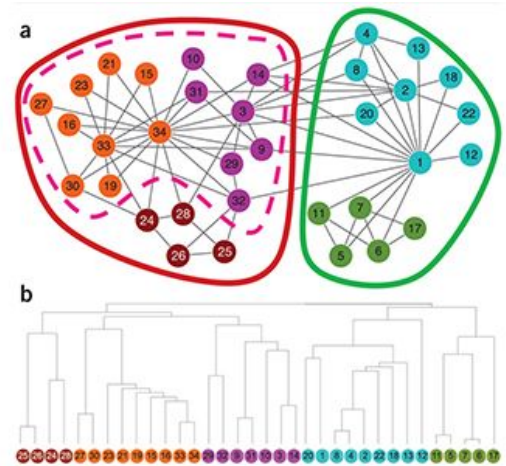
GNN - Introduction to Graph Neural Networks

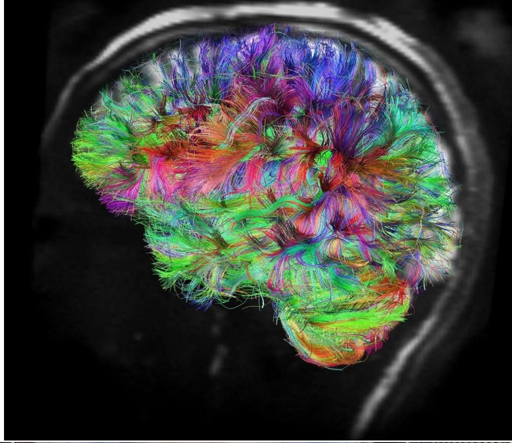
Prof. Patrick Terrematte

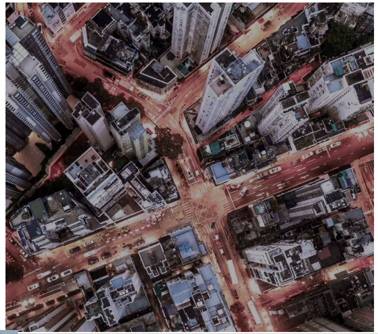
UFRN

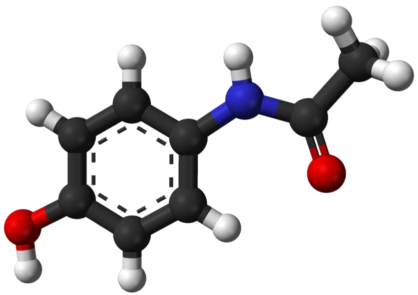
Instituto Metrópole Digital - IMD

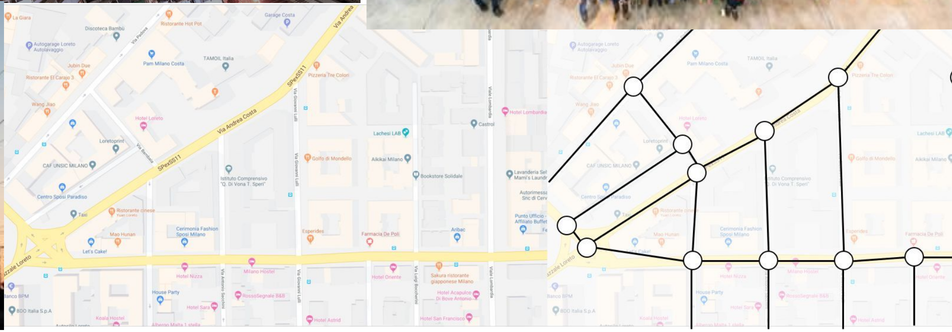
Everything is Connected!





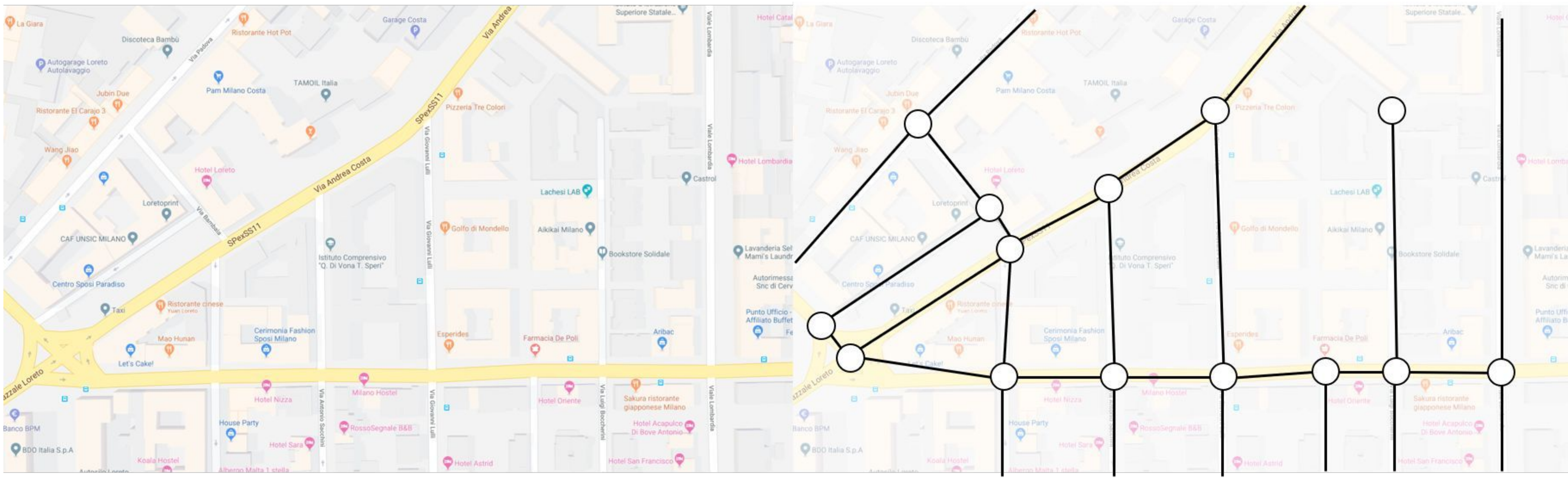






Traffic maps are graphs!

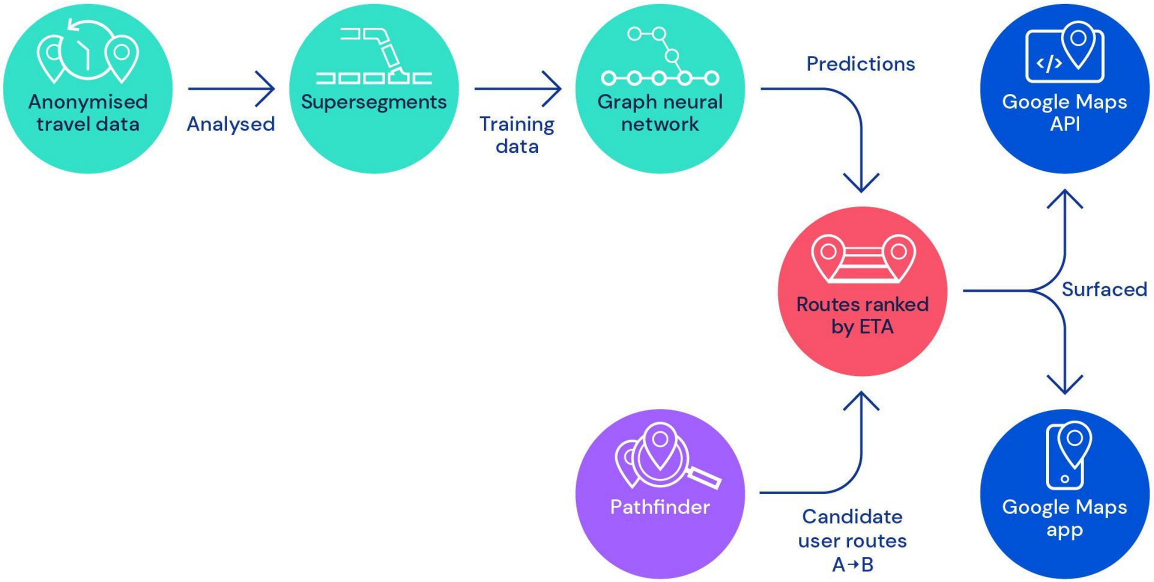
Transportation maps (e.g. the ones found on Google Maps) naturally modelled as graphs.

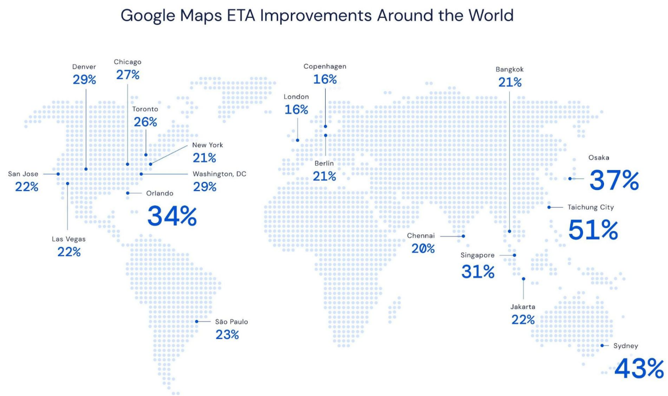


source: (Stokes et al., Cell'20)

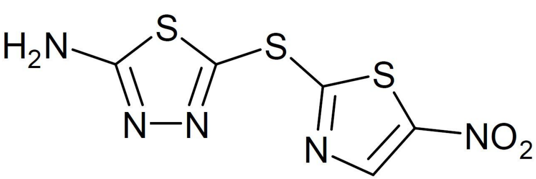
Applications in Computing

- 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



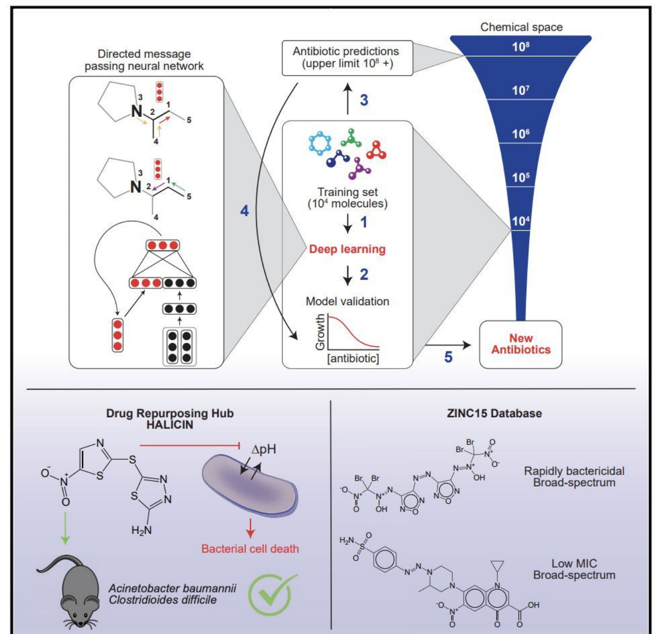
Halicin

Cell

Article

A Deep Learning Approach to Antibiotic Discovery

Graphical Abstract



Authors

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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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NEWS · 20 FEBRUARY 2020

Powerful antibiotics discovered using AI

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

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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

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Applications in biology

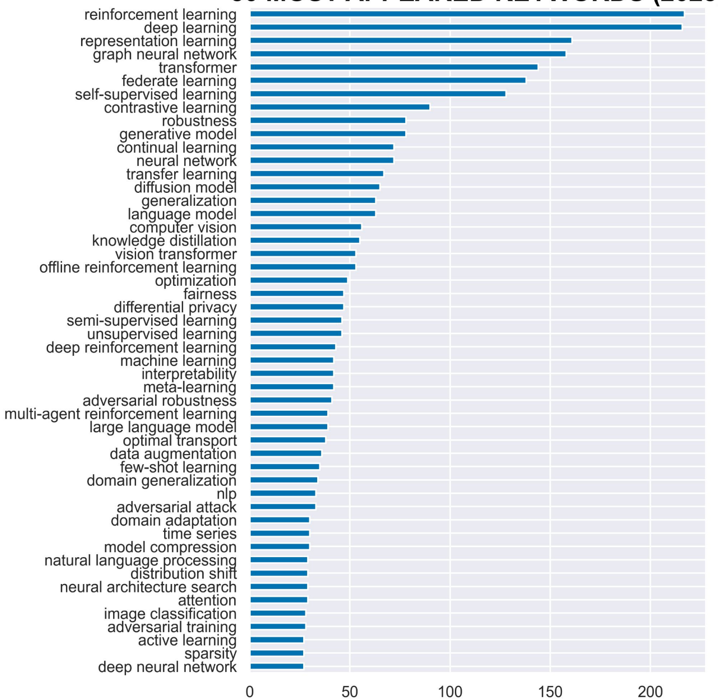
- Proteomics
  - Protein interaction prediction
  - Protein function prediction
  - Protein structure prediction
- Drug development, discovery and polypharmacy
  - Drug–target prediction
  - Prediction of drug properties
  - DDI prediction
- Disease diagnosis
- Metabolic networks and GNNs
  - Metabolic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

"Graph neural network"
Free text in full data

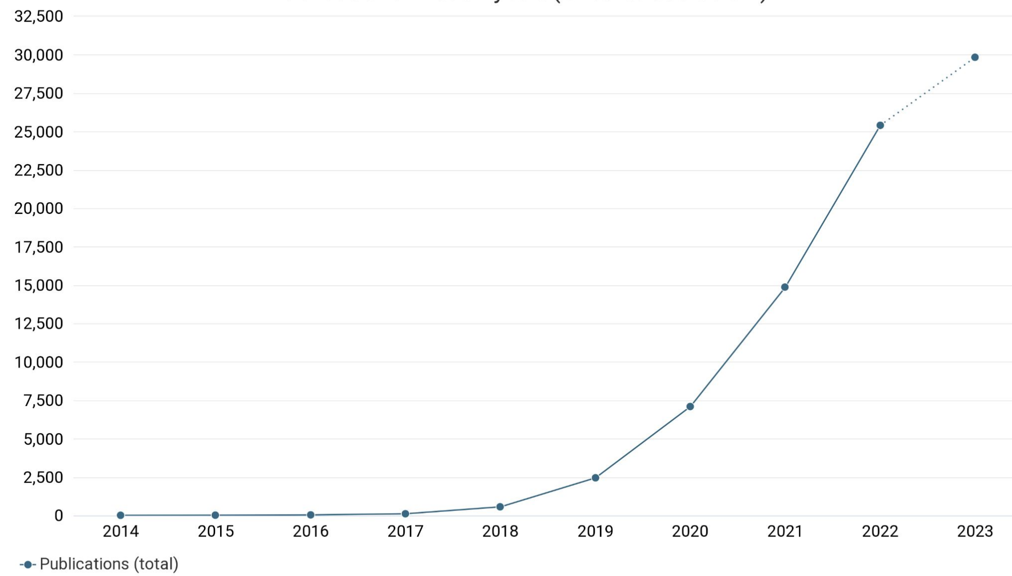
PUBLICATIONS	DATASETS	GRANTS	PATENTS	CLINICAL TRIALS	POLICY DOCUMENTS
81,155	511	411	15,293	3	13

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.

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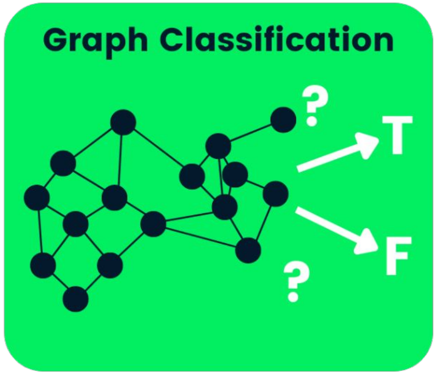
Learning tasks on graphs



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)

Convolutional Neural Network (CNN)

Convolutional Neural Network (CNN)

J. Physiol. (1959) 147, 226–238

SINGLE UNIT ACTIVITY IN STRIATE CORTEX OF UNRESTRAINED CATS

By D. H. HUBEL*

From the Department of Neurophysiology, Walter Reed Army Institute of Research, Walter Reed Army Medical Center, Washington 12, D.C., U.S.A.

(*Received* 15 *December* 1958)

A beginning has recently been made in recording single neurone activity from animals with chronically implanted electrodes (Hubel, 1957*a*; Gusel'nikov, 1957; Ricci, Doane & Jasper, 1957; Strumwasser, 1958). These methods eliminate anaesthetics, paralysing drugs, brain-stem lesions, and other acute experimental procedures. They make it possible to record electrical events in the higher central nervous system with the animal in a normal state, and to correlate these electrical events with such variables as waking state, attention, learning, and motor activity.

The present paper describes a method for unit recording from the cortex of unanaesthetized, unrestrained cats, and presents some observations from the striate cortex. The objectives have been (1) to observe maintained unit activity under various conditions such as sleep and wakefulness, and (2) to find for each unit the natural stimuli which most effectively influence firing. Of 400 units observed, some 200 are presented here because of their common characteristics. Since there is reason to believe that the remaining 200 units were afferent fibres from the lateral geniculate nucleus, these will be described in a separate paper. A preliminary account of some of this work has been given elsewhere (Hubel, 1958).

J. Physiol. (1968), 195, *pp.* 215–243
With 3 *plates and* 14 *text-figures*
Printed in Great Britain

RECEPTIVE FIELDS AND FUNCTIONAL ARCHITECTURE OF MONKEY STRIATE CORTEX

By D. H. HUBEL and T. N. WIESEL

From the Department of Physiology, Harvard Medical School, Boston, Mass., U.S.A.

(*Received* 6 *October* 1967)

SUMMARY

1. The striate cortex was studied in lightly anaesthetized macaque and spider monkeys by recording extracellularly from single units and stimulating the retinas with spots or patterns of light. Most cells can be categorized as simple, complex, or hypercomplex, with response properties very similar to those previously described in the cat. On the average, however, receptive fields are smaller, and there is a greater sensitivity to changes in stimulus orientation. A small proportion of the cells are colour coded.

2. Evidence is presented for at least two independent systems of columns extending vertically from surface to white matter. Columns of the first type contain cells with common receptive-field orientations. They are similar to the orientation columns described in the cat, but are probably smaller in cross-sectional area. In the second system cells are aggregated into columns according to eye preference. The ocular dominance columns are larger than the orientation columns, and the two sets of boundaries seem to be independent.

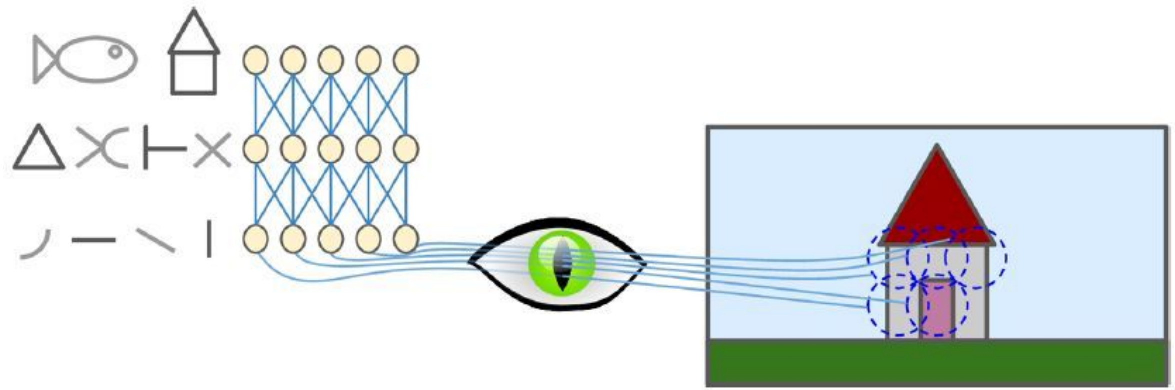
3. There is a tendency for cells to be grouped according to symmetry of responses to movement; in some regions the cells respond equally well to the two opposite directions of movement of a line, but other regions contain a mixture of cells favouring one direction and cells favouring the other.

4. A horizontal organization corresponding to the cortical layering can also be discerned. The upper layers (II and the upper two-thirds of III) contain complex and hypercomplex cells, but simple cells are virtually absent. The cells are mostly binocularly driven. Simple cells are found deep in layer III, and in IV A and IV B. In layer IV B they form a large proportion of the population, whereas complex cells are rare. In layers IV A and IV B one finds units lacking orientation specificity; it is not

Convolutional Neural Network (CNN)

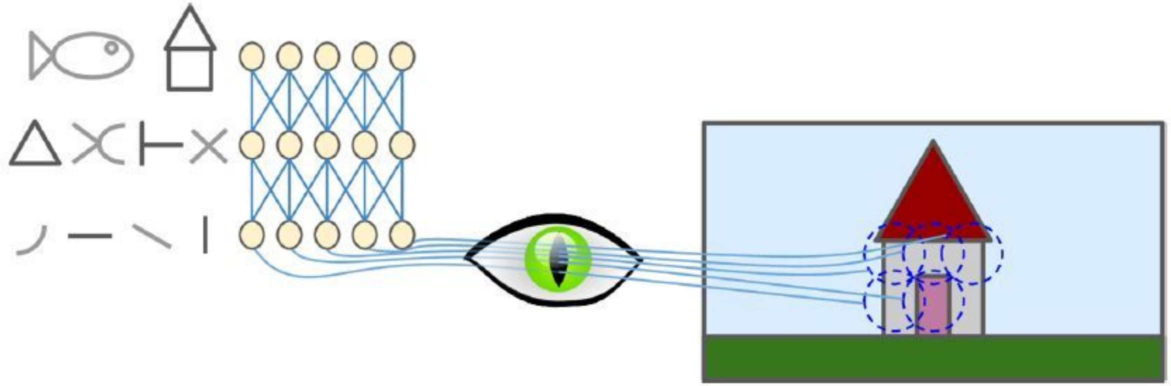
1. Hubel & Wiesel showed that **many neurons in the visual cortex have a small local receptive field**, meaning they react only to visual stimuli **located in a limited region**

2. The receptive fields of **different neurons may overlap**



Convolutional Neural Network (CNN)

3. **Some neurons** react only to images of **horizontal lines**
4. Some neurons have larger receptive fields, and they **react to more complex patterns** that are combinations of the lower-level patterns.
5. **Higher-level** neurons are based on the **outputs of neighboring** lower-level neurons



Convolutional Neural Network (CNN)

PROC. OF THE IEEE, NOVEMBER 1998 1

Gradient-Based Learning Applied to Document Recognition

Yann LeCun, Léon Bottou, Yoshua Bengio, and Patrick Haffner

Abstract—
Multilayer Neural Networks trained with the backpropagation algorithm constitute the best example of a successful Gradient-Based Learning technique. Given an appropriate network architecture, Gradient-Based Learning algorithms can be used to synthesize a complex decision surface that can classify high-dimensional patterns such as handwritten characters, with minimal preprocessing. This paper reviews various methods applied to handwritten character recognition and compares them on a standard handwritten digit recognition task. Convolutional Neural Networks, that are specifically designed to deal with the variability of 2D shapes, are shown to outperform all other techniques.

Real-life document recognition systems are composed of multiple modules including field extraction, segmentation, recognition, and language modeling. A new learning paradigm, called Graph Transformer Networks (GTN), allows such multi-module systems to be trained globally using Gradient-Based methods so as to minimize an overall performance measure.

Two systems for on-line handwriting recognition are described. Experiments demonstrate the advantage of global training, and the flexibility of Graph Transformer Networks.

A Graph Transformer Network for reading bank check is also described. It uses Convolutional Neural Network character recognizers combined with global training techniques to provides record accuracy on business and personal checks. It is deployed commercially and reads several million checks per day.

Keywords— Neural Networks, OCR, Document Recognition, Machine Learning, Gradient-Based Learning, Convolutional Neural Networks, Graph Transformer Networks, Finite State Transducers.

Nomenclature

- GT Graph transformer.

I. Introduction

Over the last several years, machine learning techniques, particularly when applied to neural networks, have played an increasingly important role in the design of pattern recognition systems. In fact, it could be argued that the availability of learning techniques has been a crucial factor in the recent success of pattern recognition applications such as continuous speech recognition and handwriting recognition.

The main message of this paper is that better pattern recognition systems can be built by relying more on automatic learning, and less on hand-designed heuristics. This is made possible by recent progress in machine learning and computer technology. Using character recognition as a case study, we show that hand-crafted feature extraction can be advantageously replaced by carefully designed learning machines that operate directly on pixel images. Using document understanding as a case study, we show that the traditional way of building recognition systems by manually integrating individually designed modules can be replaced by a unified and well-principled design paradigm, called *Graph Transformer Networks*, that allows training all the modules to optimize a global performance criterion.

Since the early days of pattern recognition it has been known that the variability and richness of natural data, be it speech, glyphs, or other types of patterns, make it almost impossible to build an accurate recognition system entirely by hand. Consequently, most pattern recognition systems are built using a combination of automatic learn-

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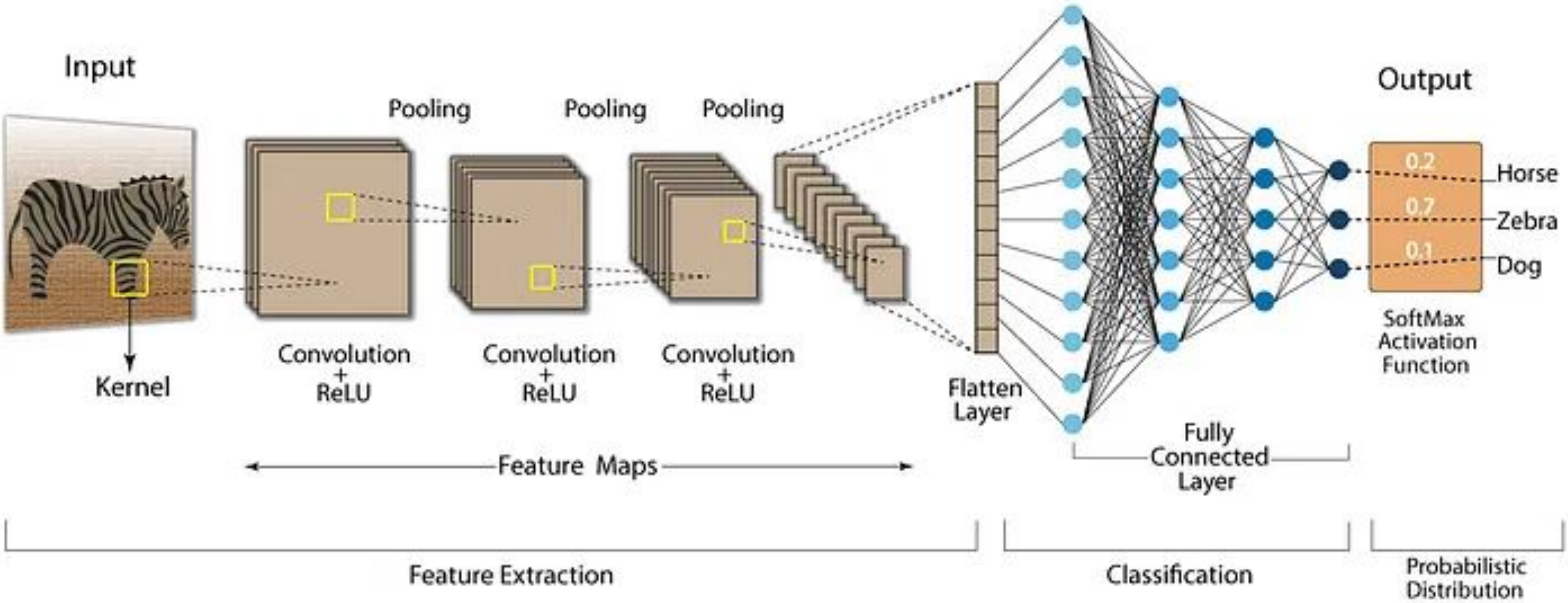
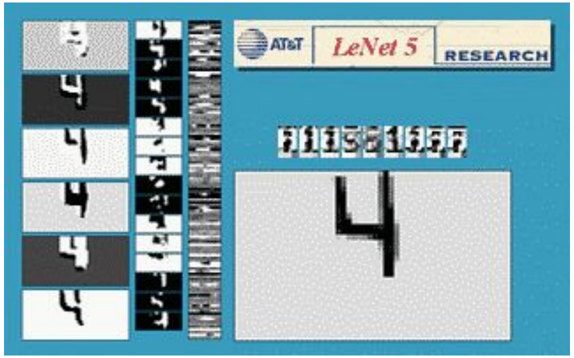
Convolutional Neural Network (CNN)

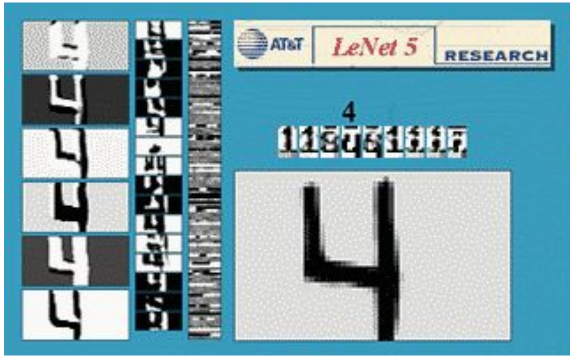


LeNet-5

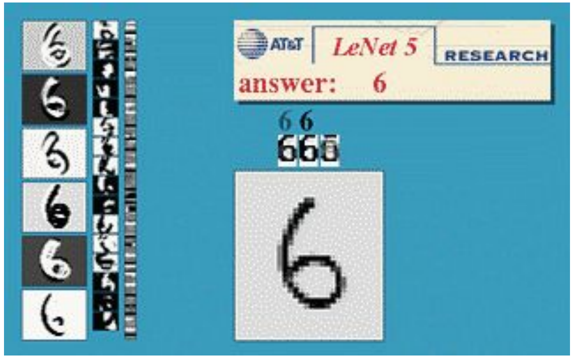
Shift Invariance



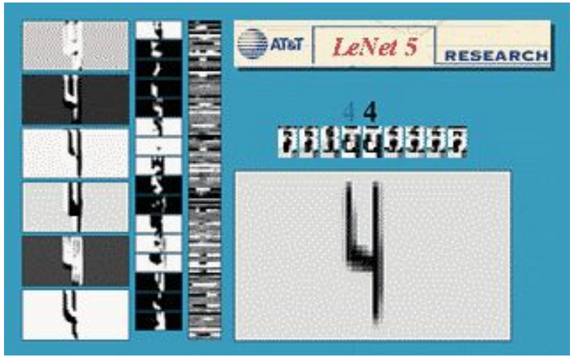
Scale Invariance



Stroke Width Invariance



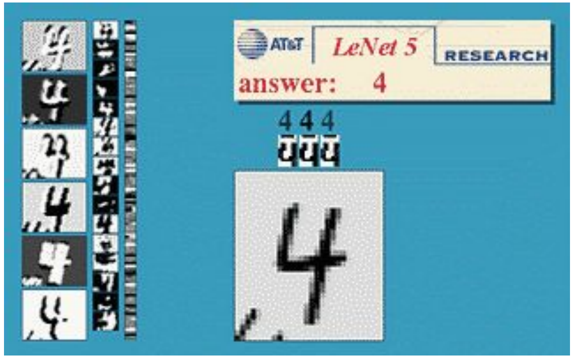
Squeezing Invariance



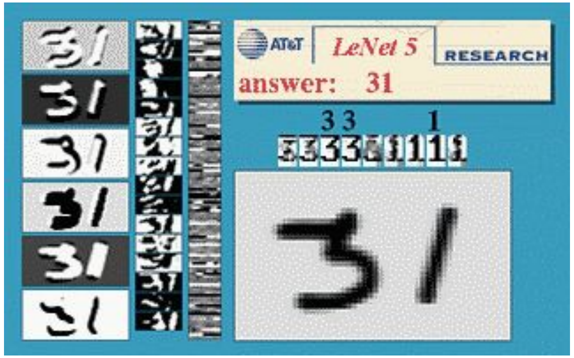
LeNet-5

Overlapping Characters

Robustness to Noise

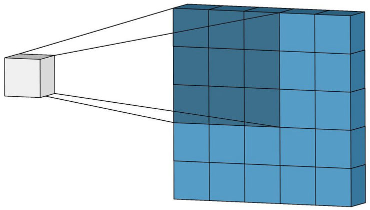


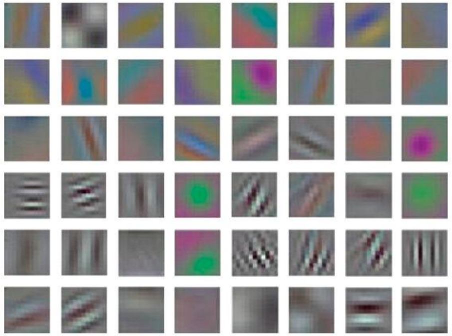
Overlapping Characters

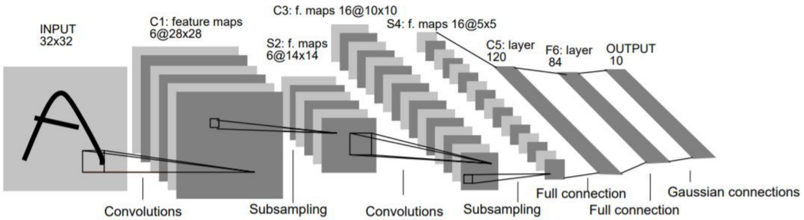


Convolutional Neural Network (CNN)

- locality
- aggregation
- composition







Simuladores de CNN e Deep Learning

- **Tensorflow – Neural Network Playground** https://playground.tensorflow.org/
- **Initializing neural networks**

  https://www.deeplearning.ai/ai-notes/initialization/index.html
- **Parameter optimization in neural networks** https://www.deeplearning.ai/ai-notes/optimization/index.html
- **CNN Explainer** https://poloclub.github.io/cnn-explainer/

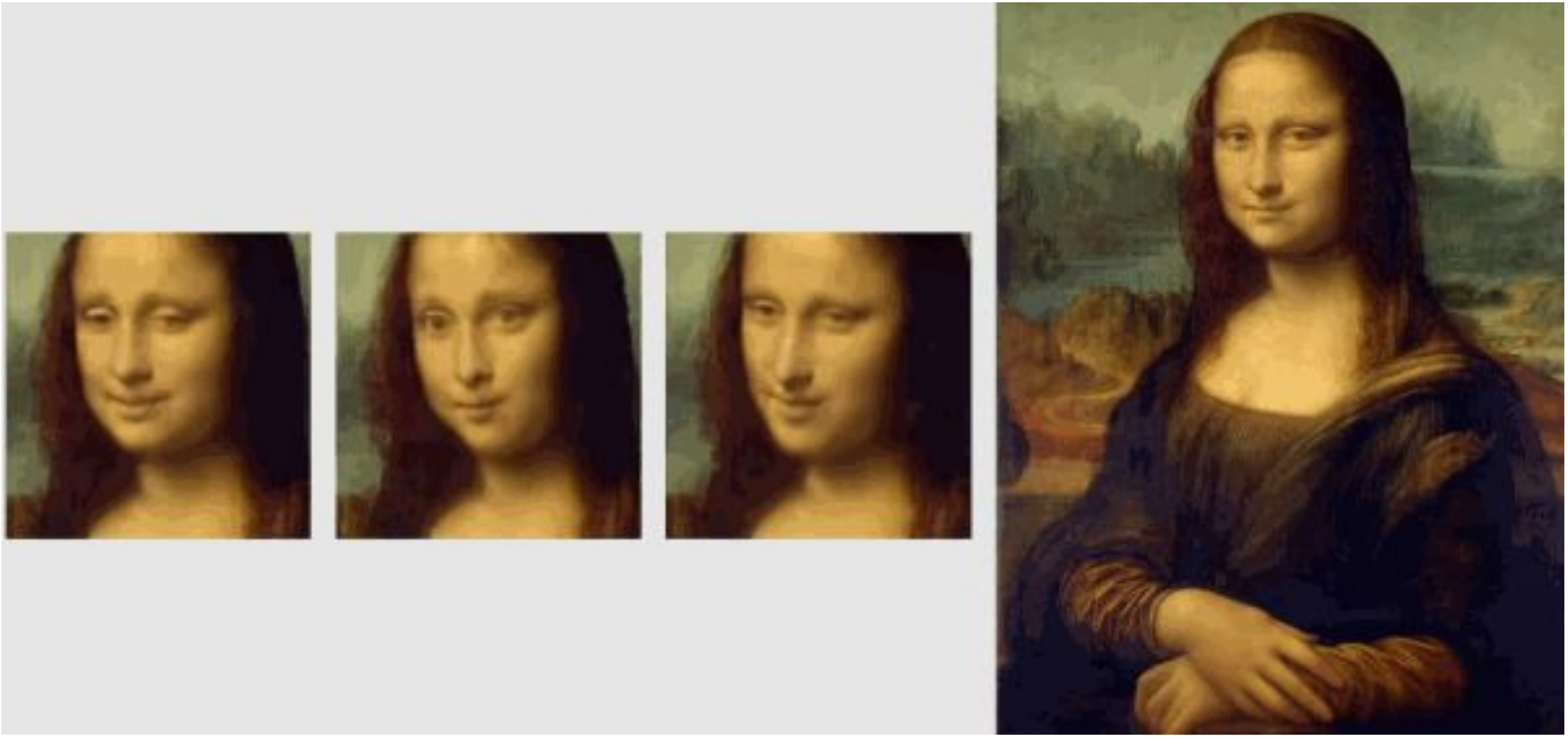
TensorFlow

Open in Colab

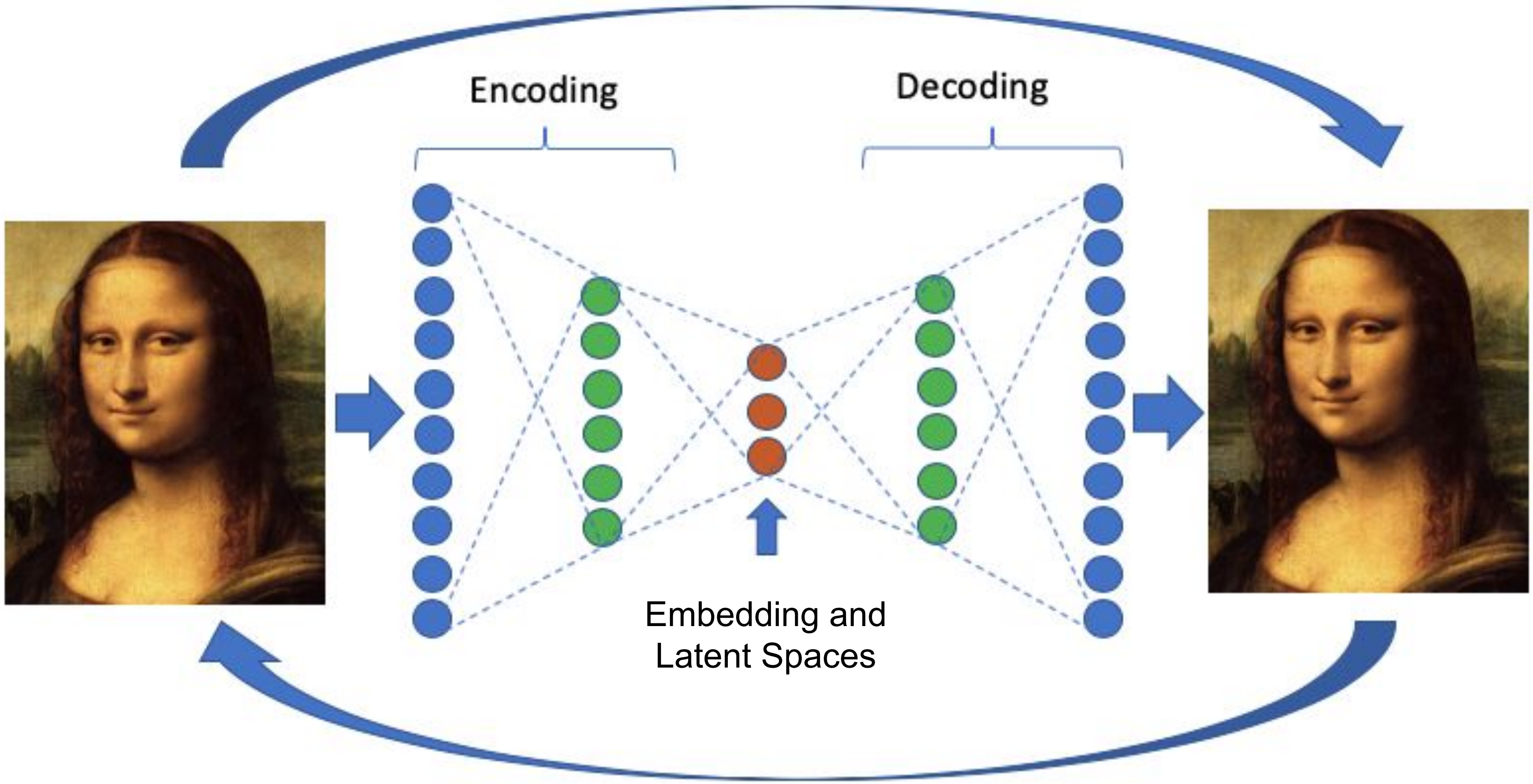
https://colab.research.google.com/github/tensorflow/tensorboard/blob/master/docs/get_started.ipynb

TensorBoard

Autoencoder



Autoencoder



21st IEEE Conference on Computational Intelligence in Bioinformatics and Computational Biology

Prof. Dr. Renan Cipriano Moioli

https://cmte.ieee.org/cis-bbtc/cibcb2024/

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27-29 August 2024

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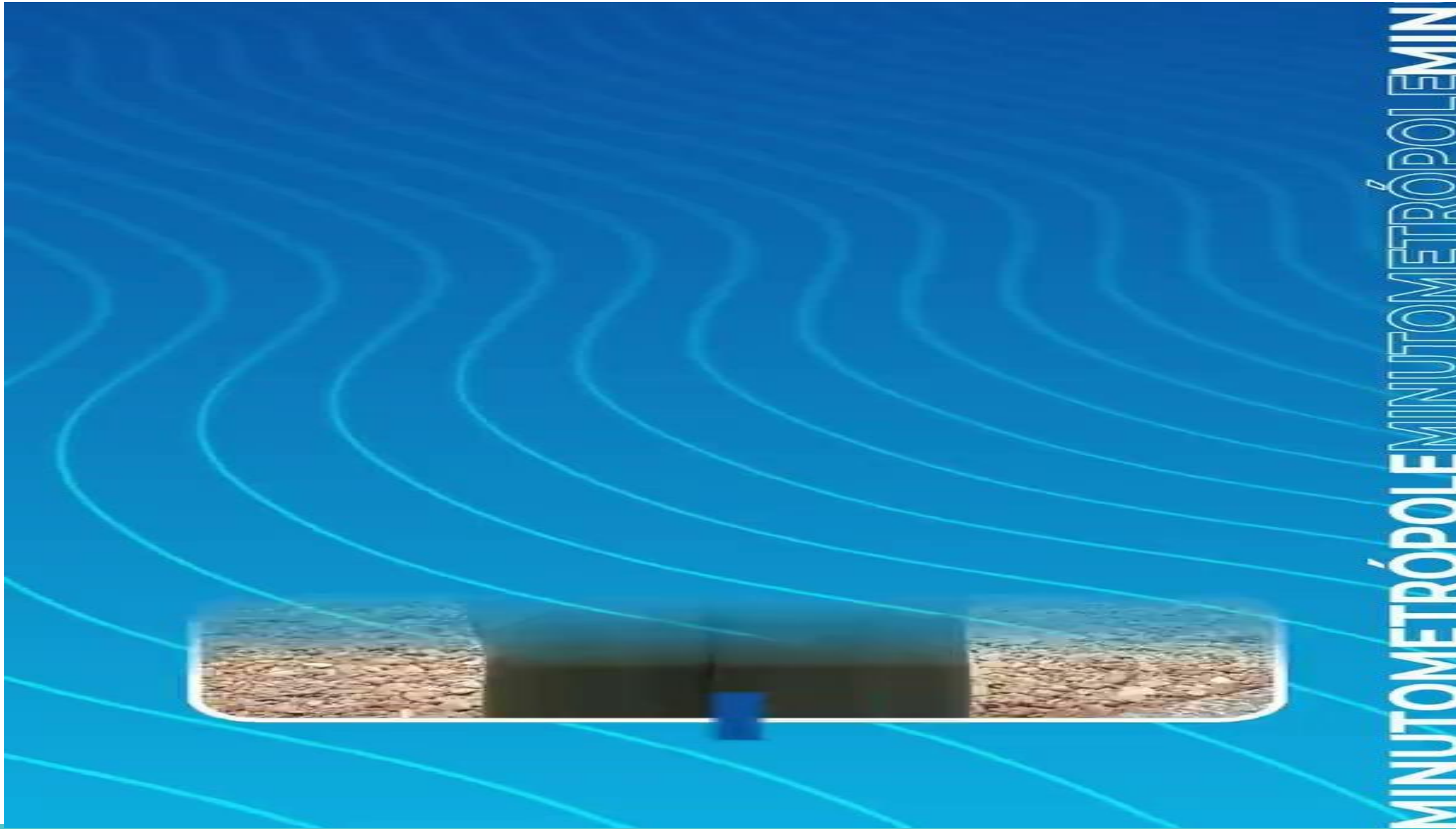
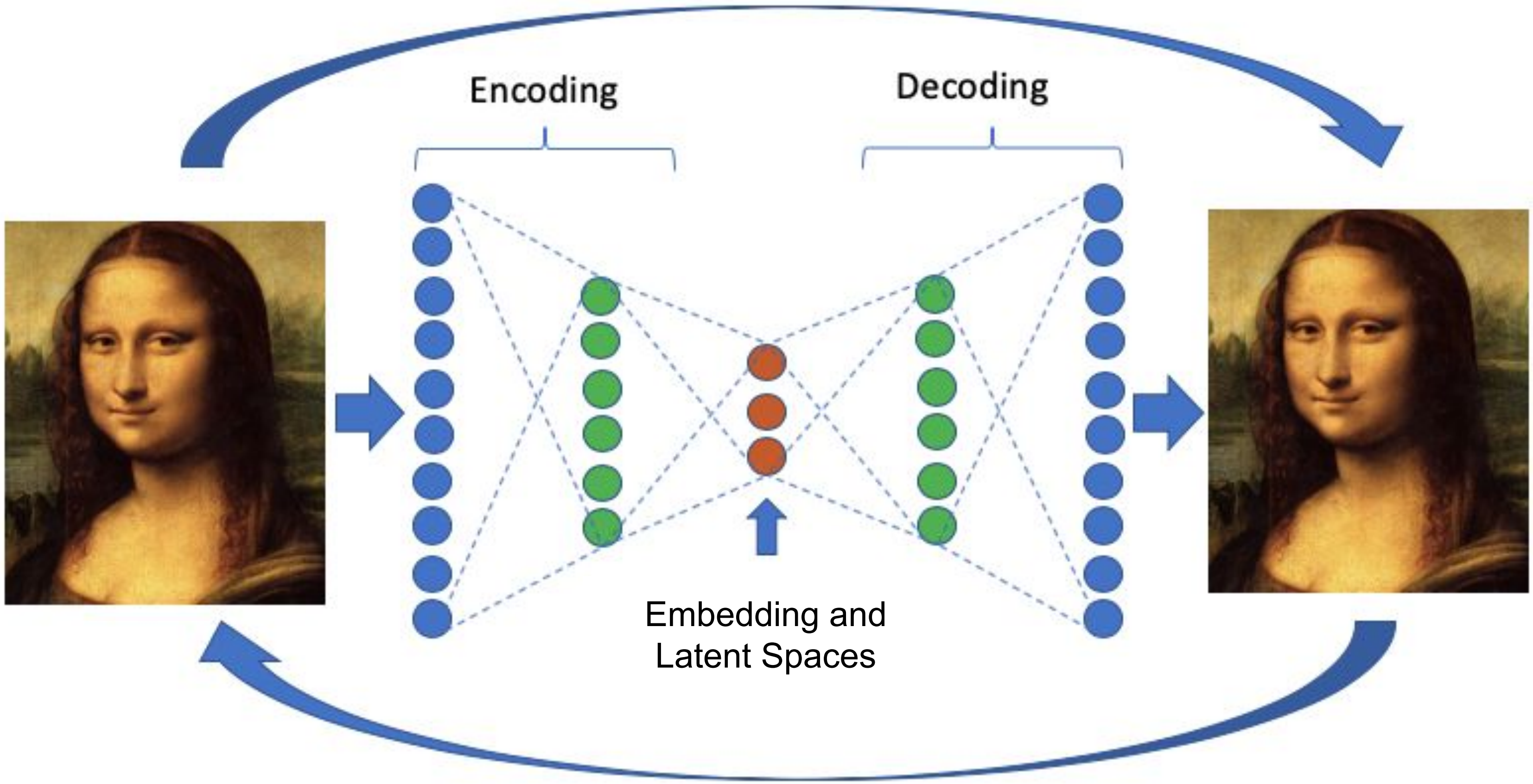
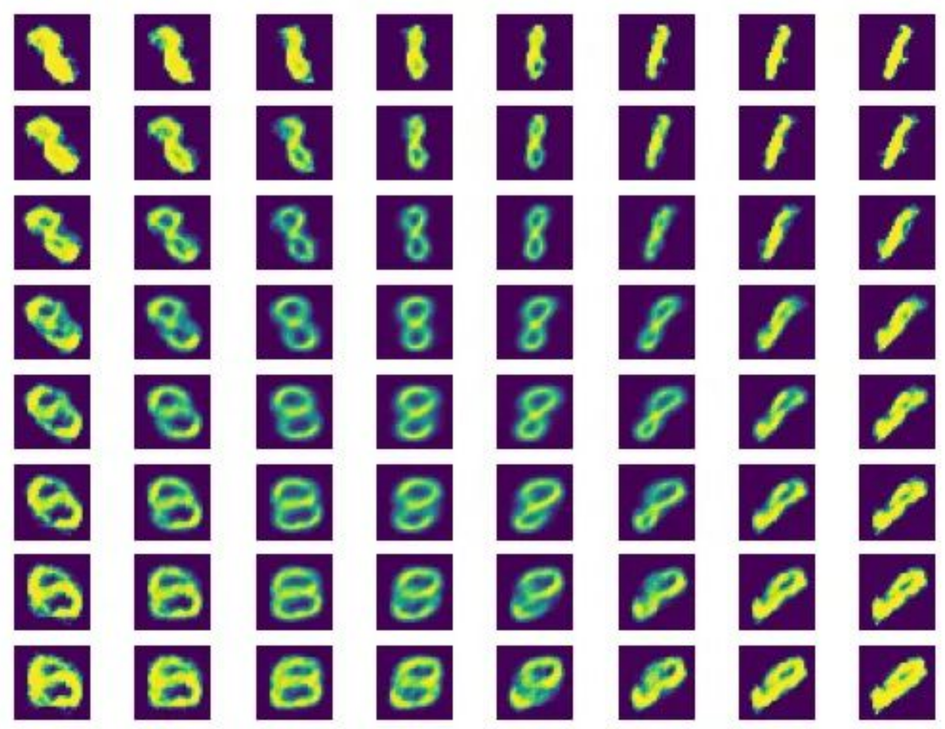
Pausa para Divulgação



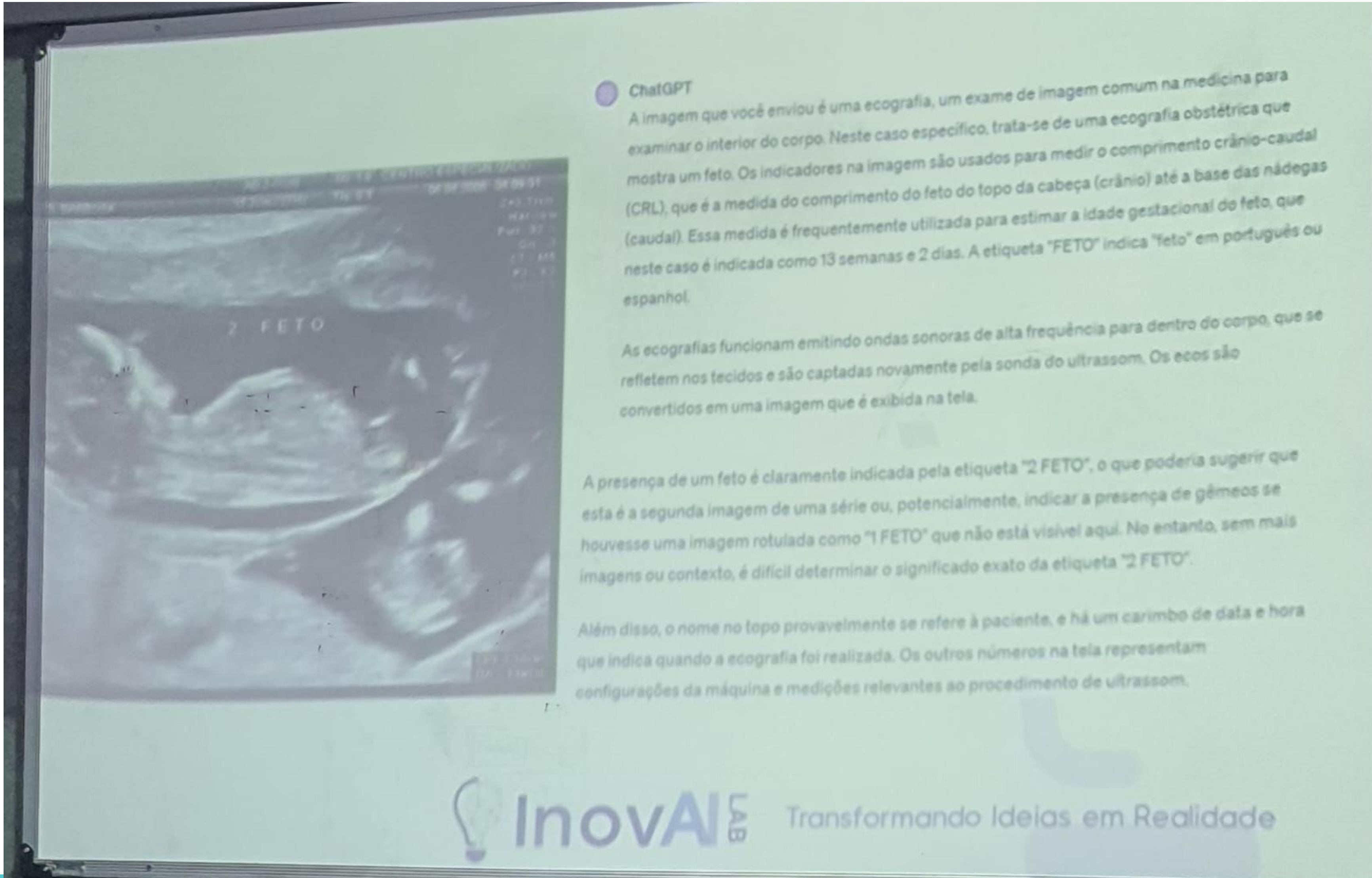
Autoencoder



Autoencoder

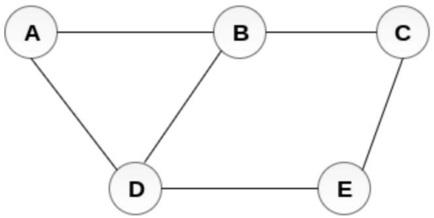


https://towardsdatascience.com/conditional-variational-autoencoders-with-learnable-conditional-embeddings-e22ee5359a2a

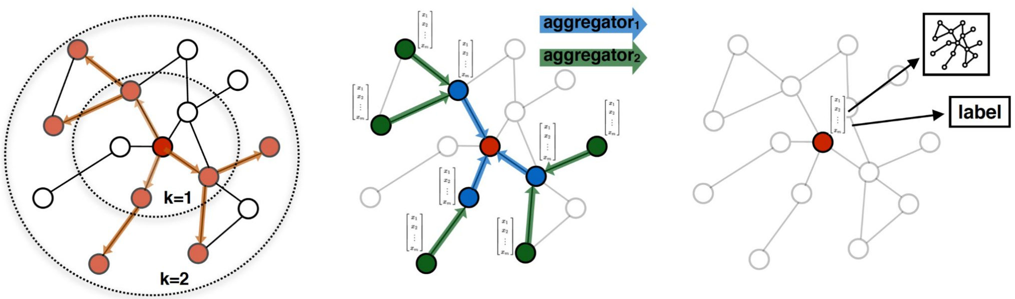

2 FETO
ChatGPT
A imagem que você enviou é uma ecografia, um exame de imagem comum na medicina para examinar o interior do corpo. Neste caso específico, trata-se de uma ecografia obstétrica que mostra um feto. Os indicadores na imagem são usados para medir o comprimento crânio-caudal (CRL), que é a medida do comprimento do feto do topo da cabeça (crânio) até a base das nádegas (caudal). Essa medida é frequentemente utilizada para estimar a idade gestacional do feto, que neste caso é indicada como 13 semanas e 2 dias. A etiqueta "FETO" indica "feto" em português ou espanhol.
As ecografias funcionam emitindo ondas sonoras de alta frequência para dentro do corpo, que se refletem nos tecidos e são captadas novamente pela sonda do ultrassom. Os ecos são convertidos em uma imagem que é exibida na tela.
A presença de um feto é claramente indicada pela etiqueta "2 FETO", o que poderia sugerir que esta é a segunda imagem de uma série ou, potencialmente, indicar a presença de gêmeos se houvesse uma imagem rotulada como "1 FETO" que não está visível aqui. No entanto, sem mais imagens ou contexto, é difícil determinar o significado exato da etiqueta "2 FETO".
Além disso, o nome no topo provavelmente se refere à paciente, e há um carimbo de data e hora que indica quando a ecografia foi realizada. Os outros números na tela representam configurações da máquina e medições relevantes ao procedimento de ultrassom.
InovAI LAB
Transformando Ideias em Realidade

Graphs

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

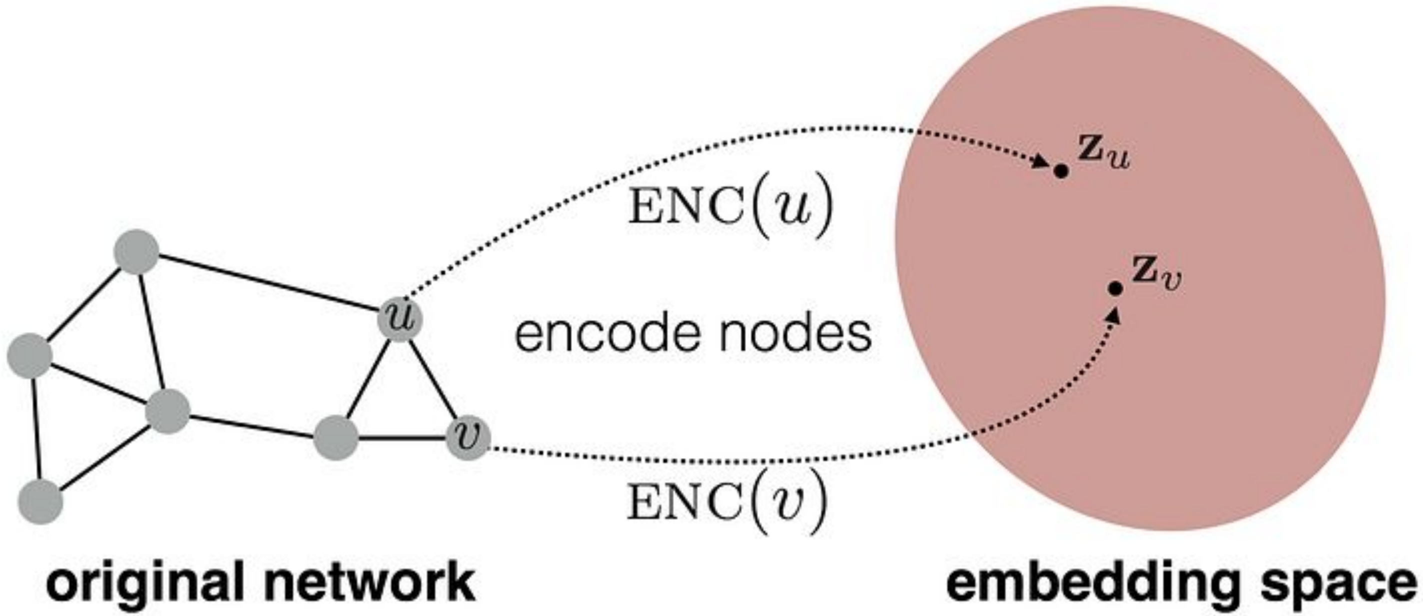


	A	B	C	D	E
A	0	1	0	1	0
B	1	0	1	1	0
C	0	1	0	0	1
D	1	1	0	0	1
E	0	0	1	1	0

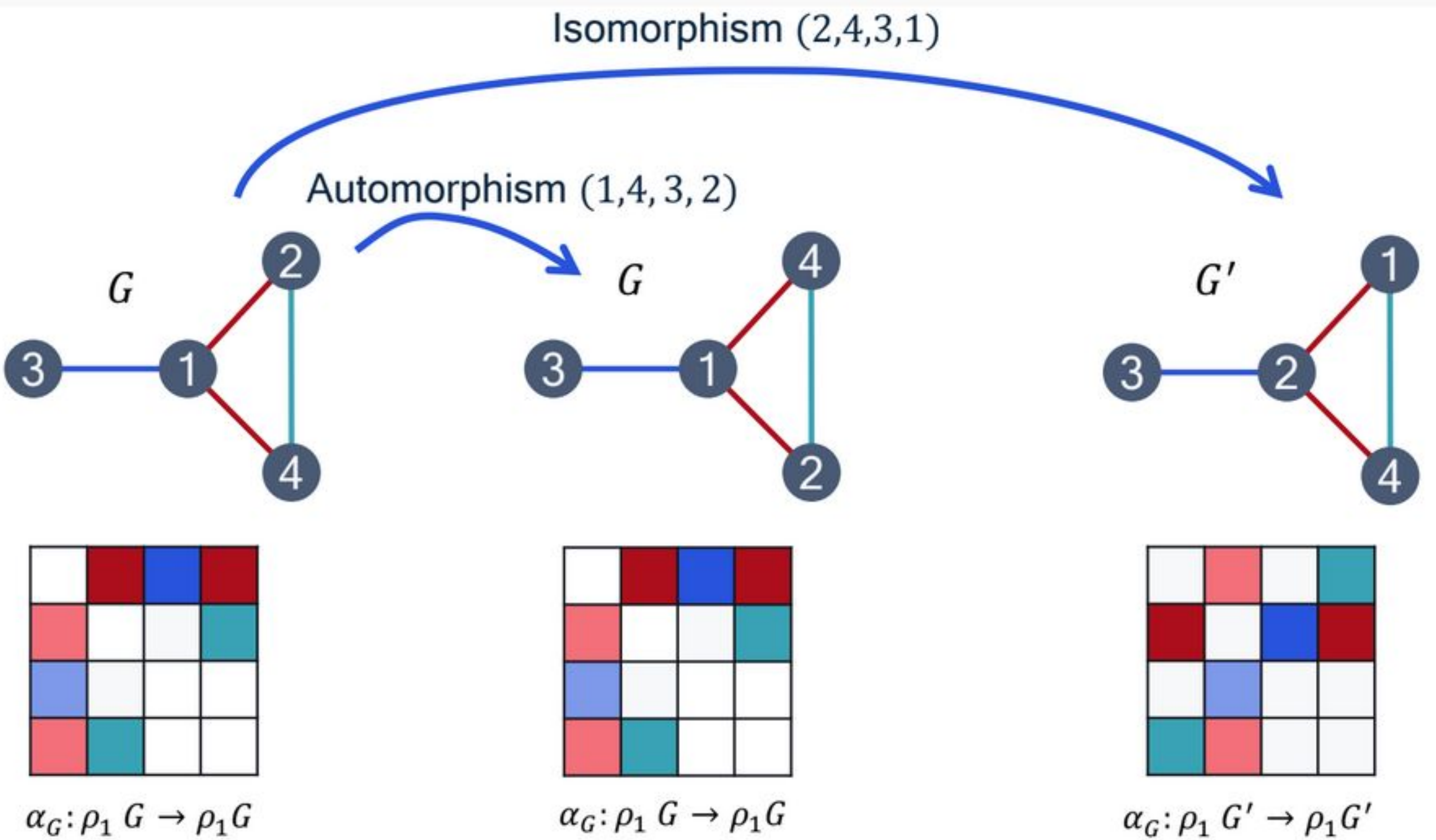


1. Sample neighborhood
2. Aggregate feature information from neighbors
3. Predict graph context and label using aggregated information

source: snap.stanford.edu/graphsage



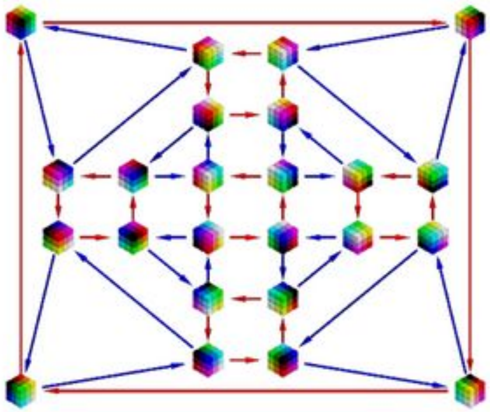
source: salmanfaroz.medium.com



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 $gg^{-1} = g^{-1}g = e$

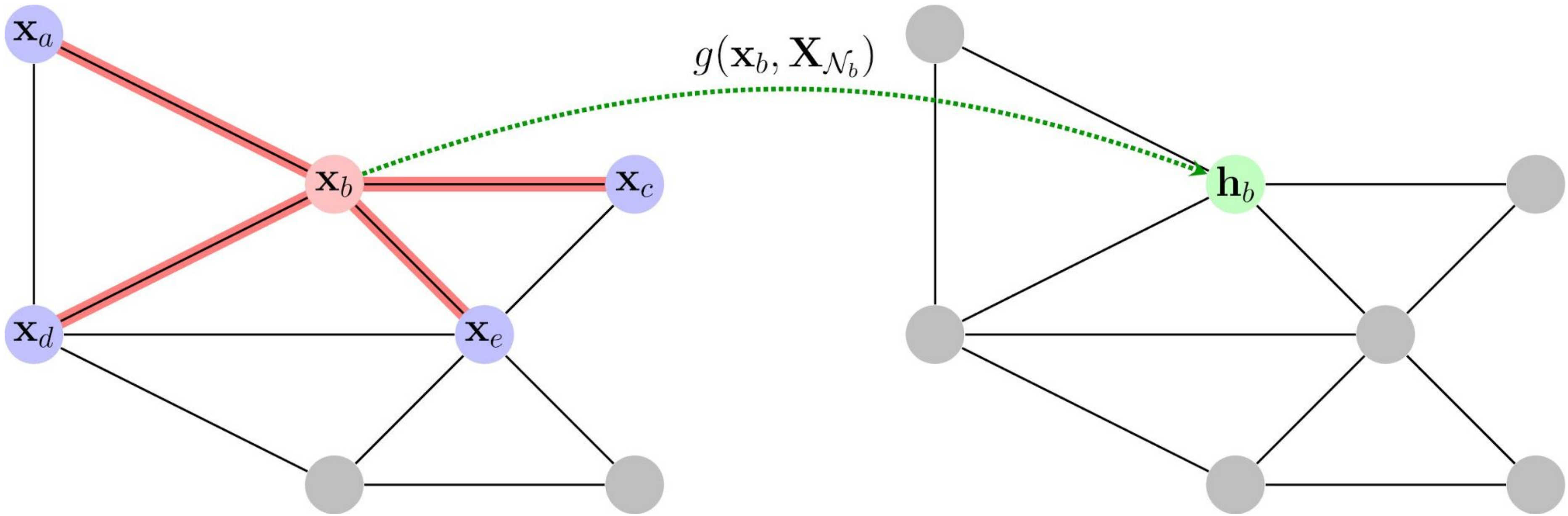


Rotational symmetries of the cube (group O_h)

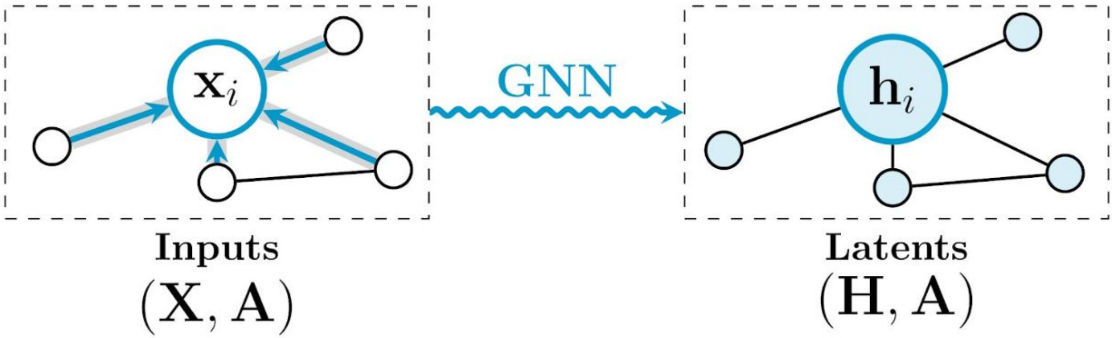
A group $\mathbf{B}G$ is a groupoid with a unique object $\star$.

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

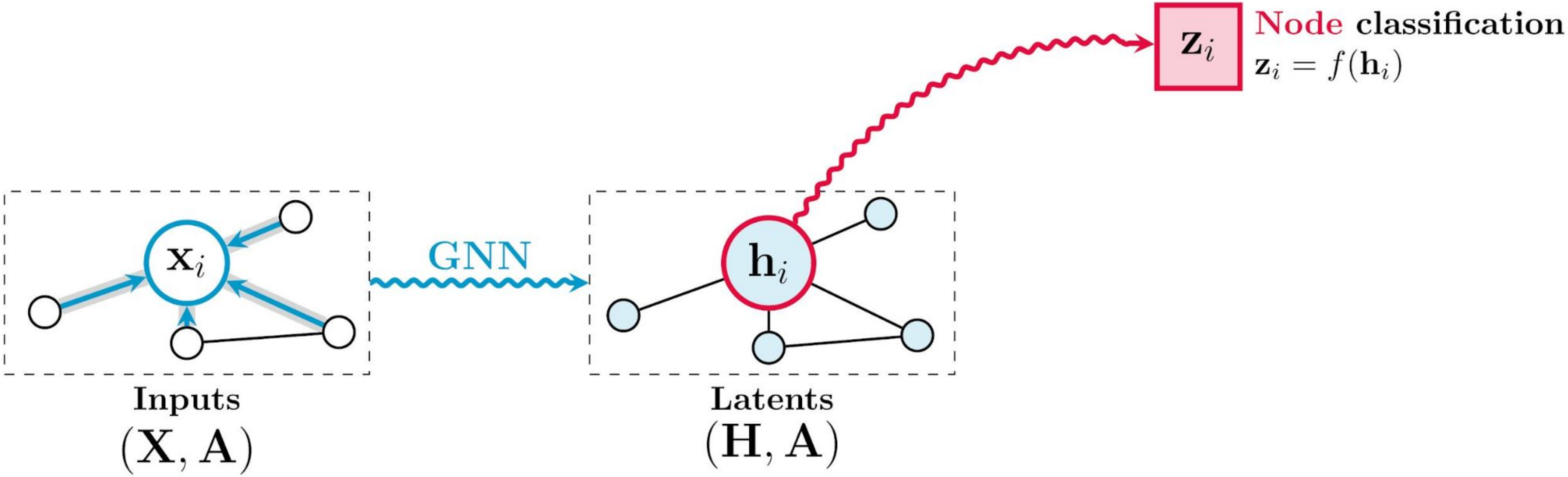
For any groupoid $\mathcal{G}$, object A, the automorphisms $f: A \to A \in \mathrm{Aut}_{\mathcal{G}}(A)$ form a group.



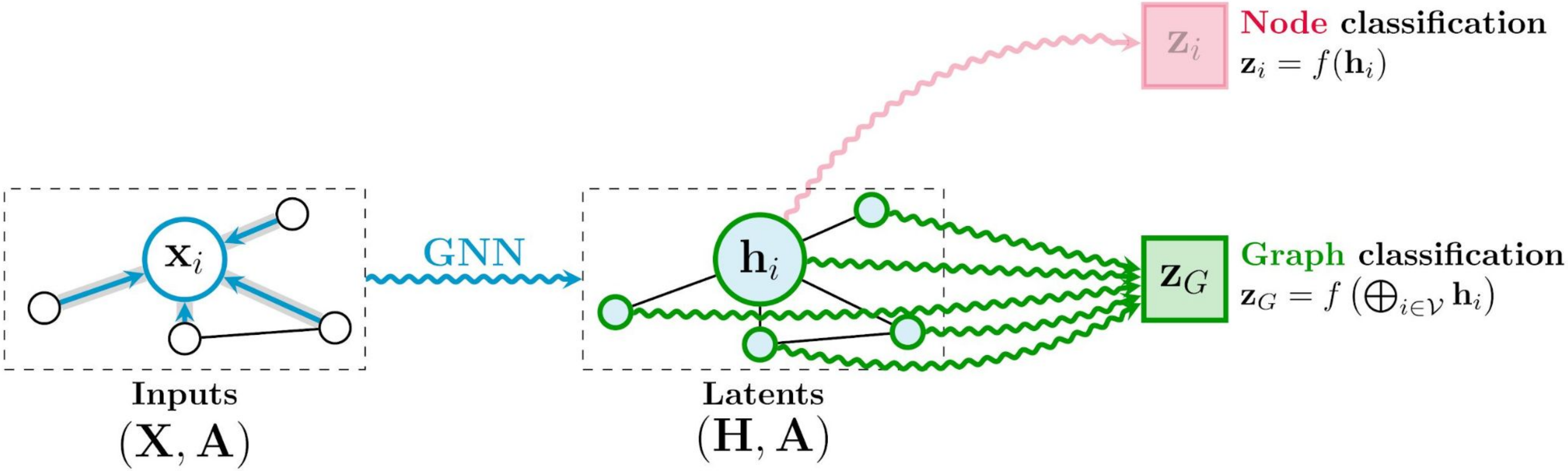
source: Petar Veličković, MLinPL2021



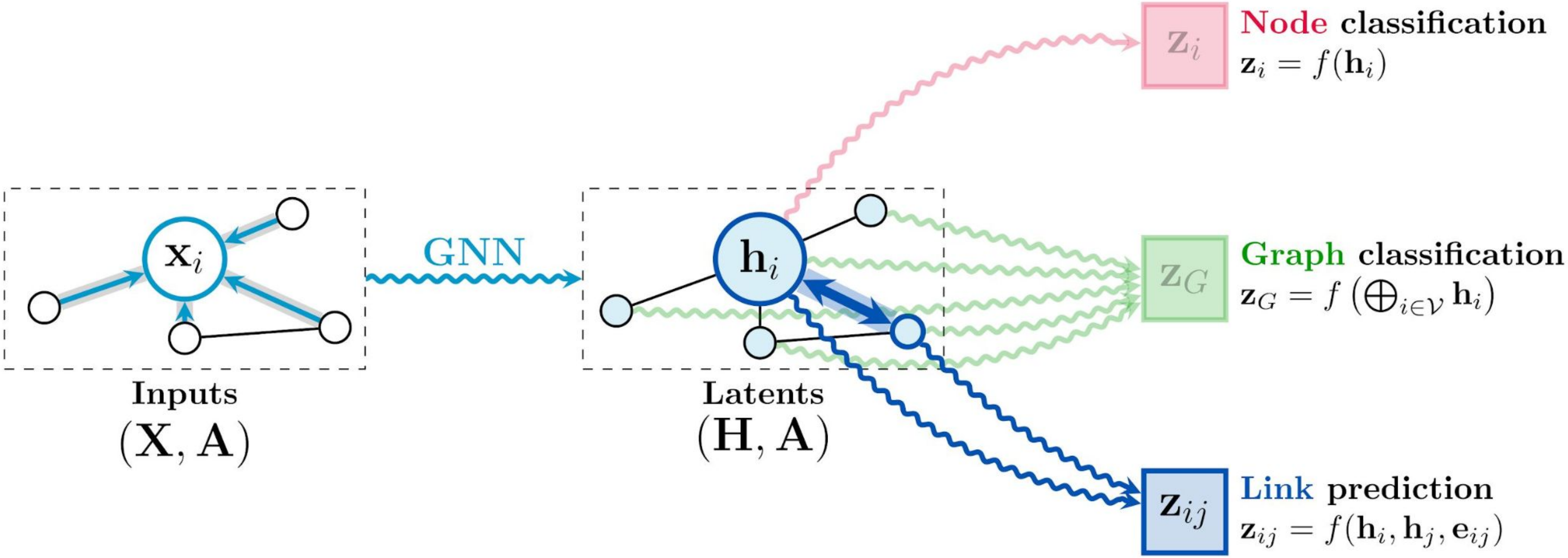
source: Petar Veličković, MLinPL2021



source: Petar Veličković, MLinPL2021

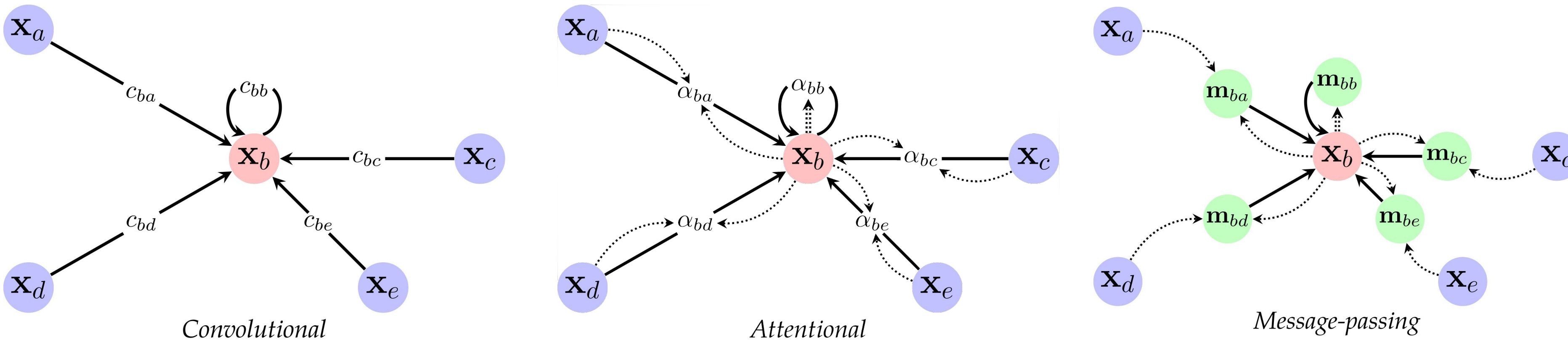


source: Petar Veličković, MLinPL2021



source: Petar Veličković, MLinPL2021

GNN layers



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

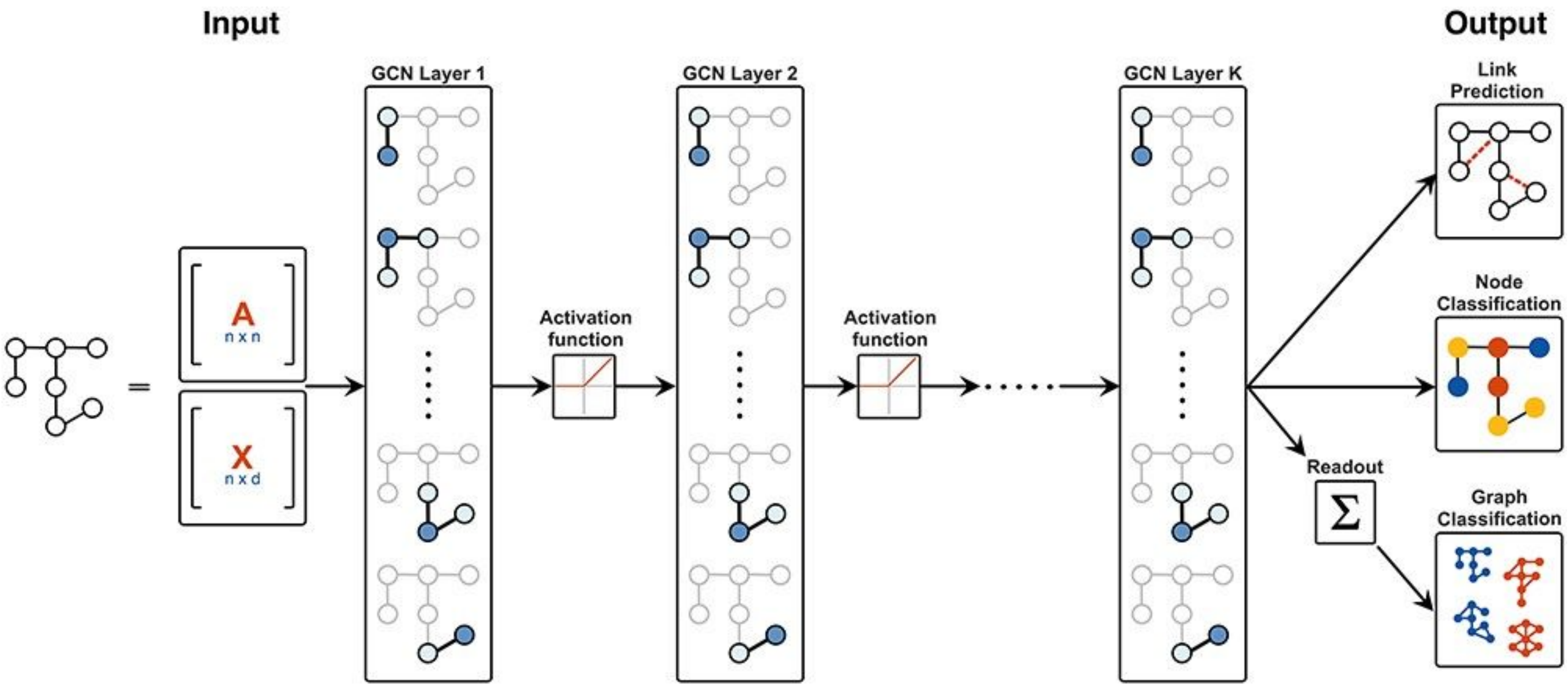
$$\mathbf{h}_i = \phi\left(\mathbf{x}_i, \bigoplus_{j\in\mathcal{N}_i} a(\mathbf{x}_i, \mathbf{x}_j)\psi(\mathbf{x}_j)\right)$$

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

source: Petar Veličković, MLinPL2021

k-layer GCN

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



Frameworks

PyTorch geometric

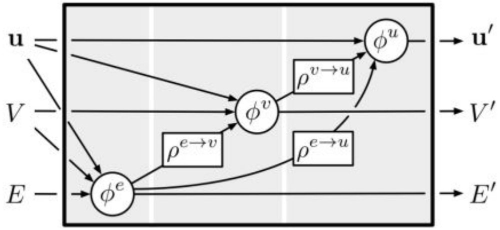
github.com/rusty1s/pytorch_geometric

Spektral

graphneural.network

DGL

dgl.ai



github.com/deepmind/graph_nets

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/

https://cats.for.ai/

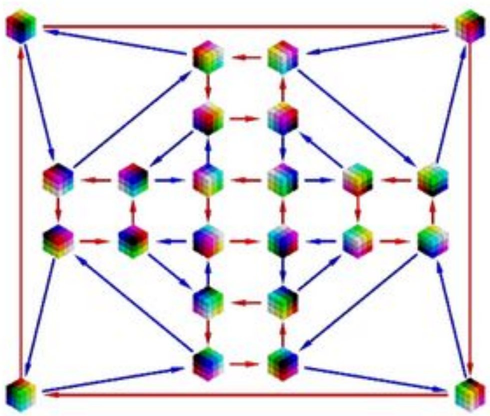
A group G is a set with a binary operation $G \times G \to G$ satisfying:

- **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)

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