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Theoretical Foundations of Graph Neural Networks

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CST Wednesday Seminar
17 February 2021

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In this talk:
Neural networks for **graph-structured data**

*(Graph Neural Networks; **GNNs**)*

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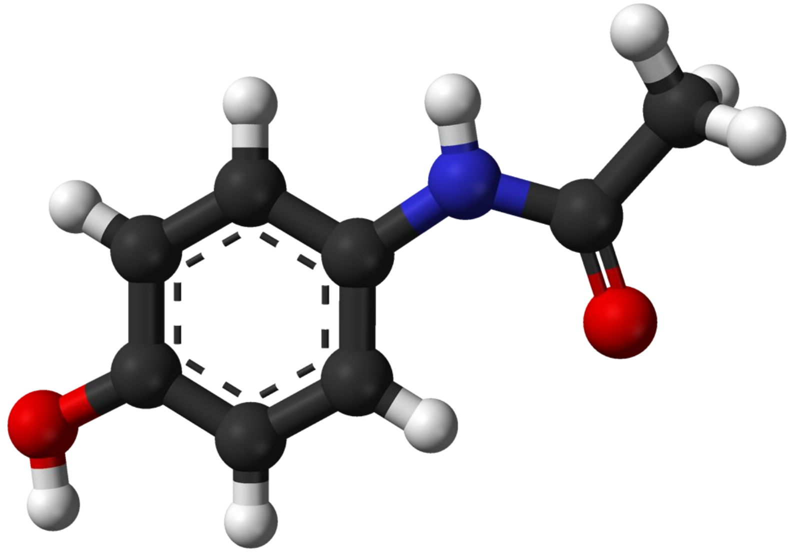
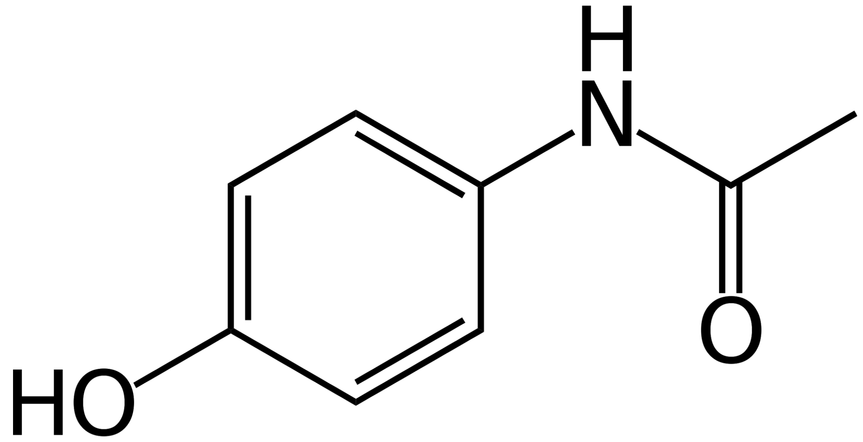
1 Fantastic GNNs in the Wild

Molecules are graphs!

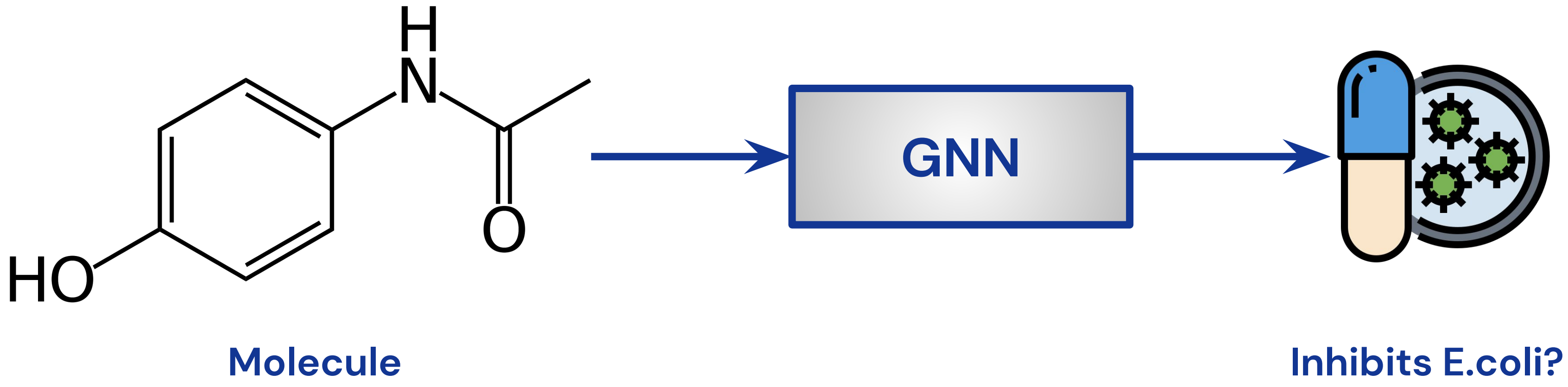
- A very natural way to represent molecules is as a **graph**
  - **Atoms** as nodes, **bonds** as edges
  - Features such as **atom type**, **charge**, **bond type**...





GNNs for molecule classification

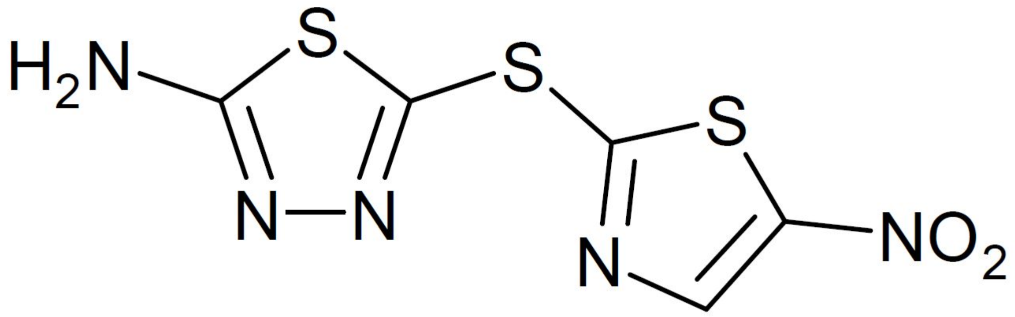
- Interesting task to predict is, for example, whether the molecule is a potent **drug**.
  - Can do *binary classification* on whether the drug will inhibit certain bacteria. (*E.coli*)
  - Train on a **curated dataset** for compounds where response is known.



Follow-up study

- Once trained, the model can be applied to *any* molecule.
  - Execute on a large dataset of known candidate molecules.
  - Select the *~top-100* candidates from your GNN model.
  - Have chemists thoroughly investigate those (after some additional filtering).

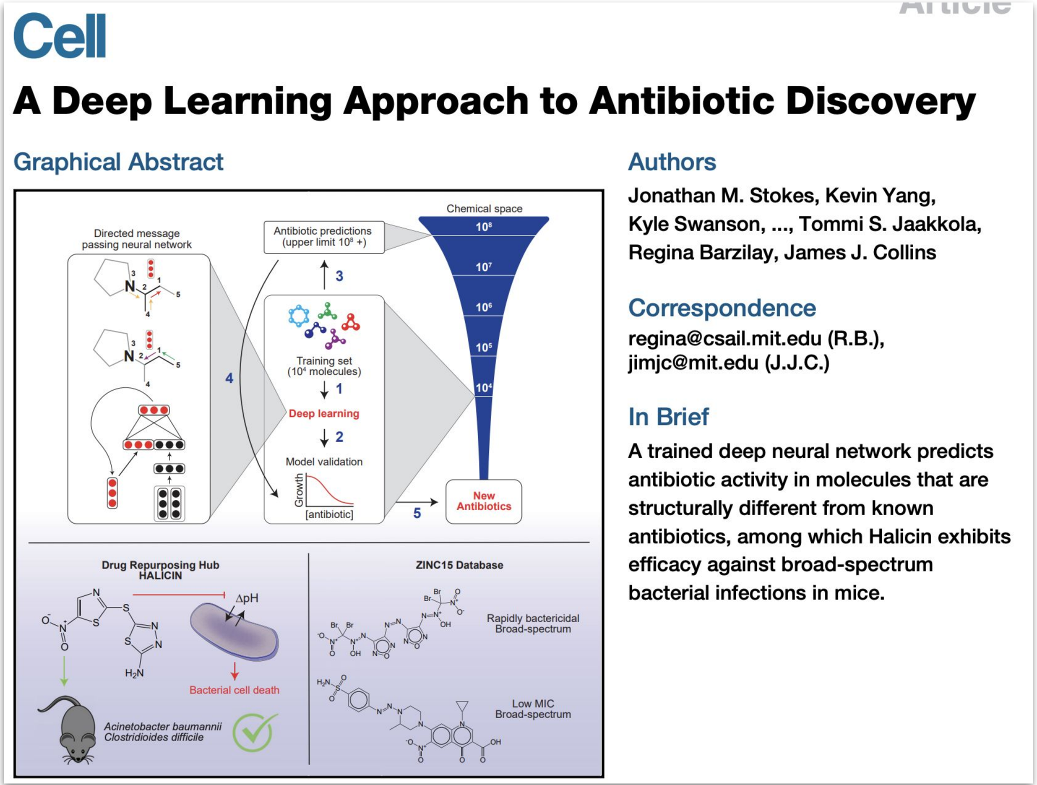
- Discover a previously overlooked compound that is a **highly potent** antibiotic!



Halicin

…Achieve wide acclaim!

Arguably the most popularised **success story** of graph neural networks to date!

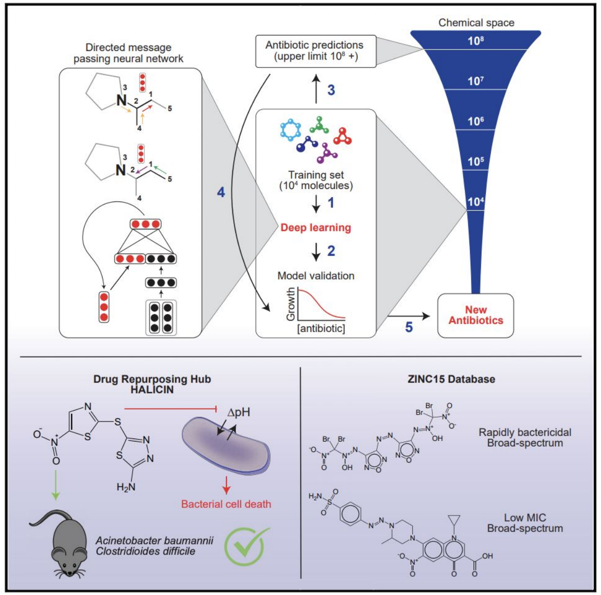


Article

Cell

A Deep Learning Approach to Antibiotic Discovery

Graphical Abstract



Directed message passing neural network
Antibiotic predictions (upper limit 10^8 +)
Chemical space
10^8
10^7
10^6
10^5
10^4
3
4
Training set (10^4 molecules)
1
Deep learning
2
Model validation
Growth
[antibiotic]
5
New Antibiotics
Drug Repurposing Hub HALICIN
ΔpH
Bacterial cell death
Acinetobacter baumannii Clostridioides difficile
ZINC15 Database
Rapidly bactericidal Broad-spectrum
Low MIC Broad-spectrum

Authors

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

Correspondence

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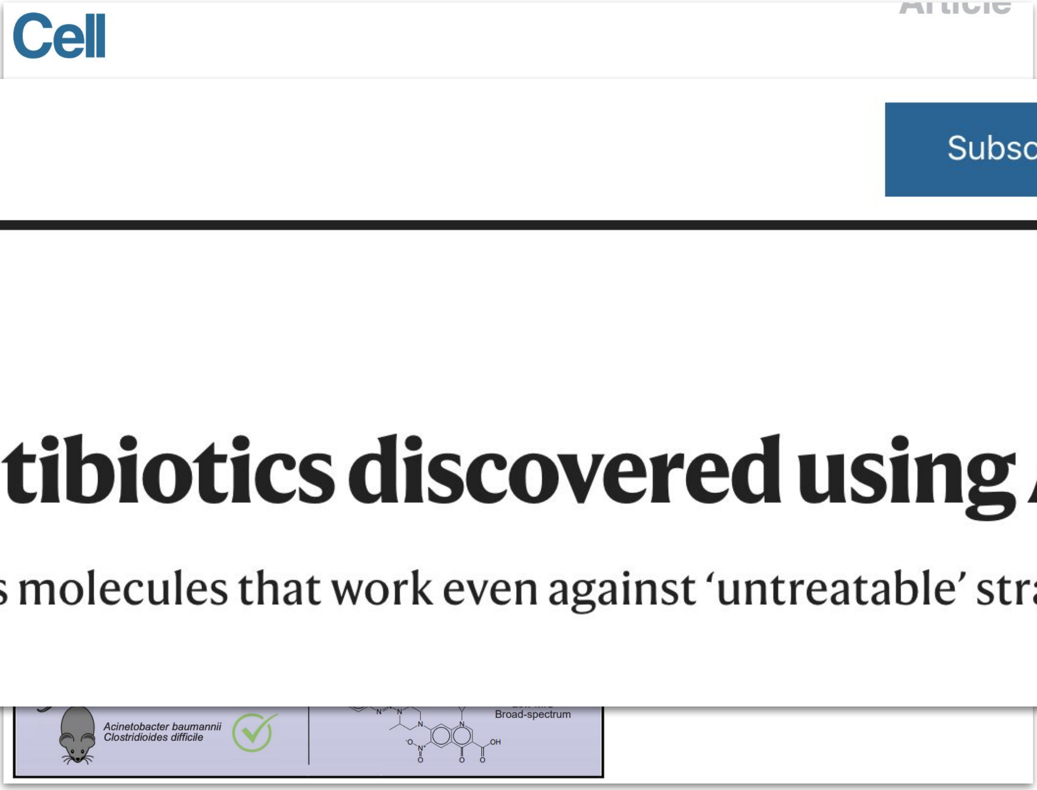
In Brief

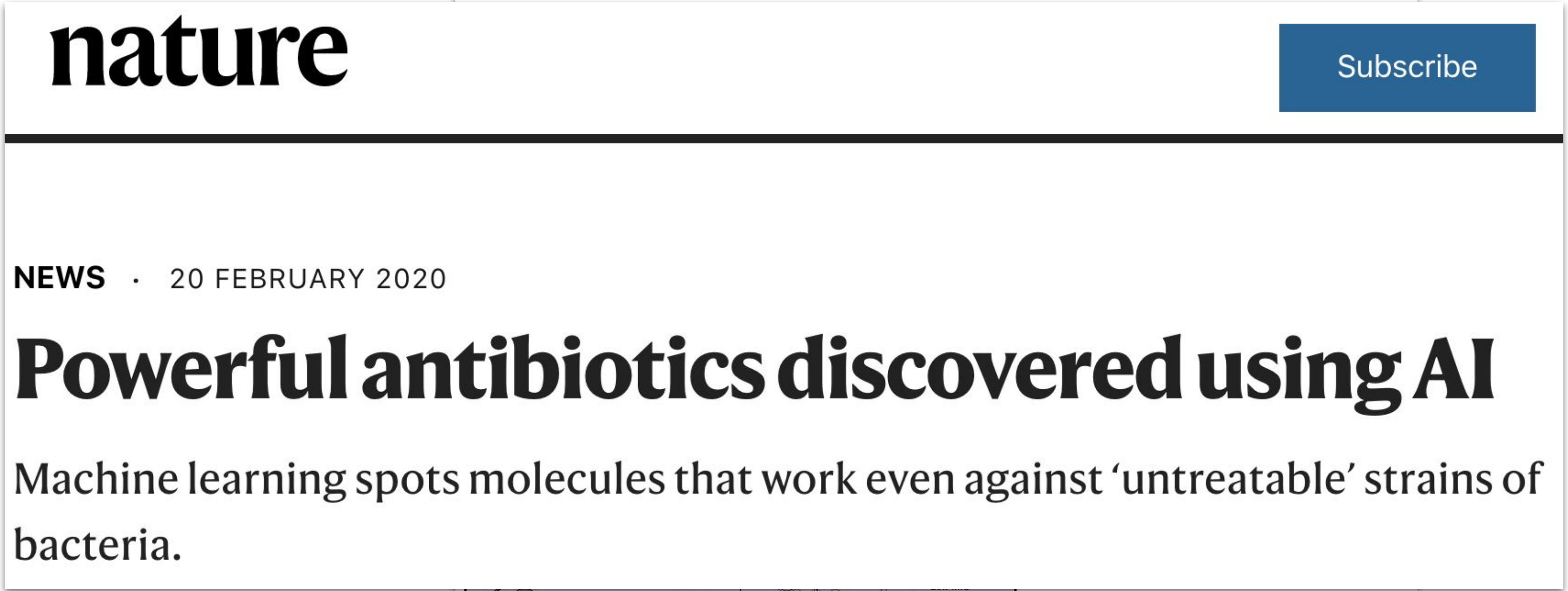
A trained deep neural network predicts antibiotic activity in molecules that are structurally different from known antibiotics, among which Halicin exhibits efficacy against broad-spectrum bacterial infections in mice.

(Stokes *et al.*, Cell'20)

…Achieve wide acclaim!

Arguably the most popularised **success story** of graph neural networks to date!





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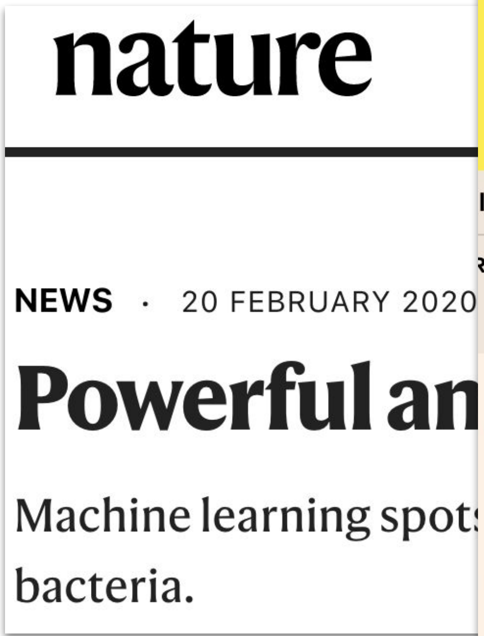
Powerful antibiotics discovered using AI

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

(Stokes *et al.*, Cell’20)

…Achieve wide acclaim!

Arguably the most popula



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Powerful an

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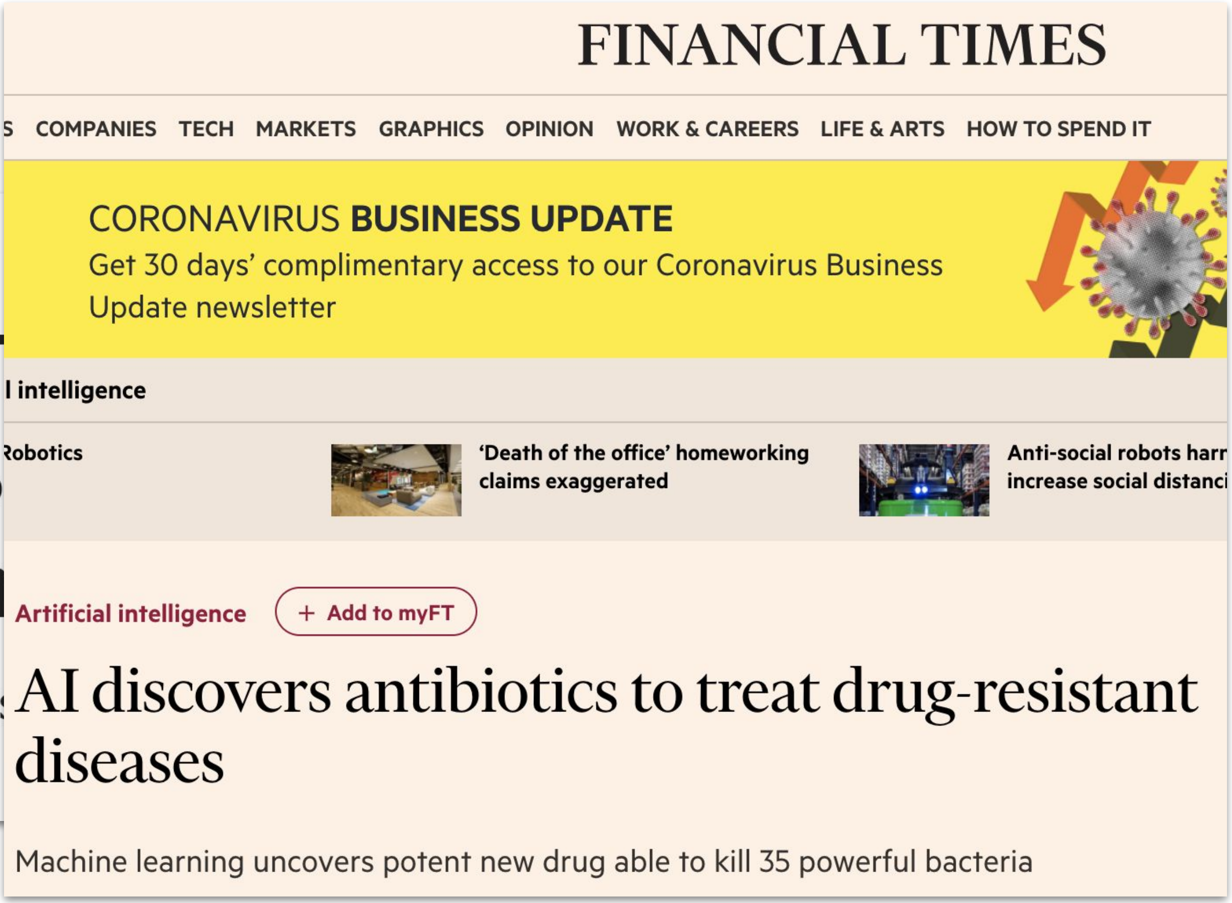

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Anti-social robots harr increase social distanci

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AI discovers antibiotics to treat drug-resistant diseases

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

…Achieve wide acclaim!

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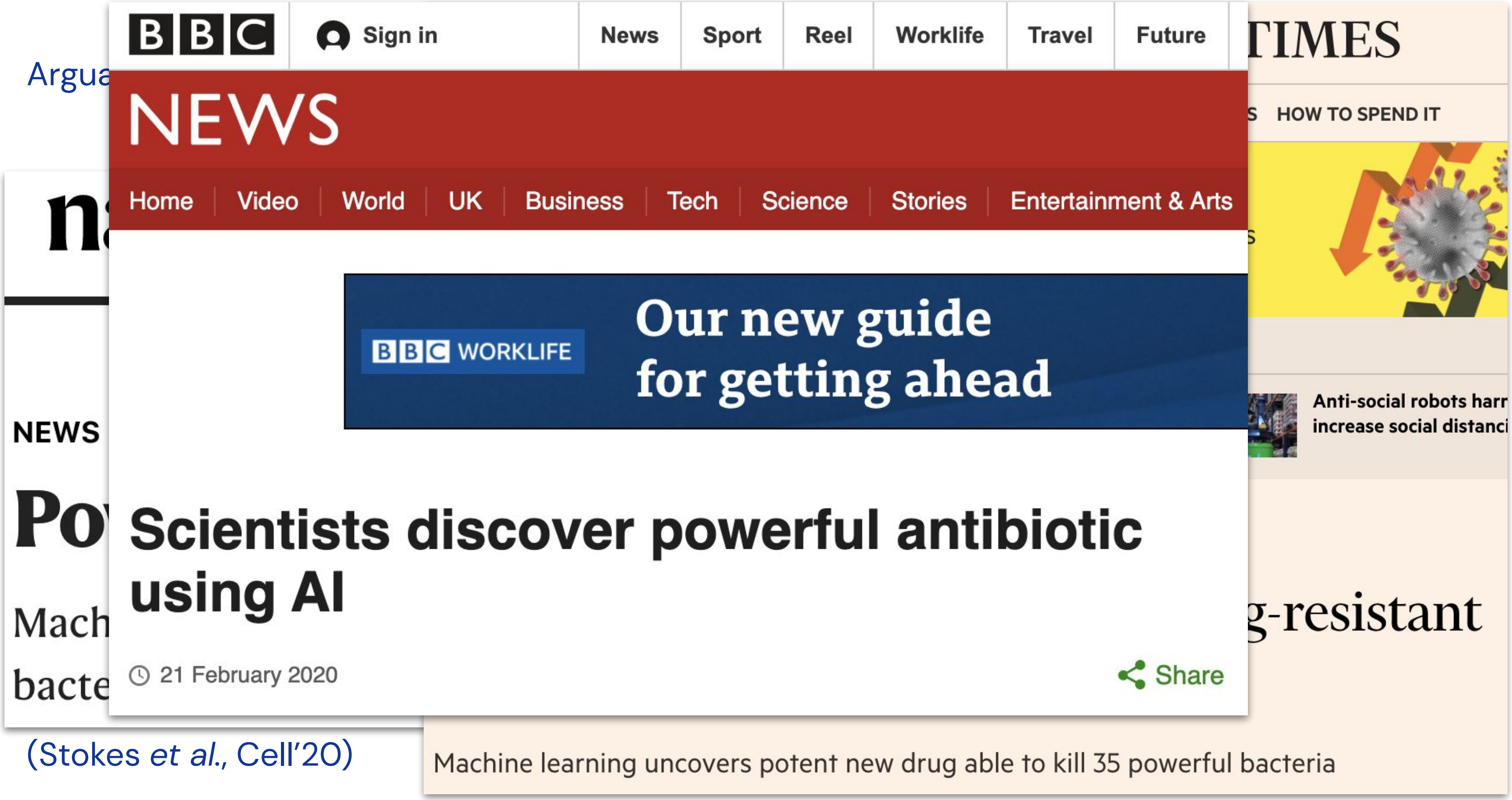

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Machine learning uncovers potent new drug able to kill 35 powerful bacteria

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Scientists discover powerful antibiotic using AI

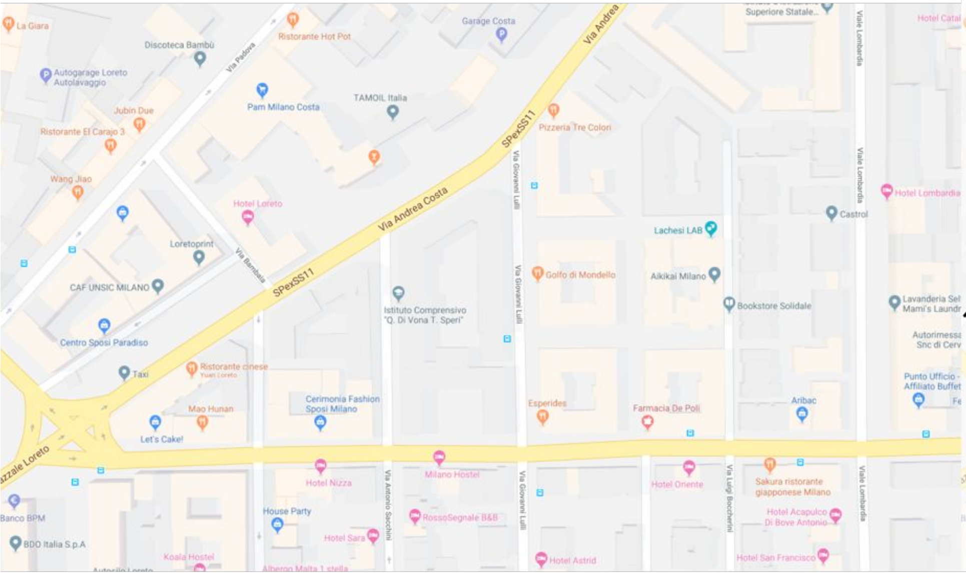
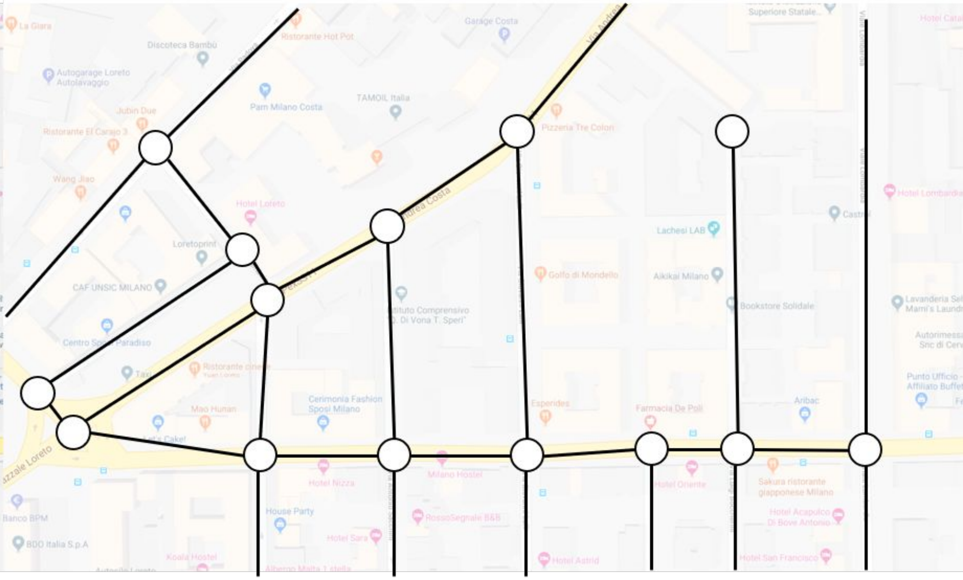
21 February 2020

Share

(Stokes *et al.*, Cell'20)

Traffic maps are graphs!

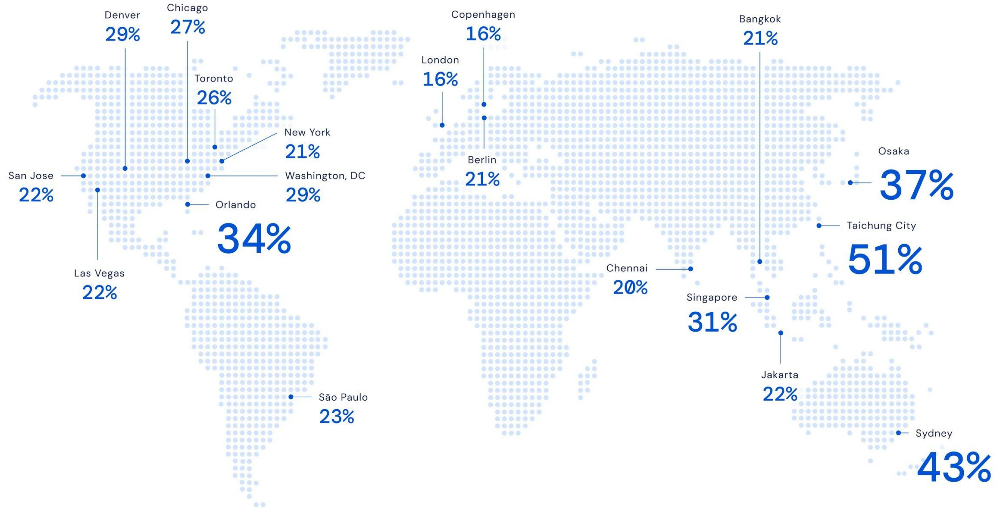
Transportation maps (e.g. the ones found on *Google Maps*) naturally modelled as **graphs**.

Nodes could be **intersections**, and edges could be **roads**. (Relevant **node features**: road *length*, *current speeds*, *historical speeds*)

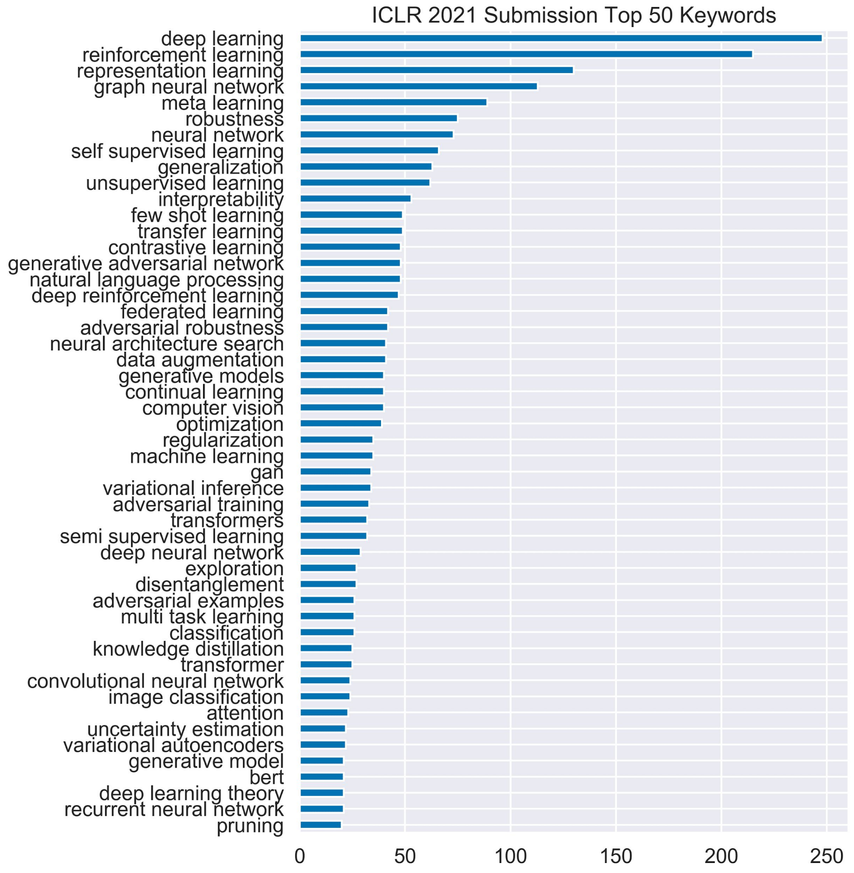
DeepMind's ETA Prediction using GNNs in Google Maps

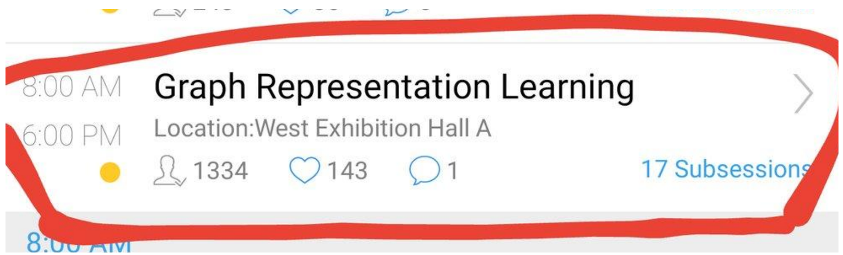
Run GNN on **supersegment** graph to estimate **time of arrival** (ETA) (*graph regression*).

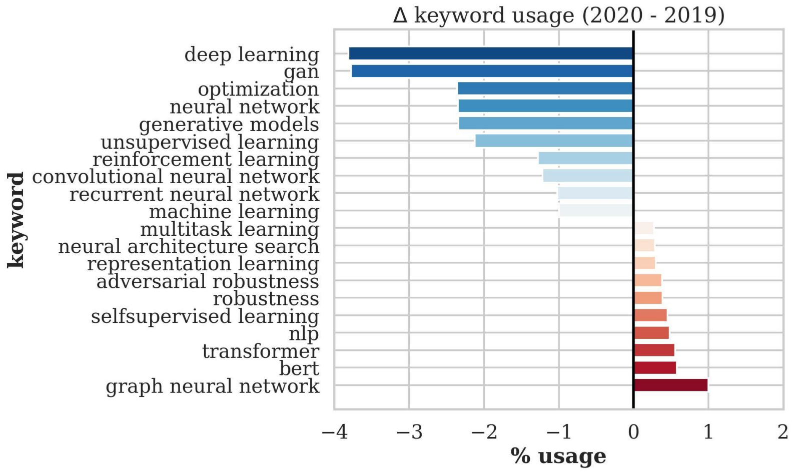


Already **deployed** in several major cities, significantly reducing negative ETA outcomes!

GNNs are a **very hot** research topic




8:00 AM Graph Representation Learning
6:00 PM Location:West Exhibition Hall A
1334 143 1 17 Subsessions



GNNs are currently experiencing their "ImageNet" moment

Rich **ecosystem** of **libraries**

PyTorch geometric

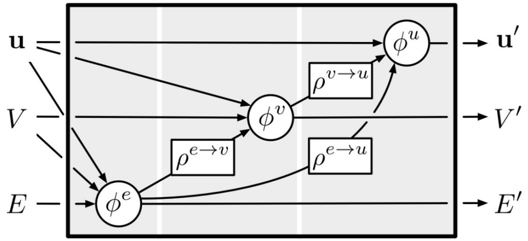
`github.com/rusty1s/pytorch_geometric`

Spektral

`graphneural.network`

DGL

`dgl.ai`



`github.com/deepmind/graph_nets`

`github.com/deepmind/jraph`

Rich **ecosystem** of **datasets**

OGB

ogb.stanford.edu

PyTorch geometric

https://pytorch-geometric.readthedocs.io/en/latest/modules/datasets.html

TUDataset

graphlearning.io

Benchmarking Graph Neural Networks

github.com/graphdeeplearning/benchmarking-gnns

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2 Talk roadmap

What will we cover today?

- Hopefully I've given you a convincing argument for **why** GNNs are useful to study
  - For more details and applications, please see e.g. my *EEML 2020* talk

- My aim for today: provide good **blueprints** and **contexts** for studying the field
  - Derive GNNs from first principles
  - Position this in context of several *independently-studied* derivations of GNNs
    - Often using *drastically* different mathematical tools…
  - Look to the *past*: how GNN-like models emerged in historical ML research
  - Look to the *present*: some *immediate* lines of research interest
  - Look to the *future*: how our blueprint *generalises* beyond graph-structured inputs

- Hopefully my perspective is of use both to newcomers and seasoned GNN practitioners
  - **Any** and **all** feedback *very welcome*!

What is the content **based** on?

- GNN derivation + further horizons inspired by my work on **geometric deep learning**
    - Ongoing collaboration with Joan Bruna, Michael Bronstein and Taco Cohen
- Various contexts of GNN study inspired by Will Hamilton's **GRL Textbook** (esp. Chapter 7)
    - https://www.cs.mcgill.ca/~wlh/grl_book/
    - **Highly** recommended!
- Historical contexts developed with input of several researchers
    - Thanks to Yoshua Bengio, Marco Gori, Jürgen Schmidhuber, Christian Merkwirth and Marwin Segler
- But of course, any errors and omissions are mine alone.

Disclaimer before advancing

- My talk **content** is geared to a ***general*** Computer Science audience
  - We will construct “useful” functions operating over graphs
  - We will use concepts commonly encountered in a CS curriculum

- **Implementation** requires background in machine learning with deep neural networks
  - Useful resource to get started: **“Deep Learning”** by Goodfellow, Bengio and Courville
    - https://www.deeplearningbook.org/

- I recently compiled a list of many useful GNN resources in a **Twitter thread**
  - https://twitter.com/PetarV_93/status/1306689702020382720

- When you feel ready, I **highly** recommend Aleksa Gordić’s GitHub repository on GATs:
  - https://github.com/gordicaleksa/pytorch-GAT
  - Arguably the most *gentle* introduction to GNN implementations

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3 Towards GNNs from first principles

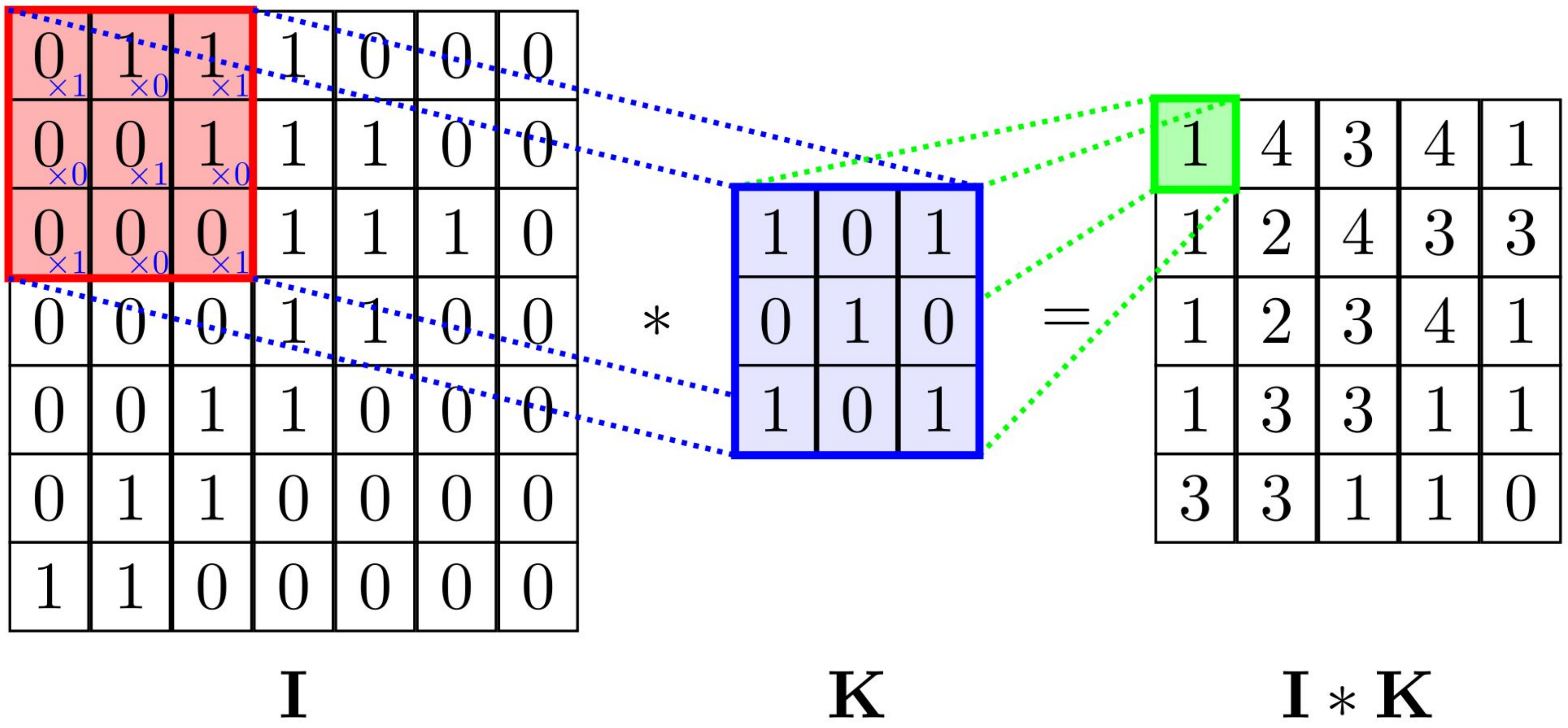
Towards a **neural network** for **graphs**

- We will now work towards defining a GNN from first principles

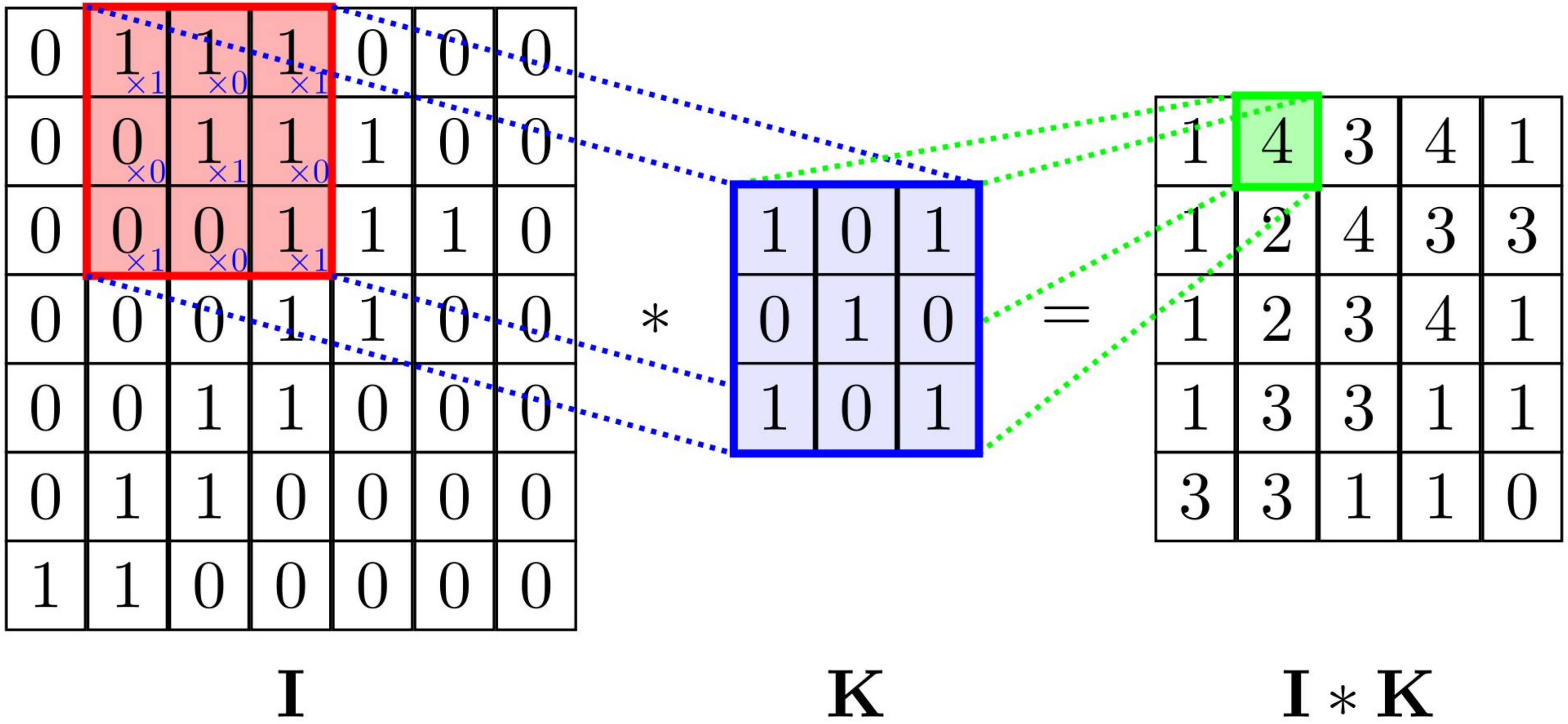
- What properties are useful for operating meaningfully on graphs?

- Specifically: what **symmetries** and **invariances** must a GNN preserve?
    - Let's revisit a known example...

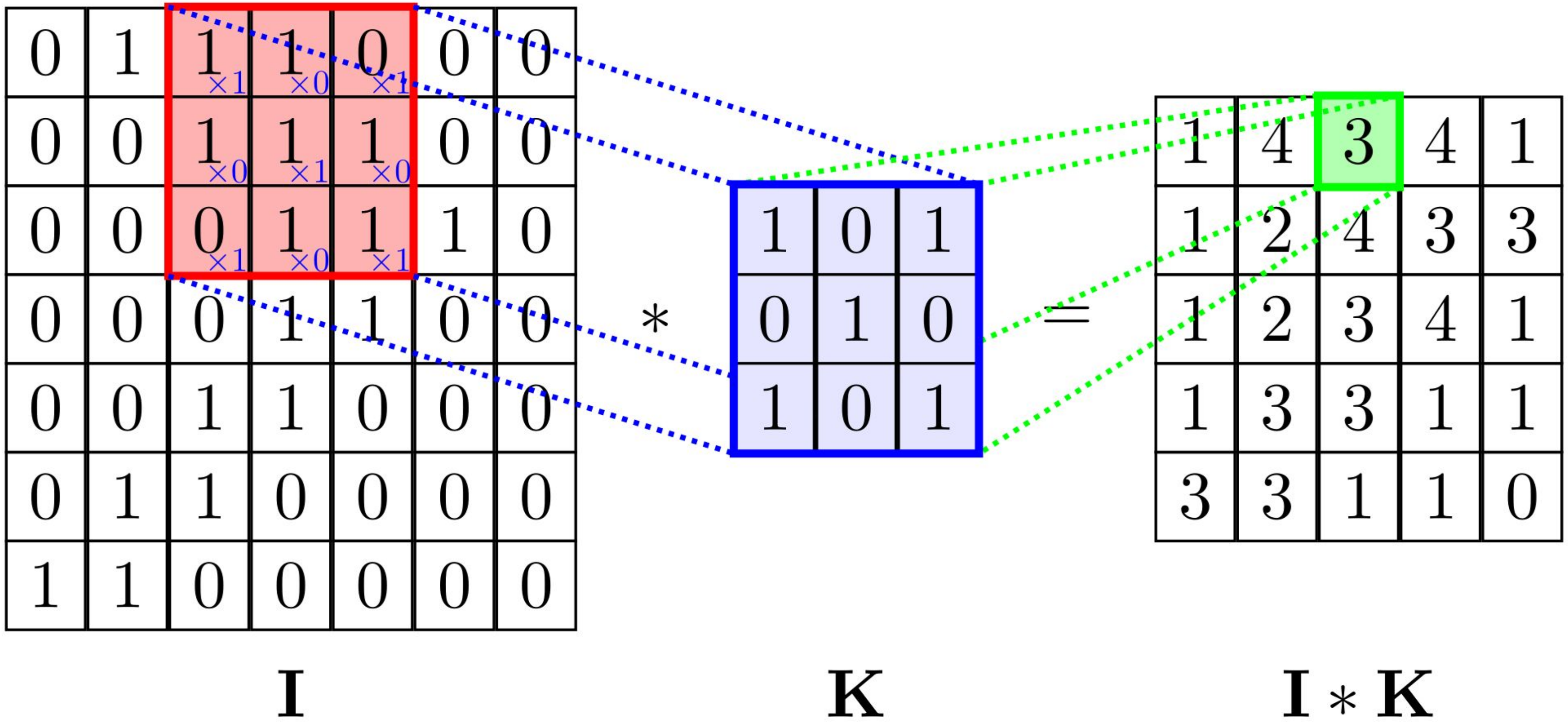
Convolution on images



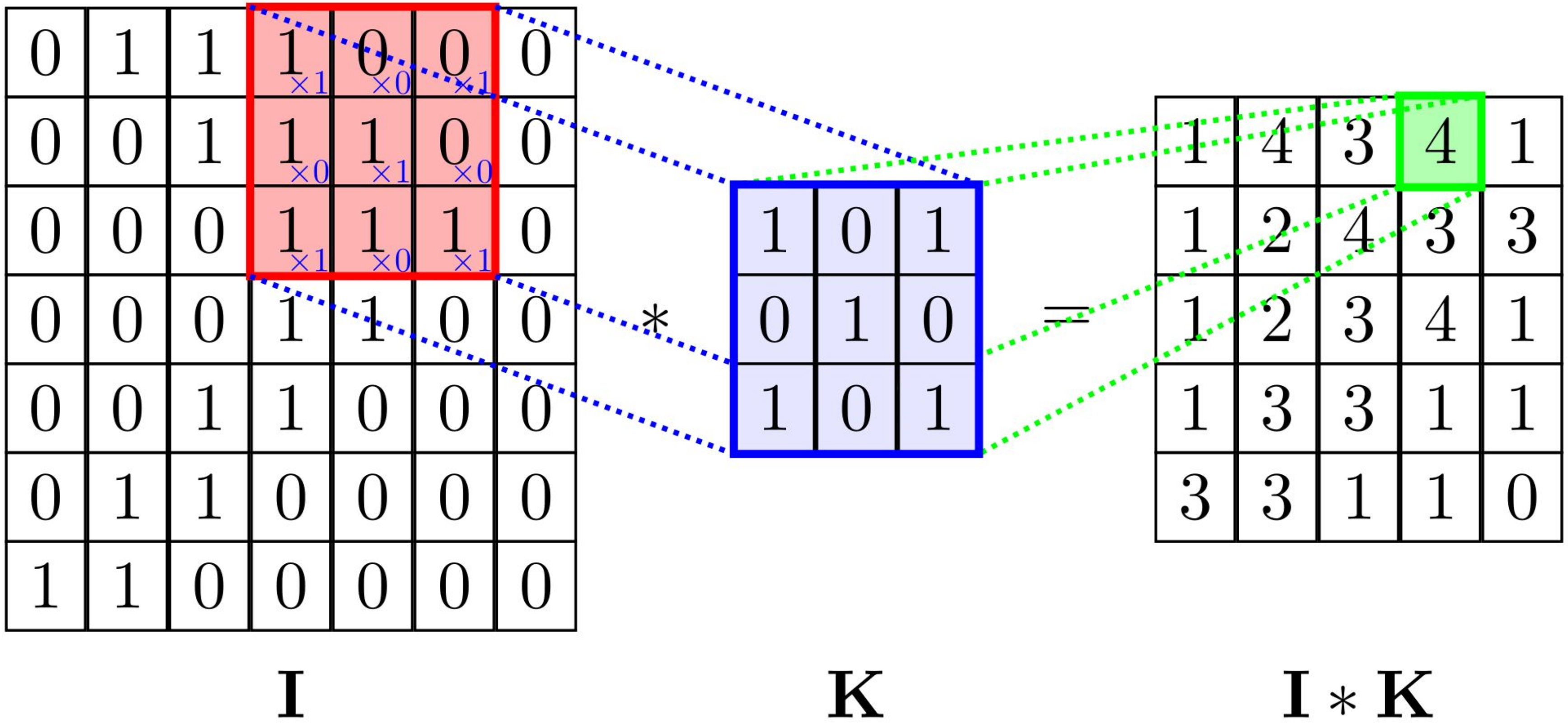
Convolution on images



Convolution on images



Convolution on images

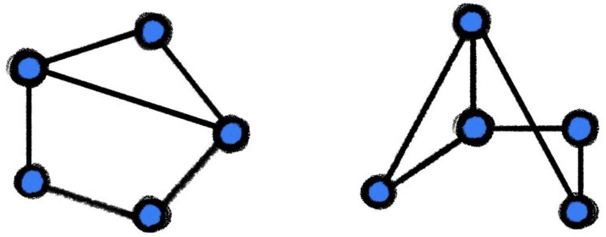


Convolutional neural network invariances

- Convolutional neural nets respect **translational invariance**
- Patterns are interesting irrespective of *where* they are in the image
- **Locality**: neighbouring pixels relate much more strongly than distant ones
- What about **arbitrary** graphs?

Isomorphism-preserving transformation

- The nodes of a graph are not assumed to be in any order
- That is, we would like to get the same results for two isomorphic graphs



- To see how to enforce this, we will define new terms...

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4 Permutation invariance and equivariance

Learning on sets: Setup

- For now, assume the graph **has no edges** (e.g. *set* of nodes, V).
- Let $\mathbf{x}_i \in \mathbb{R}^k$ be the features of node *i*.
- We can stack them into a node feature matrix of shape *n* x *k*:

$$\mathbf{X} = (\mathbf{x}_1, \ldots, \mathbf{x}_n)^\top$$

- That is, the *i*th row of **X** corresponds to $\mathbf{x}_i$
- Note that, by doing so, we have specified a **node ordering**!
    - We would like the result of any neural networks to not depend on this.

Permutations and permutation matrices

- It will be useful to think about the operations that **change** the node order
  - Such operations are known as **permutations** (there are **n!** of them)
  - e.g. a permutation (2, 4, 1, 3) means $\mathbf{y}_1 \leftarrow \mathbf{x}_2$, $\mathbf{y}_2 \leftarrow \mathbf{x}_4$, $\mathbf{y}_3 \leftarrow \mathbf{x}_1$, $\mathbf{y}_4 \leftarrow \mathbf{x}_3$.

- To stay within linear algebra, each permutation defines an *n* x *n* **matrix**
  - Such matrices are called **permutation matrices**
  - They have exactly one 1 in every row and column, and zeros everywhere else
  - Their effect when left-multiplied is to permute the rows of **X**, like so:

$$\mathbf{P}_{(2,4,1,3)}\mathbf{X} = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} — & \mathbf{x}_1 & — \\ — & \mathbf{x}_2 & — \\ — & \mathbf{x}_3 & — \\ — & \mathbf{x}_4 & — \end{bmatrix} = \begin{bmatrix} — & \mathbf{x}_2 & — \\ — & \mathbf{x}_4 & — \\ — & \mathbf{x}_1 & — \\ — & \mathbf{x}_3 & — \end{bmatrix}$$

Permutation ***invariance***

- We want to design functions f(**X**) over sets that will not depend on the order

- Equivalently, applying a permutation matrix shouldn't modify the result!

- We arrive at a useful notion of **permutation invariance**. We say that f(**X**) is permutation *invariant* if, for *all* permutation matrices **P**:

$$f(\mathbf{PX}) = f(\mathbf{X})$$

- One very generic form is the *Deep Sets* model (Zaheer et al., NeurIPS'17): $f(\mathbf{X}) = \phi\left(\sum_{i \in \mathcal{V}} \psi(\mathbf{x}_i)\right)$ where ψ and ϕ are (learnable) functions, e.g. MLPs.
    - The **sum** aggregation is *critical*! (other choices possible, e.g. **max** or **avg**)

Permutation ***equivariance***

- Permutation-*invariant* models are a good way to obtain set-level outputs

- What if we would like answers at the **node** level?
    - We want to still be able to **identify** node outputs, which a permutation-invariant aggregator would destroy!

- We may instead seek functions that don't **change** the node order
    - i.e. if we permute the nodes, it doesn't matter if we do it **before** or **after** the function!

- Accordingly, we say that f(**X**) is **permutation equivariant** if, for all permutation matrices **P**:

$$f(\mathbf{PX}) = \mathbf{P}f(\mathbf{X})$$

General blueprint for learning on **sets**

- Equivariance mandates that each node's row is unchanged by f. That is, we can think of equivariant set functions as transforming each node input $\mathbf{x}_i$ into a *latent* vector $\mathbf{h}_i$:

$$\mathbf{h}_i = \boxed{\psi(\mathbf{x}_i)}$$

where ψ is any function, applied in isolation to every node. Stacking $\mathbf{h}_i$ yields $\mathbf{H} = f(\mathbf{X})$.

- We arrive at a general blueprint: (stacking) **equivariant** function(s), potentially with an **invariant** tail---yields (m)any useful functions on sets!

$$f(\mathbf{X}) = \boxed{\phi\left(\bigoplus_{i\in\mathcal{V}} \boxed{\psi\left(\mathbf{x}_i\right)}\right)}$$

Here, $\bigoplus$ is a permutation-invariant **aggregator** (such as sum, avg or max).

(remark: this is typically **as far** as we can get with sets, without assuming or inferring additional structure)

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5 Learning on graphs

Learning on graphs

- Now we augment the set of nodes with **edges** between them.
  - That is, we consider general E ⊆ V x V.

- We can represent these edges with an **adjacency matrix**, **A**, such that:

$$a_{ij} = \begin{cases} 1 & (i,j) \in \mathcal{E} \\ 0 & \text{otherwise} \end{cases}$$

- Further additions (e.g. *edge features*) are possible but **ignored** for simplicity.

- Our main desiderata (*permutation {in,equi}variance*) still hold!

Permutation invariance and equivariance on **graphs**

- The main difference: node permutations now also accordingly act on the **edges**

- We need to appropriately permute both **rows** and **columns** of **A**
    - When applying a permutation matrix **P**, this amounts to **PAP**$^\top$

- We arrive at updated definitions of suitable functions f(**X, A**) over graphs:

Invariance: $$f(\mathbf{PX}, \mathbf{PAP}^\top) = f(\mathbf{X}, \mathbf{A})$$

Equivariance: $$f(\mathbf{PX}, \mathbf{PAP}^\top) = \mathbf{P}f(\mathbf{X}, \mathbf{A})$$

Locality on graphs: **neighbourhoods**

- On **sets**, we enforced equivariance by applying functions to every node **in isolation**

- **Graphs** give us a broader context: a node's **neighbourhood**
    - For a node *i*, its (1-hop) neighbourhood is commonly defined as follows:

$$\mathcal{N}_i = \{j : (i,j) \in \mathcal{E} \vee (j,i) \in \mathcal{E}\}$$

N.B. we do not explicitly consider *directed* edges, and often we assume $i \in N_i$

- Accordingly, we can extract the *multiset* of **features** in the neighbourhood

$$\mathbf{X}_{\mathcal{N}_i} = \{\{\mathbf{x}_j : j \in \mathcal{N}_i\}\}$$

and define a *local* function, g, as operating over this multiset: $g(\mathbf{x}_i, \mathbf{X}_{N_i})$.

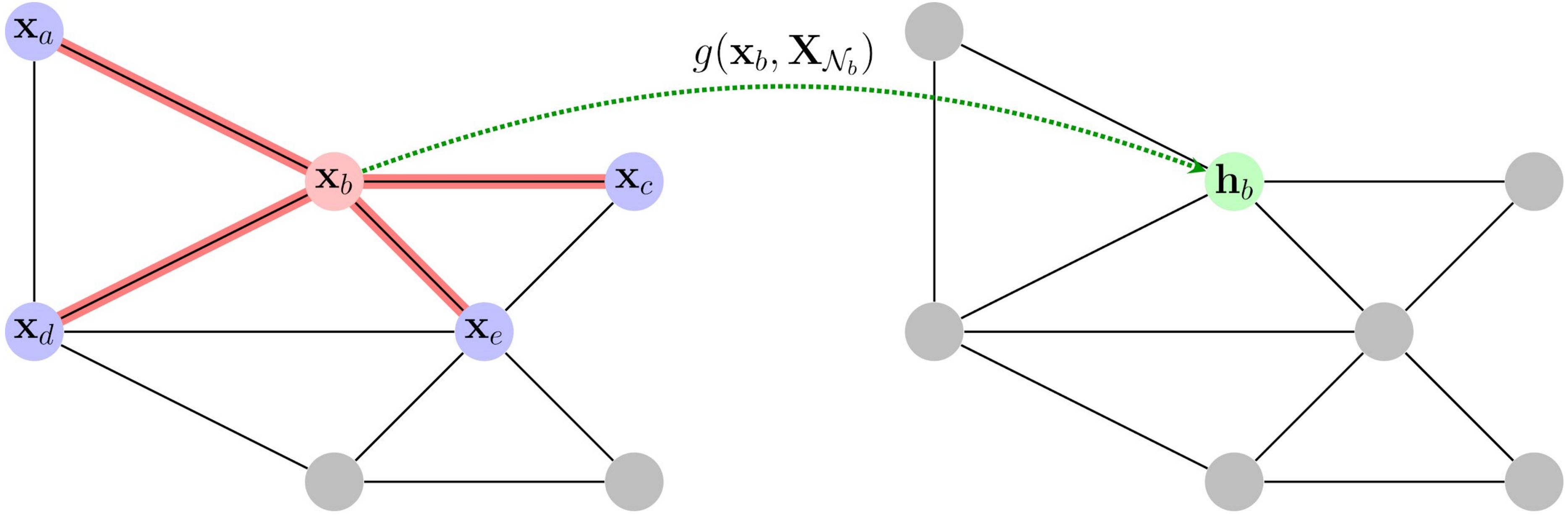
A recipe for **graph** neural networks

- Now we can construct permutation equivariant functions, f(**X, A**), by appropriately applying the local function, g, over *all* neighbourhoods:

$$f(\mathbf{X}, \mathbf{A}) = \begin{bmatrix} — & g(\mathbf{x}_1, \mathbf{X}_{\mathcal{N}_1}) & — \\ — & g(\mathbf{x}_2, \mathbf{X}_{\mathcal{N}_2}) & — \\ & \vdots & \\ — & g(\mathbf{x}_n, \mathbf{X}_{\mathcal{N}_n}) & — \end{bmatrix}$$

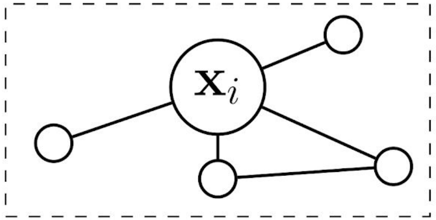
- To ensure equivariance, we need g to not depend on the **order** of the vertices in $\mathbf{X}_{\mathrm{N}i}$
  - Hence, g should be permutation **invariant**!

A recipe for **graph** neural networks, visualised



$$\mathbf{X}_{\mathcal{N}_b} = \{\!\{\mathbf{x}_a, \mathbf{x}_b, \mathbf{x}_c, \mathbf{x}_d, \mathbf{x}_e\}\!\}$$

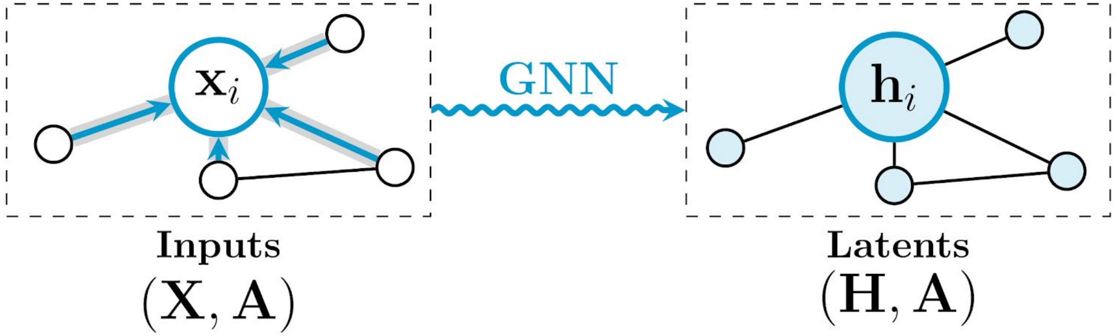
How to use GNNs?



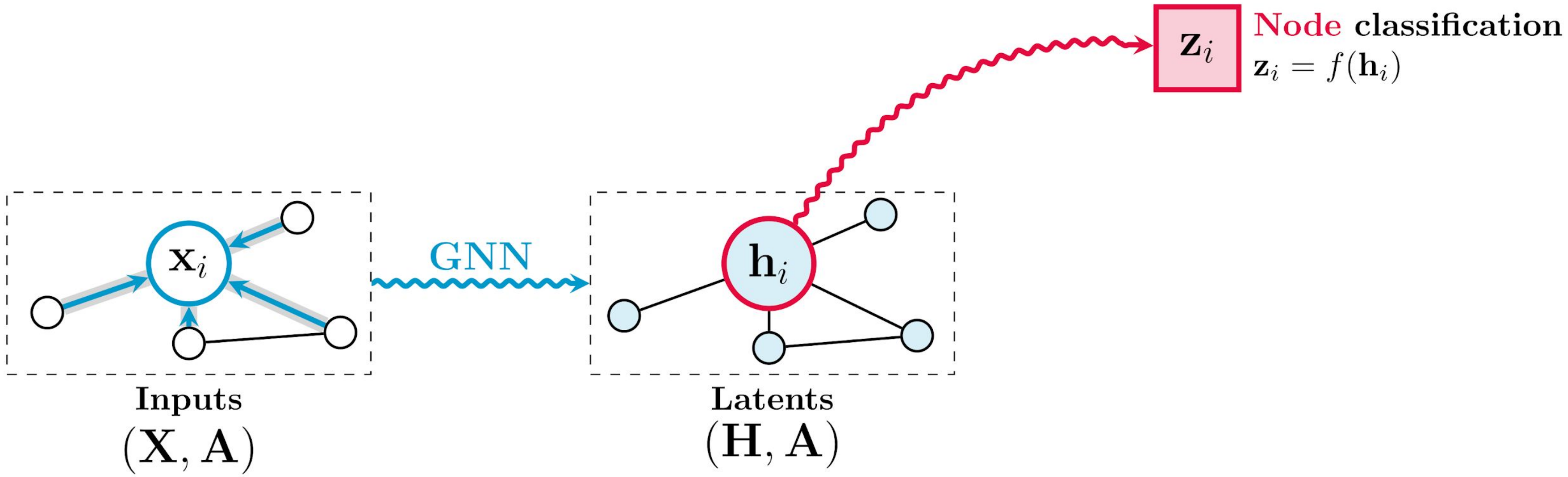
Inputs

$(\mathbf{X}, \mathbf{A})$

How to use GNNs?

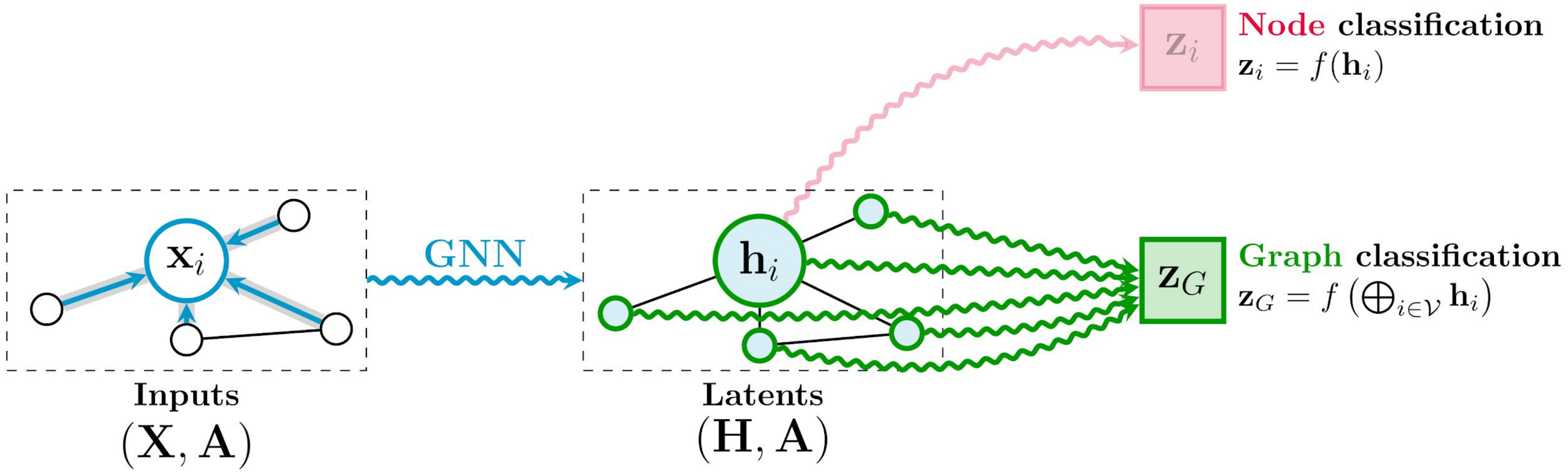


How to use GNNs?

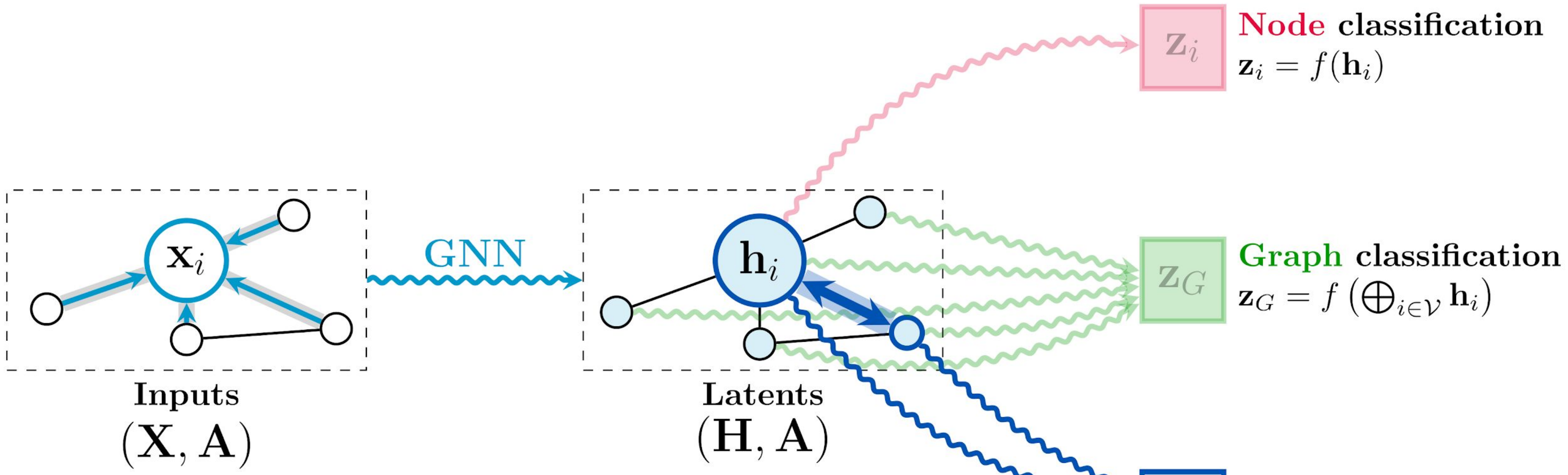


$\mathbf{x}_i$
GNN
$\mathbf{h}_i$
$\mathbf{z}_i$
Node classification
$\mathbf{z}_i = f(\mathbf{h}_i)$
Inputs
$(\mathbf{X}, \mathbf{A})$
Latents
$(\mathbf{H}, \mathbf{A})$

How to use GNNs?


$\mathbf{x}_i$
GNN
$\mathbf{h}_i$
Inputs
$(\mathbf{X}, \mathbf{A})$
Latents
$(\mathbf{H}, \mathbf{A})$
$\mathbf{z}_i$
Node classification
$\mathbf{z}_i = f(\mathbf{h}_i)$
$\mathbf{z}_G$
Graph classification
$\mathbf{z}_G = f\left(\bigoplus_{i \in \mathcal{V}} \mathbf{h}_i\right)$

How to use GNNs?


$\mathbf{z}_i$
Node classification
$\mathbf{z}_i = f(\mathbf{h}_i)$
$\mathbf{x}_i$
GNN
$\mathbf{h}_i$
$\mathbf{z}_G$
Graph classification
$\mathbf{z}_G = f\left(\bigoplus_{i \in \mathcal{V}} \mathbf{h}_i\right)$
Inputs
$(\mathbf{X}, \mathbf{A})$
Latents
$(\mathbf{H}, \mathbf{A})$
$\mathbf{z}_{ij}$
Link prediction
$\mathbf{z}_{ij} = f(\mathbf{h}_i, \mathbf{h}_j, \mathbf{e}_{ij})$

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6 Message passing on graphs

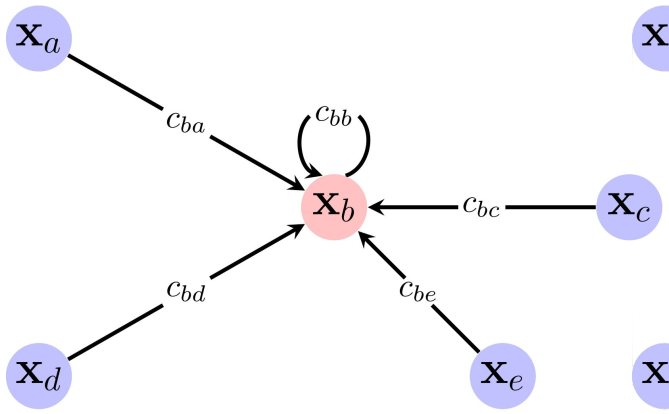
What's in a GNN layer?

- As mentioned, we construct permutation-equivariant functions $f(\mathbf{X}, \mathbf{A})$ over graphs by shared application of a local permutation-invariant $g(\mathbf{x}_i, \mathbf{X}_{\mathcal{N}_i})$.
    - We often refer to f as "GNN layer", g as "diffusion", "propagation", "message passing"

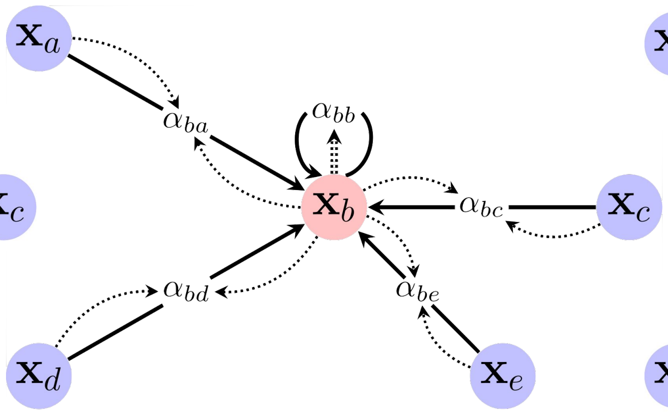
- Now we look at ways in which we can actually concretely **define** g.
    - **Very intense** area of research!

- Fortunately, *almost all* proposed layers can be classified as one of three ***spatial*** "*flavours*".

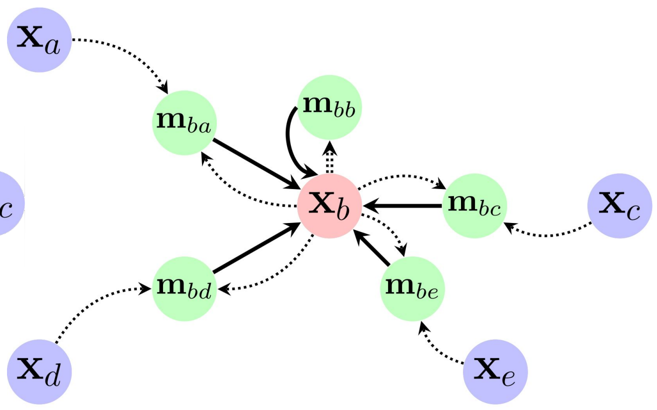
The three "flavours" of GNN layers



Convolutional



Attentional



Message-passing

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

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

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

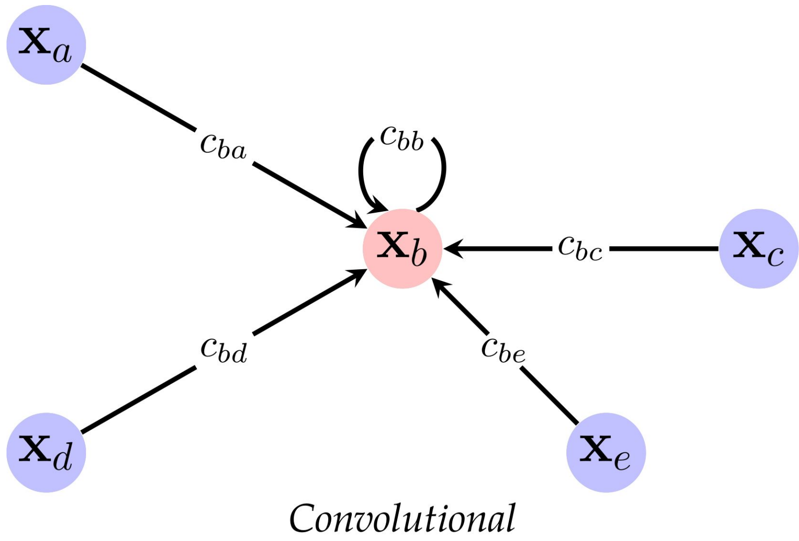
Convolutional GNN

- Features of neighbours aggregated with fixed weights, c_{ij}

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

- Usually, the weights depend directly on **A**.
  - ChebyNet (Defferrard *et al.*, NeurIPS'16)
  - GCN (Kipf & Welling, ICLR'17)
  - SGC (Wu *et al.*, ICML'19)

- Useful for **homophilous** graphs and **scaling up**
  - When edges encode *label similarity*



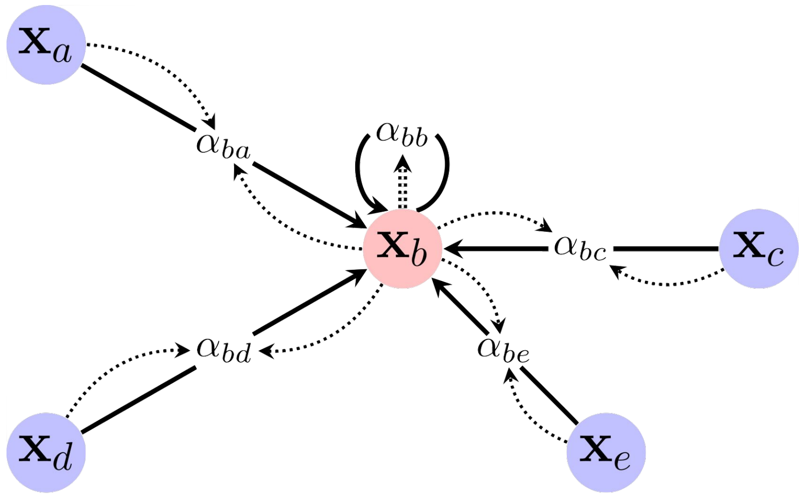
Attentional GNN

- Features of neighbours aggregated with **implicit** weights (via *attention*)

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

- Attention weight computed as $\alpha_{ij} = a(\mathbf{x}_i, \mathbf{x}_j)$
  - MoNet (Monti *et al.*, CVPR'17)
  - GAT (Veličković *et al.*, ICLR'18)
  - GaAN (Zhang *et al.*, UAI'18)

- Useful as "middle ground" w.r.t. **capacity** and **scale**
  - Edges need not encode homophily
  - But still compute *scalar* value in each edge



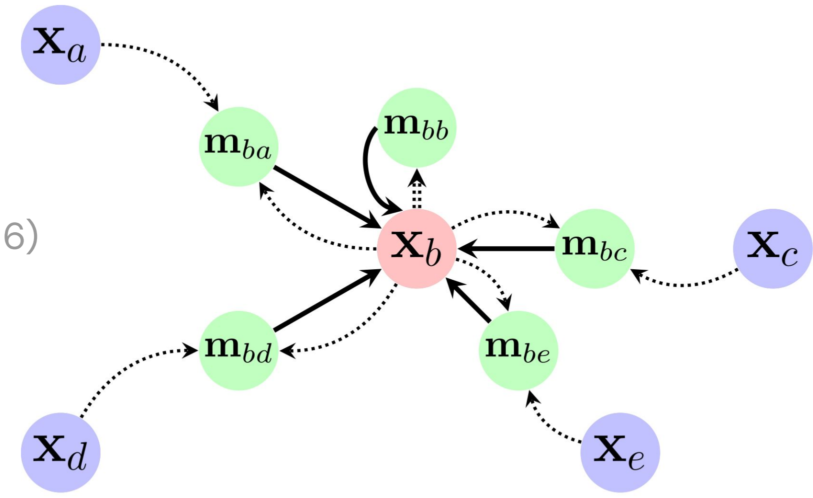
Attentional

Message-passing GNN

- Compute **arbitrary vectors** (*"messages"*) to be sent across edges

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

- Messages computed as $\mathbf{m}_{ij} = \psi(\mathbf{x}_i, \mathbf{x}_j)$
  - Interaction Networks (Battaglia *et al.*, NeurIPS'16)
  - MPNN (Gilmer *et al.*, ICML'17)
  - GraphNets (Battaglia *et al.*, 2018)



Message-passing

- Most **generic** GNN layer
  - May have *scalability* or *learnability* issues
  - Ideal for *computational chemistry*, *reasoning* and *simulation*

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7 Perspectives on GNNs

This framework looks quite clean, *but*...

- We didn't ***start*** researching GNNs from a blueprint like this.
- Graphs naturally arise **across** the sciences
    - Different disciplines found different tools to process them
- To give you a feel of the scale of diversity, I will now **survey** several prior and concurrent approaches to graph representation learning + to what extent they map to this blueprint.
- If you've read up on graph machine learning before, there's a good chance you will have seen at least some of these.

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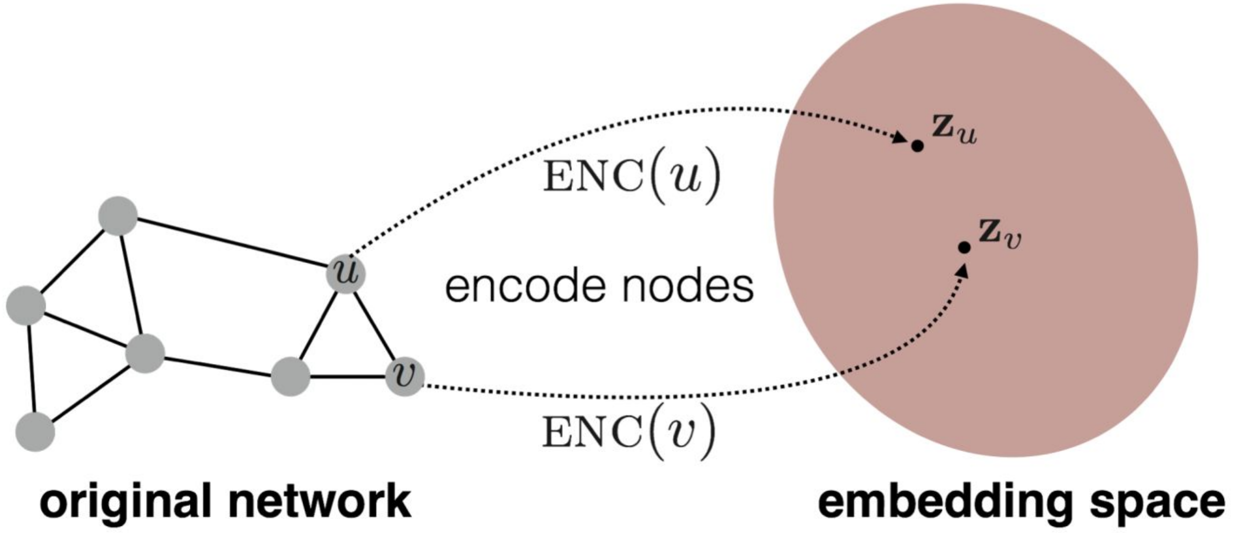
I Node embedding techniques

Node embedding techniques

- Some of the earliest "successes" of deep learning on graphs relied on finding good ways to **embed** nodes into vectors $\mathbf{h}_u$ (below: $\mathbf{z}_u$) using an *encoder function*
  - At the time, implemented as a **look-up table**!



Credits to **Will Hamilton**

What's in a *good* representation?

- What makes an embedding "good"?
  - Graphs carry interesting **structure**!
  - Good node representations should **preserve** it.

- Simplest notion of graph structure is an *edge*.
  - Features of nodes *i* and *j* should be predictive of existence of edge (*i*, *j*)!

- Yields a straightforward unsupervised objective
  - Optimise $\mathbf{h}_i$ and $\mathbf{h}_j$ to be **nearby** iff $(i, j) \in E$.
  - Can use standard *binary cross-entropy* loss:

$$\sum_{(i,j)\in E} \log \sigma\left(\mathbf{h}_i^\top \mathbf{h}_j\right) + \sum_{(i,j)\notin E} \log\left(1 - \sigma\left(\mathbf{h}_i^\top \mathbf{h}_j\right)\right)$$

Random-walk objectives

- This link-prediction objective is a special case of **random-walk** objectives.

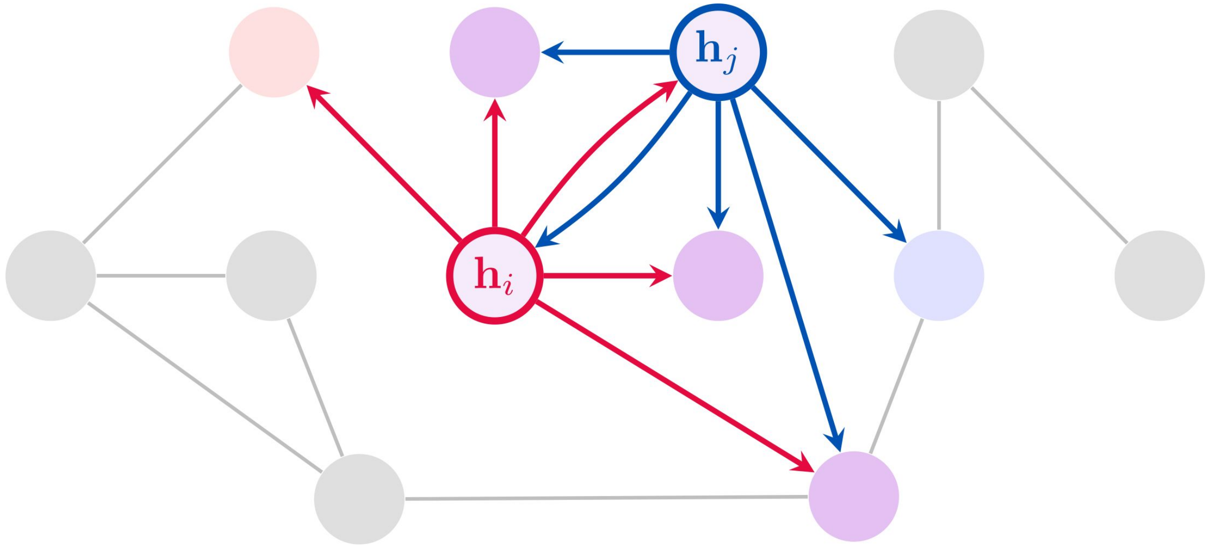
- **Redefine** the condition from $(i, j) \in E$ to *i* and *j* co-occur in a (short) random walk.

- Dominated unsupervised graph representation learning prior to GNNs!
    - DeepWalk (Perozzi *et al.*, KDD'14)
    - node2vec (Grover & Leskovec, KDD'16)
    - LINE (Tang *et al.*, WWW'15)

Local objectives **emulate** Conv-GNNs

- Random walk objectives inherently capture **local** similarities.

- But a (convolutional) GNN *summarises local patches* of the graph!
  - Neighbouring nodes tend to highly overlap in *n*-step neighbourhoods;
  - Therefore, a conv-GNN enforces similar features for neighbouring nodes **by design**.



Local objectives **emulate** Conv-GNNs

- Random walk objectives inherently capture **local** similarities.

- But a (convolutional) GNN *summarises local patches* of the graph!
  - Neighbouring nodes tend to highly overlap in *n*-step neighbourhoods;
  - Therefore, a conv-GNN enforces similar features for neighbouring nodes **by design**.

- From a representation perspective, DeepWalk-style models **emulate** a convolutional GNN!

- **Corollary 1:** Random-walk objectives can **fail** to provide useful signal to GNNs!
- **Corollary 2:** At times, DeepWalk can be matched by an **untrained conv-GNN**!
  - First spotted within DGI (Veličković *et al.*, ICLR'19)
  - Independently verified by SGC (Wu *et al.*, ICML'19)

Parallels to NLP

- Note clear **correspondence** between *node embedding* techniques and **word embedding** techniques in NLP
    - nodes ~ words
    - random walks ~ sentences
    - “node2vec” ~ “word2vec”
    - The optimisation objectives are *near-equal*!

- This correspondence continues even nowadays, with recent unsupervised graph representation learning techniques borrowing concepts from BERT.

  (**“Strategies for pre-training graph neural networks”**; Hu, Liu *et al.*, ICLR’20)

- Speaking of NLP...

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II Natural Language Processing

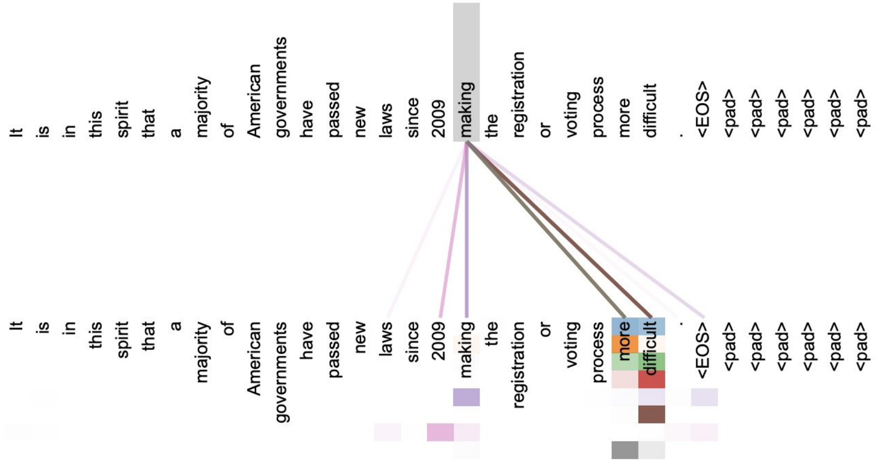
Parallels from NLP

- It’s not only that NLP feeds into GNN design…

- Words in a sentence **interact**
  - Nontrivially and **non-sequentially**
  - We may want to use a **graph** over them
  - But *what* is this graph?

- A common assumption is to assume a ***complete* graph**
  - Then let the network *infer* relations

- If you’re at all involved with NLP, this should sound **familiar**…



A note on Transformers

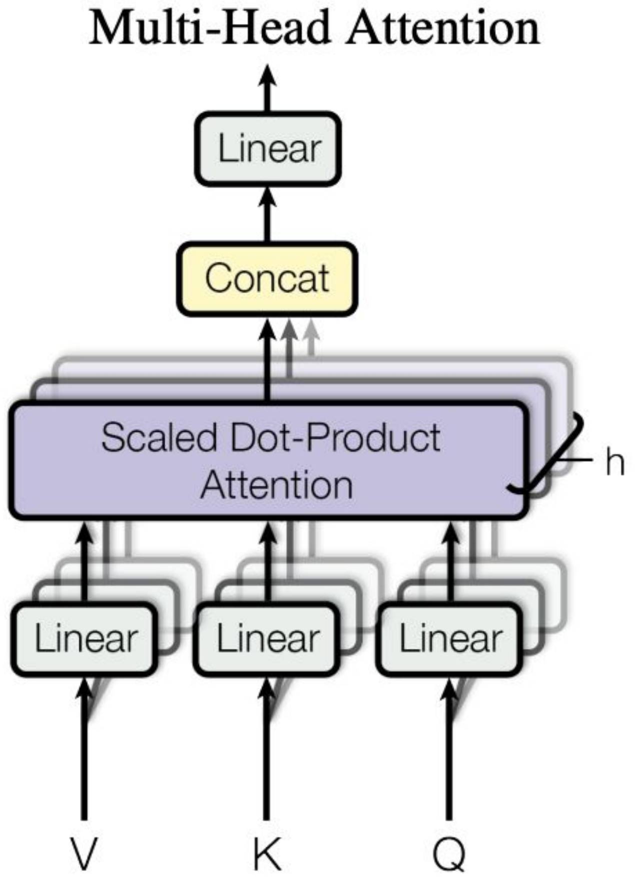
Transformers **are** Graph Neural Networks!

- Fully-connected graph
- Attentional flavour

The sequential structural information is injected through the **positional embeddings**. Dropping them yields a fully-connected GAT model.

Attention can be seen as inferring **soft adjacency**.

See Joshi (The Gradient; 2020).



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III Spectral GNNs

Look to the Fourier transform

- The **convolution theorem** defines a very attractive identity:

$$(x \star y)(\xi) = \hat{x}(\xi) \cdot \hat{y}(\xi) \qquad \hat{x}(\xi) = \int_{-\infty}^{+\infty} x(u) e^{-\mathrm{i}\xi u} du$$

"convolution in the time domain is multiplication in the frequency domain"

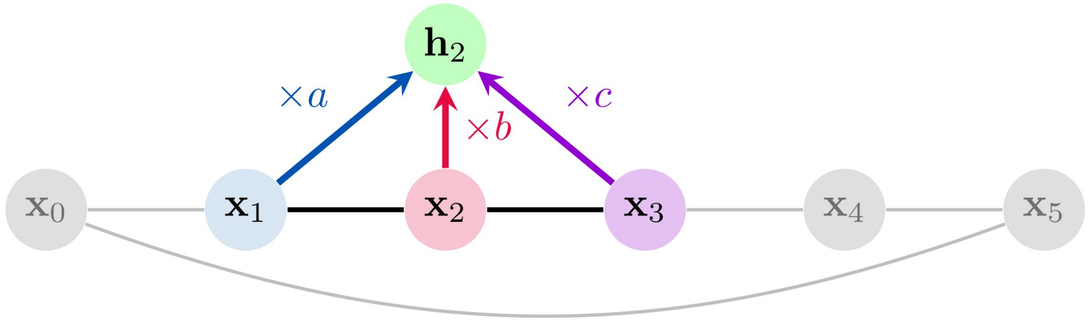
- This could give us a 'detour' to defining convolutions on graphs
  - Pointwise multiplication is **easy**!
  - But what are the 'domains' in this case?

- We will first see how graphs arise in ***discrete*** sequences.

Rethinking the convolution on *sequences*

*for easier handling of boundary conditions

- We can imagine a sequence as a *cyclical **grid** graph*, and a **convolution** over it:



- NB this defines a **circulant** matrix **C**([*b*, *c*, 0, 0, ..., 0, *a*]) s.t. **H** = f(**X**) = **CX**

$$f(\mathbf{X}) = \begin{bmatrix} b & c & & & a \\ a & b & c & & \\ & \ddots & \ddots & \ddots & \\ & & a & b & c \\ c & & & a & b \end{bmatrix} \begin{bmatrix} — & \mathbf{x}_0 & — \\ — & \mathbf{x}_1 & — \\ & \vdots & \\ — & \mathbf{x}_{n-2} & — \\ — & \mathbf{x}_{n-1} & — \end{bmatrix}$$

Properties of circulants, and their eigenvectors

- Circulant matrices **commute**!
  - That is, **C**(**v**)**C**(**w**) = **C**(**w**)**C**(**v**), for *any* parameter vectors **v**, **w**.

- Matrices that commute are **jointly diagonalisable**.
  - That is, the eigenvectors of one are eigenvectors of *all* of them!

- Conveniently, the eigenvectors of circulants are the *discrete Fourier basis*

$$\phi_\ell = \frac{1}{\sqrt{n}}\left(1, e^{\frac{2\pi \mathrm{i}\ell}{n}}, e^{\frac{4\pi \mathrm{i}\ell}{n}}, \ldots, e^{\frac{2\pi \mathrm{i}(n-1)\ell}{n}}\right)^\top, \qquad \ell = 0, 1, \ldots, n-1$$

- This can be easily computed by studying **C**([0, 1, 0, 0, 0, ...]), which is the **shift** matrix.

The DFT and the convolution theorem

- If we stack these Fourier basis vectors into a matrix: $\mathbf{\Phi} = (\phi_0, \dots, \phi_{n-1})$
  - We recover the *discrete Fourier transform* (DFT), as multiplication by $\mathbf{\Phi}^*$. (conjugate transpose)

- We can now eigendecompose *any* circulant as $\mathbf{C}(\boldsymbol{\theta}) = \mathbf{\Phi}\mathbf{\Lambda}\mathbf{\Phi}^*$
  - Where $\mathbf{\Lambda}$ is a diagonal matrix of its eigenvalues, $\hat{\boldsymbol{\theta}}$

- The convolution theorem naturally follows:

$$f(\mathbf{X}) = \mathbf{C}(\boldsymbol{\theta})\mathbf{X} = \mathbf{\Phi}\mathbf{\Lambda}\mathbf{\Phi}^*\mathbf{X} = \mathbf{\Phi}\begin{bmatrix} \hat{\theta}_0 & & \\ & \ddots & \\ & & \hat{\theta}_{n-1} \end{bmatrix}\mathbf{\Phi}^*\mathbf{X} = \mathbf{\Phi}(\hat{\boldsymbol{\theta}} \circ \hat{\mathbf{X}})$$

- Now, as long as we know $\mathbf{\Phi}$, we can express our convolution using $\hat{\boldsymbol{\theta}}$ rather than $\boldsymbol{\theta}$

What we have covered so far

Spatial

$$\begin{tikzcd}
\mathbf{X} \arrow[r, "\text{Circulant matrix}", "\mathbf{C}(\theta)"'] \arrow[d, "\text{DFT}"', "\mathbf{\Phi}^*"] & f(\mathbf{X}) \\
\hat{\mathbf{X}} \arrow[r, "\text{Elementwise product}", "\begin{bmatrix} \hat{\theta}_0 & & & \\ & \hat{\theta}_1 & & \\ & & \ddots & \\ & & & \hat{\theta}_{n-1} \end{bmatrix}"'] & \widehat{f(\mathbf{X})} \arrow[u, "\mathbf{\Phi}", "\text{IDFT}"']
\end{tikzcd}$$

Spectral

Key idea: we don't **need** to know the circulant if we know its eigenvalues!

Credits to **Michael Bronstein**

What about *graphs*?

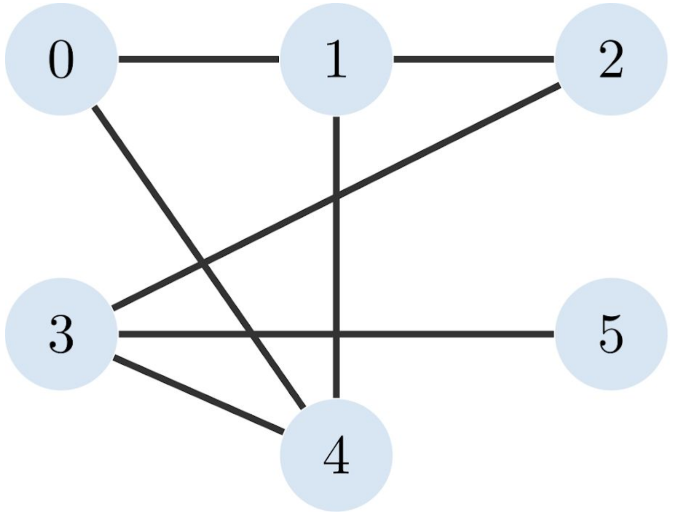
- On graphs, convolutions of interest need to be more generic than circulants.
    - But we can still use the concept of **joint eigenbases**!
    - If we know a "graph Fourier basis", $\mathbf{\Phi}$, we can only focus on learning the eigenvalues.

- For grids, we wanted our convolutions to commute with *shifts*.
    - We can think of the shift matrix as an **adjacency matrix** of the grid
    - This generalises to non-grids!
    - For the grid convolution on n nodes, $\mathbf{\Phi}$ was always the same (n-way DFT).
    - Now **every graph** will have its own $\mathbf{\Phi}$!

- Want our convolution to commute with **A**, but we cannot always eigendecompose **A**!

- Instead, use the **graph Laplacian matrix**, $\mathbf{L} = \mathbf{D} - \mathbf{A}$, where **D** is the degree matrix.
    - Captures all adjacency properties in mathematically convenient way!

Example Laplacian



$$\mathbf{L} = \begin{bmatrix} 2 & -1 & 0 & 0 & -1 & 0 \\ -1 & 3 & -1 & 0 & -1 & 0 \\ 0 & -1 & 2 & -1 & 0 & 0 \\ 0 & 0 & -1 & 3 & -1 & -1 \\ -1 & -1 & 0 & -1 & 3 & 0 \\ 0 & 0 & 0 & -1 & 0 & 1 \end{bmatrix}$$

Graph Fourier Transform

- Assuming undirected graphs, **L** is:
  - **Symmetric** ($\mathbf{L}^T = \mathbf{L}$)
  - **Positive semi-definite** ($\mathbf{x}^T\mathbf{L}\mathbf{x} \geq 0$ for all $\mathbf{x} \in \mathbb{R}^{|V|}$)
  - This means we will be able to *eigendecompose* it!

- This allows us to re-express $\mathbf{L} = \mathbf{\Phi}\mathbf{\Lambda}\mathbf{\Phi}^*$, as before.
  - Changing the eigenvalues in $\mathbf{\Lambda}$ expresses ***any*** operation that commutes with **L**.
  - Commonly referred to as the **graph Fourier transform** (Bruna *et al.*, ICLR'14)

- Now, to convolve with some feature matrix **X**, do as follows (the diagonal can be ***learnable***):

$$f(\mathbf{X}) = \mathbf{\Phi} \begin{bmatrix} \hat{\theta}_0 & & \\ & \ddots & \\ & & \hat{\theta}_{n-1} \end{bmatrix} \mathbf{\Phi}^* \mathbf{X}$$

Spectral GNNs in practice

- However, directly learning the eigenvalues is typically inappropriate:
  - Not **localised**, doesn't **generalise** to other graphs, computationally **expensive**, etc.

- Instead, a common solution is to make the eigenvalues related to $\mathbf{\Lambda}$, the eigenvalues of **L**
  - Commonly by a degree-*k* polynomial function, p_k
  - Yielding $f(\mathbf{x}) = \mathbf{\Phi} p_k(\mathbf{\Lambda})\mathbf{\Phi}^*\mathbf{x} = p_k(\boldsymbol{L})\mathbf{x}$
  - Popular choices include:
    - *Cubic splines* (Bruna *et al.*, ICLR'14)
    - *Chebyshev polynomials* (Defferrard *et al.*, NeurIPS'16)
    - *Cayley polynomials* (Levie *et al.*, Trans. Sig. Proc.'18)

- **NB** by using a polynomial in **L**, we have defined a **conv-GNN**!
  - With coefficients defined by $c_{ij} = (p_k(\mathbf{L}))_{ij}$
  - Most efficient spectral approaches "*spatialise*" themselves in similar ways
  - The "spatial-spectral" divide is often ***not really a divide***!

The Transformer positional encodings and beyond

- Lastly, another look at Transformers.

- Transformers signal that the input is a **sequence** of words by using *positional embeddings*
  - Sines/cosines sampled depending on position

$$PE_{(pos,2i)} = sin(pos/10000^{2i/d_{\text{model}}})$$
$$PE_{(pos,2i+1)} = cos(pos/10000^{2i/d_{\text{model}}})$$

- **Very** similar to the DFT eigenvectors!

- Positional embeddings could hence be interpreted as eigenvectors of the grid graph
  - Which is the only assumed 'underlying' connectivity between the words

- We can use this idea to run Transformers over *general* graph structures!
  - Just feed some eigenvectors of the graph Laplacian (columns of $\mathbf{\Phi}$)
  - See the ***Graph Transformer*** from Dwivedi & Bresson (2021)

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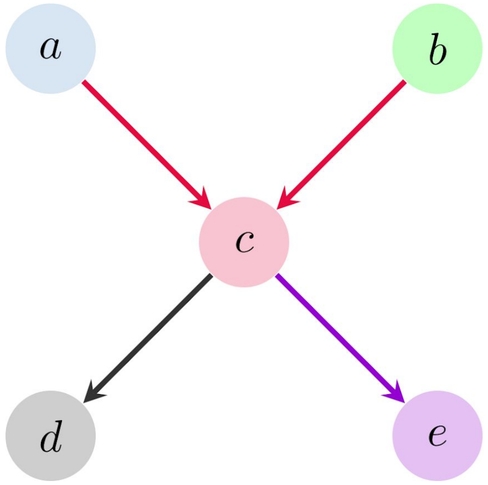
IV Probabilistic Graphical Models

Probabilistic modelling

- We've so far used edges in a graph to mean any kind of relation between nodes

- Taking a more **probabilistic** view, we can treat nodes as *random variables*, and interpret edges as *dependencies* between their distributions.
    - This gives rise to **probabilistic graphical models** (PGMs)
    - They help us *ignore* relations between variables when computing **joint** probabilities



$$p(a, b, c, d, e) = p(a)p(b)p(c|a, b)p(d|c)p(e|c)$$

Markov random fields

- One particular PGM of interest here is the *Markov random field* (**MRF**).
    - It allows us to decompose the joint into a product of *edge potentials*

- Specifically, we assume nodes are represented by inputs **X** and latents **H**
    - Inputs and latents are related for every node in isolation
    - Latents are related according to the edges of the graph

- This yields the following decomposition of the joint

$$p(\mathbf{X}, \mathbf{H}) \propto \prod_{u \in \mathcal{V}} \Phi(\mathbf{x}_u, \mathbf{h}_u) \prod_{(u,v) \in \mathcal{E}} \Psi(\mathbf{h}_u, \mathbf{h}_v)$$

where $\mathbf{\Phi}$ and $\mathbf{\Psi}$ are real-valued *potential functions*.

Mean-field inference

- To embed nodes, we need to sample from the *posterior*, p(**H** | **X**).
    - Generally *intractable*, even if we know the exact potential functions.

- One popular method of resolving this is ***mean-field*** *variational inference*
    - Assume that posterior can be approximated by a product of node-level densities

$$p(\mathbf{H}|\mathbf{X}) \approx \prod_{u \in \mathcal{V}} q(\mathbf{h}_u)$$

where *q* is a well-defined density, that is easy to compute and sample (e.g. Gaussian).

- We then obtain the parameters of *q* by minimising the distance (e.g. KL-divergence) to the true posterior, KL($\mathbf{\Pi}_u$ q($\mathbf{h}_u$) || p(**H** | **X**))

- Minimising the KL is intractable, but it admits a favourable approximate algorithm

GNNs strike again!

- Using variational inference techniques (out of scope), we can *iteratively* update *q*, starting from some initial guess $q^{(0)}(\mathbf{h})$, as follows:

$$\log q^{(t+1)}(\mathbf{h}_i) = c_i + \log \Phi(\mathbf{x}_i, \mathbf{h}_i) + \sum_{j \in \mathcal{N}_i} \int_{\mathbb{R}^k} q^{(t)}(\mathbf{h}_j) \log \Psi(\mathbf{h}_i, \mathbf{h}_j) \, \mathrm{d}\mathbf{h}_i$$

- See anything familiar? :)

GNNs strike again!

- Using variational inference techniques (out of scope), we can *iteratively* update q, starting from some initial guess $q^{(0)}(\mathbf{h})$, as follows:

$$\boxed{\log} q^{(t+1)}(\mathbf{h}_i) = \boxed{c_i + \log \Phi(\mathbf{x}_i, \mathbf{h}_i) + \boxed{\sum_{j \in \mathcal{N}_i}} \boxed{\int_{\mathbb{R}^k} q^{(t)}(\mathbf{h}_j) \log \Psi(\mathbf{h}_i, \mathbf{h}_j) \, \mathrm{d}\mathbf{h}_i}}$$

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

- This aligns **very nicely** with computations of a (message-passing) GNN!

GNNs and PGMs, more broadly

- Based on this idea, **structure2vec** (Dai *et al.*, ICML'16) embed mean-field inference within computations of a GNN.
  - Key difference: in PGMs, we expect potential functions specified and known upfront
  - Here, they are defined implicitly, within the latents of a GNN.

- The structure2vec GNN itself is not unlike a typical MPNN.

- Recently, there are other approaches that unify GNNs with PGM-like computations:
  - CRF-GNNs (Gao *et al.*, KDD'19)
  - GMNNs (Qu *et al.*, ICML'19)
  - ExpressGNN (Zhang *et al.*, ICLR'20)
  - Tail-GNNs (Spalević *et al.*, ICML'20 GRL+)

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V Graph Isomorphism Testing

How *powerful* are Graph Neural Networks?

- GNNs are a powerful tool for processing real-world graph data
    - But they won't solve ***any*** task specified on a graph accurately!

- Canonical example: deciding *graph isomorphism*
    - Am I able to use my GNN to **distinguish** two *non*-isomorphic graphs? ($\mathbf{h}_{G1} \neq \mathbf{h}_{G2}$)
    - If I can't, any kind of task discriminating them is *hopeless*

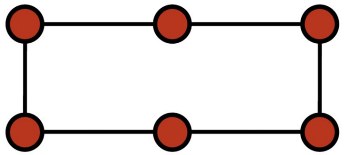
- Permutation invariance mandates that two *isomorphic* graphs will always be indistinguishable, so this case is OK.

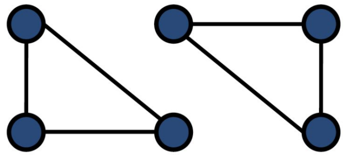
Weisfeiler-Leman Test

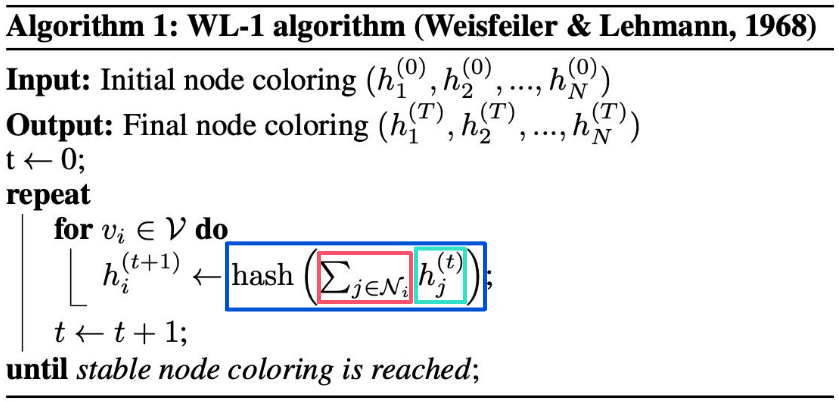
- Simple but powerful way of distinguishing: pass **random hashes** of **sums** along the edges
  - Connection to conv-GNNs spotted very early; e.g. by GCN (Kipf & Welling, ICLR'17)

- It explains why untrained GNNs work well!
  - Untrained ~ random hash

- The test does **fail** at times, however:







Algorithm 1: WL-1 algorithm (Weisfeiler & Lehmann, 1968)

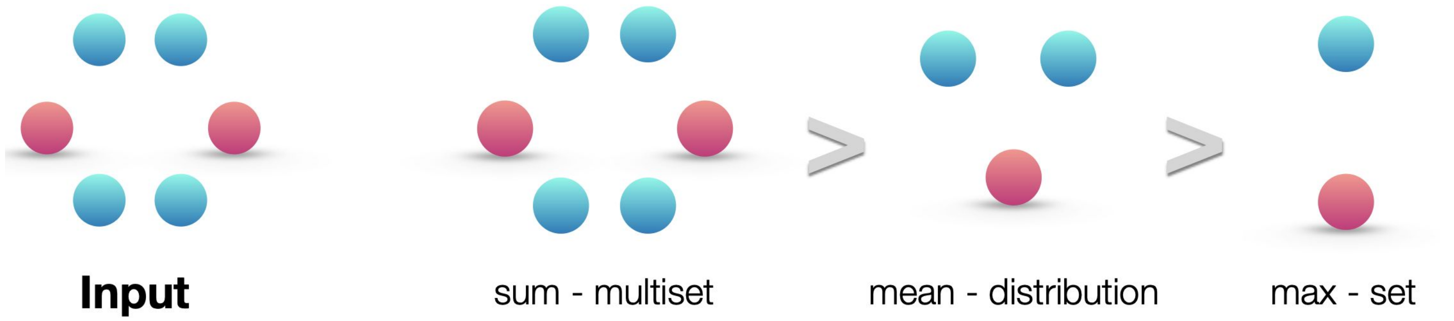
```
Input: Initial node coloring $(h_1^{(0)}, h_2^{(0)}, ..., h_N^{(0)})$
Output: Final node coloring $(h_1^{(T)}, h_2^{(T)}, ..., h_N^{(T)})$
$t \leftarrow 0$;
repeat
    for $v_i \in \mathcal{V}$ do
        $h_i^{(t+1)} \leftarrow \boxed{\text{hash}\left(\boxed{\sum_{j \in \mathcal{N}_i}} \boxed{h_j^{(t)}}\right)}$;
    $t \leftarrow t + 1$;
until stable node coloring is reached;
```

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

GNNs are **no more powerful** than 1-WL

- Over ***discrete*** *features*, GNNs can only be **as powerful** as the 1-WL test described before!

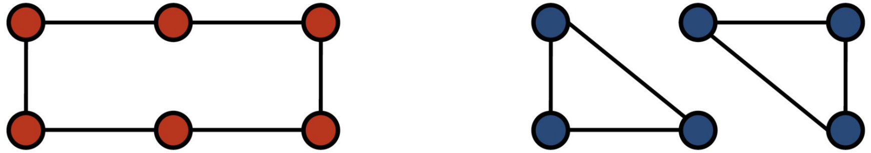
- One important condition for maximal power is an *injective* aggregator (e.g. **sum**)



- Graph isomorphism network (**GIN**; Xu *et al.*, ICLR'19) proposes a simple, maximally-expressive GNN, following this principle

$$h_v^{(k)} = \mathrm{MLP}^{(k)}\left(\left(1+\epsilon^{(k)}\right)\cdot h_v^{(k-1)} + \sum\nolimits_{u\in\mathcal{N}(v)} h_u^{(k-1)}\right)$$

Higher-order GNNs



- We can make GNNs stronger by analysing **failure cases** of 1-WL!

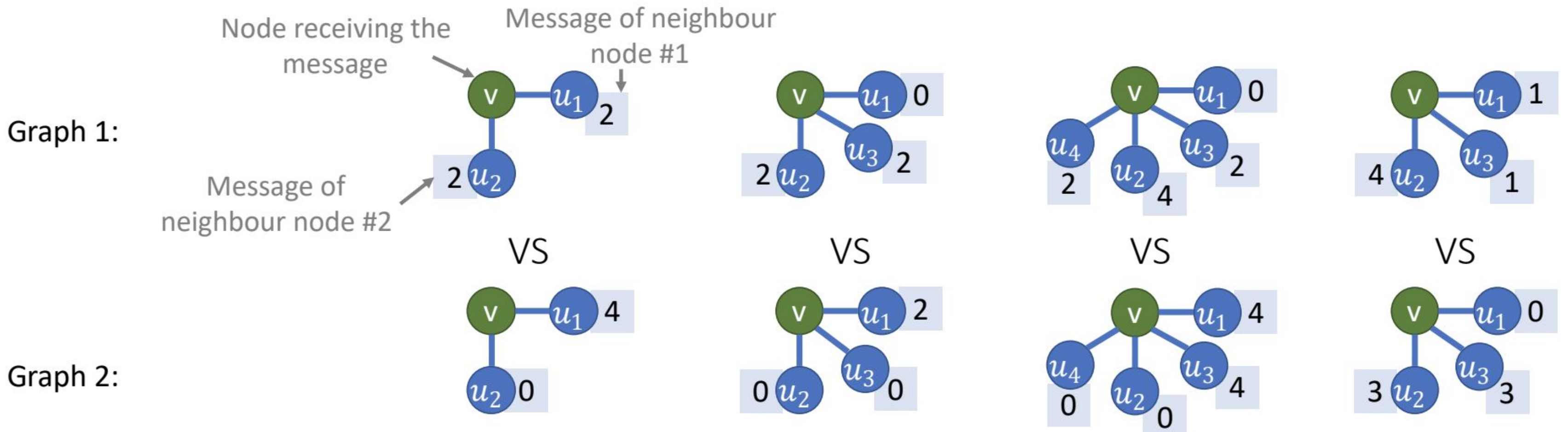
- For example, just like 1-WL, GNNs cannot detect **closed triangles**
    - Augment nodes with randomised/positional features
        - Explored by RP-GNN (Murphy *et al.*, ICML'19) and P-GNN (You *et al.*, ICML'19)
        - See also: Sato *et al.* (SDM'21)
    - Can also literally **count** interesting subgraphs (Bouritsas *et al.*, 2020)

- *k*-WL labels *subgraphs* of *k* nodes together.
    - Exploited by 1-2-3-GNNs (Morris *et al.*, AAAI'19)

- Further avenues of interest:
    - Invariant and equivariant GNNs (Maron *et al.* (ICLR'19))
    - Directional graph networks (DGNs) (Beaini, Passaro *et al.* (2020))

Going beyond *discrete* features

- What happens when features are **continuous**? (real-world apps / latent GNN states)
  - … the proof for injectivity of sum (hence GINs' expressivity) **falls apart**



Node receiving the message
Message of neighbour node #1
Message of neighbour node #2
Graph 1:
Graph 2:
VS
v
u_1
u_2
u_3
u_4

Simple aggregators that can differentiate graph 1 and 2:	Min, Max, STD	Mean	STD	Min, Max
Aggregators that fail:	Mean	Min, Max, STD	Mean, Min, Max	Mean, STD

Which is best? **Neither.**

- There doesn't seem to be a clear single "winner" aggregator here...

- In fact, we prove in the PNA paper (Corso, Cavalleri *et al.*, NeurIPS'20) that **there isn't one**!

Theorem 1 (Number of aggregators needed). *In order to discriminate between multisets of size n whose underlying set is $\mathbb{R}$, at least n aggregators are needed.*

- The proof is (in my opinion) **really cool**! (relies on **Borsuk-Ulam** theorem)

- PNA proposes empirically powerful **combination** of aggregators for general-purpose GNNs:

$$\bigoplus = \underbrace{\begin{bmatrix} I \\ S(D, \alpha = 1) \\ S(D, \alpha = -1) \end{bmatrix}}_{\text{scalers}} \otimes \underbrace{\begin{bmatrix} \mu \\ \sigma \\ \max \\ \min \end{bmatrix}}_{\text{aggregators}}$$

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VI Geometric Deep Learning

Remark on **geometric** deep learning

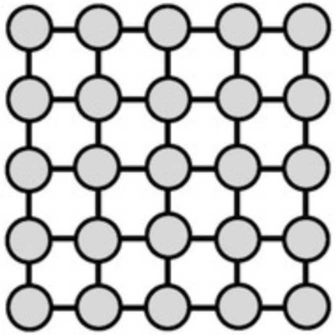
- We used the blueprint of *invariances* and *equivariances* to describe GNNs

- In fact, it is remarkably powerful! By combining an appropriate
    - **Local** and **equivariant** layer specified over *neighbourhoods*
    - Activation functions
    - (Potentially: **pooling** layers that coarsen the structure)
    - **Global** and **invariant** layer over the entire domain

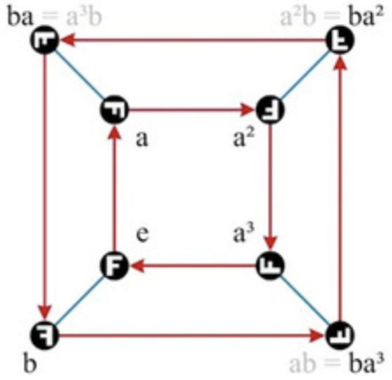
  we recover many standard architectures (including CNNs and Transformers!)

- But also a more general class of **geometric** deep learning architectures

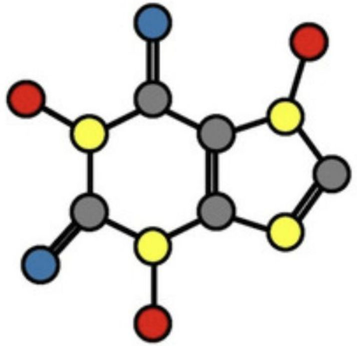
The "Four Gs" of geometric deep learning



Grids



Groups

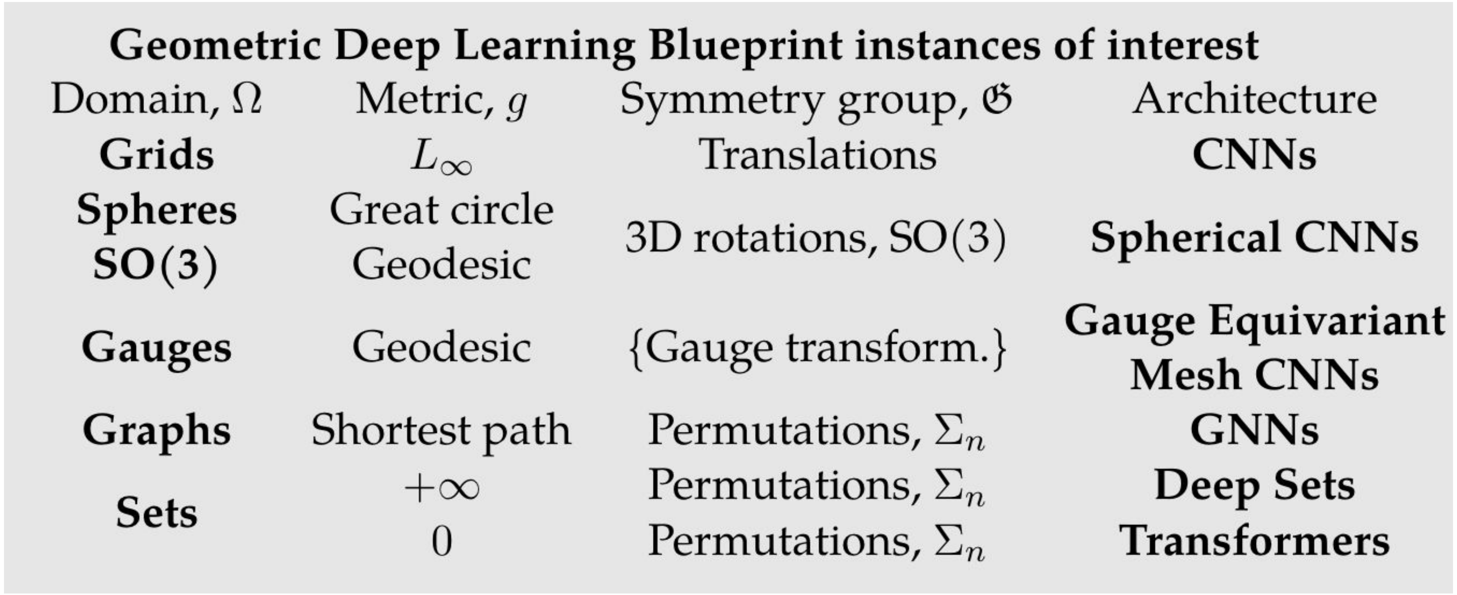


Graphs

"Gauges"

Credits to **Michael Bronstein**

Some architectures of interest



Geometric Deep Learning Blueprint instances of interest

Domain, Ω	Metric, g	Symmetry group, $\mathfrak{G}$	Architecture
Grids	L_∞	Translations	**CNNs**
Spheres	Great circle	3D rotations, $\mathrm{SO}(3)$	**Spherical CNNs**
$\mathbf{SO(3)}$	Geodesic		
Gauges	Geodesic	{Gauge transform.}	**Gauge Equivariant Mesh CNNs**
Graphs	Shortest path	Permutations, Σ_n	**GNNs**
Sets	$+\infty$	Permutations, Σ_n	**Deep Sets**
	0	Permutations, Σ_n	**Transformers**

Credits to **Taco Cohen**

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VII Historical concepts

Where did GNNs come from?

- Early forms can be traced to the **early 1990s**, often involving DAG structures.
    - Labeling RAAM (Sperduti, NeurIPS'94)
    - Backpropagation through structure (Goller & Küchler, ICNN'96)
    - Adaptive structure processing (Sperduti & Starita, TNN'97; Frasconi *et al.*, TNN'98)

- First proper treatment of **generic** graph structure processing happens in the 2000s:
    - The **GNN framework** (Gori *et al.*, IJCNN'05; Scarselli *et al.*, TNN'08)
    - The **NN4G framework** (Micheli, TNN'09)

- The GNN model of Gori, Scarselli *et al.* used primarily *recurrent*-style updates
    - Updated for modern best practices by **gated GNNs** (Li *et al.*, ICLR'16)

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VIII Computational Chemistry

“Chemistry disrupts ML, not the other way around”

- Important and **concurrent** GNN development line came from **computational chemistry**
  - Very relevant to the area, as molecules are naturally modelled as graphs

- GNN-like models of *molecular property prediction* arise, also, in the 1990s
  - Examples include **ChemNet** (Kireev, CICS’95) and (Baskin *et al.*, CICS’97)

- **“Molecular Graph Networks”** (Merkwirth and Lengauer, CIM’05) already propose many elements commonly found in modern MPNNs

- This drive continued well into the 2010s:
  - GNNs for molecular fingerprinting (Duvenaud *et al.*, NeurIPS’15)
  - GNNs for quantum chemistry (Gilmer *et al.*, ICML’17)

- Lastly, recall **(Stokes *et al.*, Cell’20)**: chemistry is to-this-day a **leading** outlet for GNNs!

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Thank you!

Questions?

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