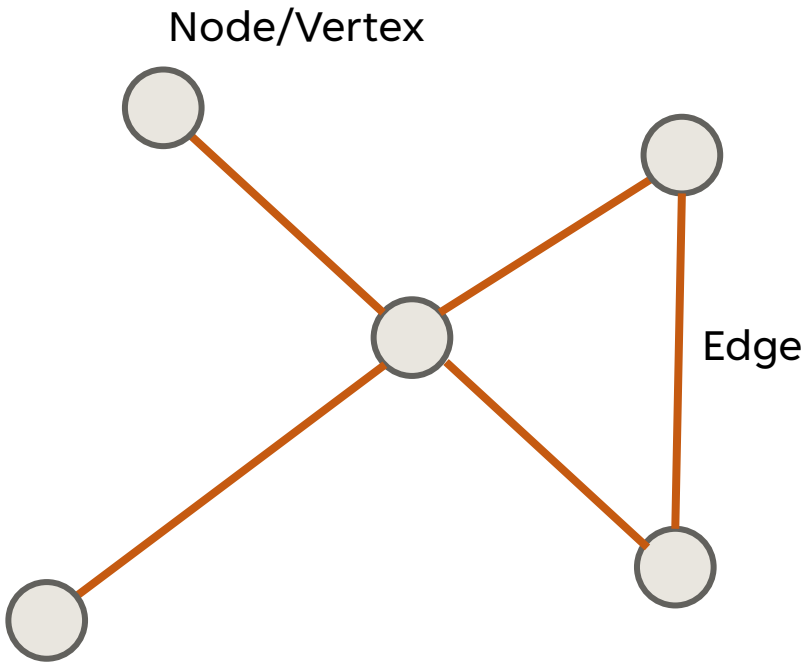
INTRODUCTION TO GRAPH NEURAL NETWORKS

Keith Butler

BEFORE WE START

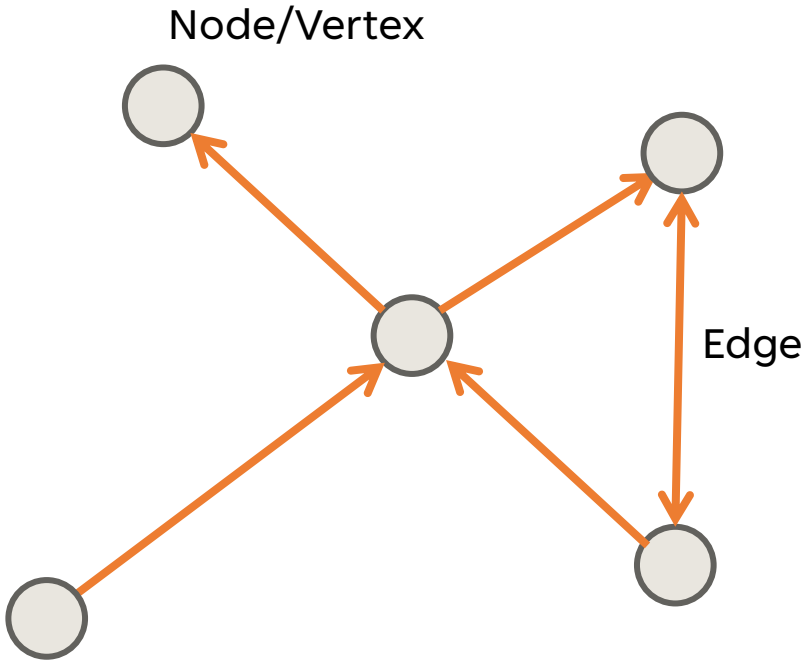
Let’s open up the exercise notebook in colab and put the dependencies loading in the background.

WHAT IS A GRAPH?



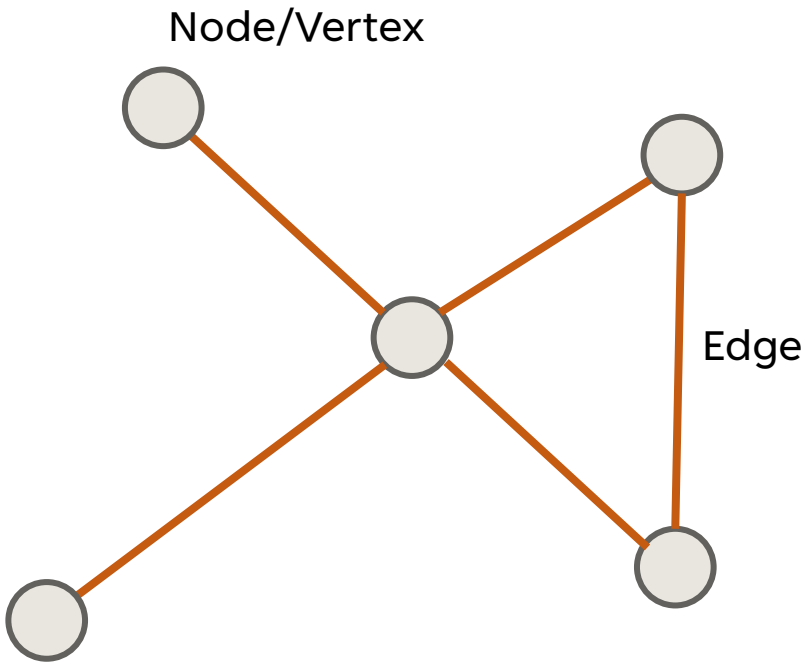
Graphs encode relations between entities.
Nodes have information about the entity.
Edges connect nodes.

WHAT IS A GRAPH?



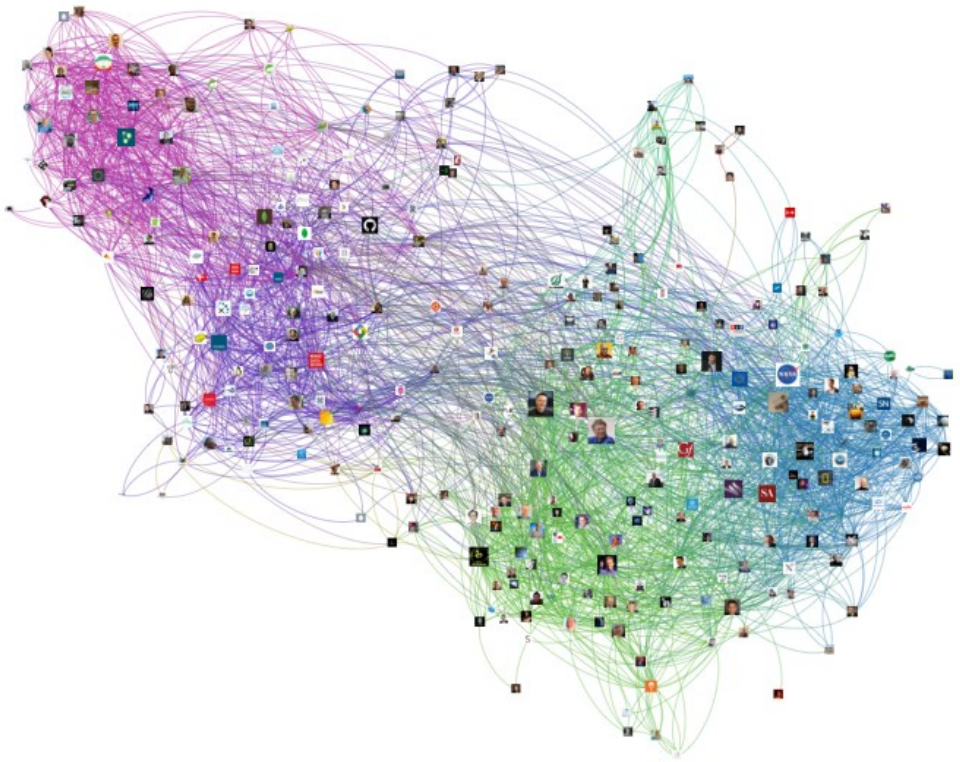
Edges can be directed or undirected.
Meaning that information can flow in either or both directions.

WHAT IS A GRAPH?

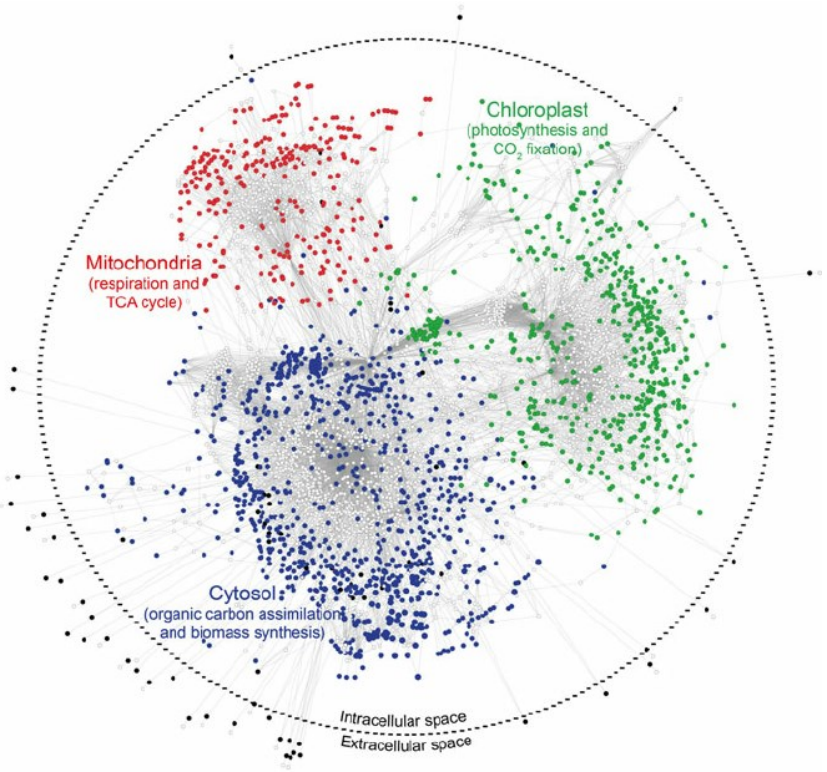


Information is stored in both nodes and edges. Information is stored as embeddings.

WHERE DO WE FIND/USE GRAPHS?

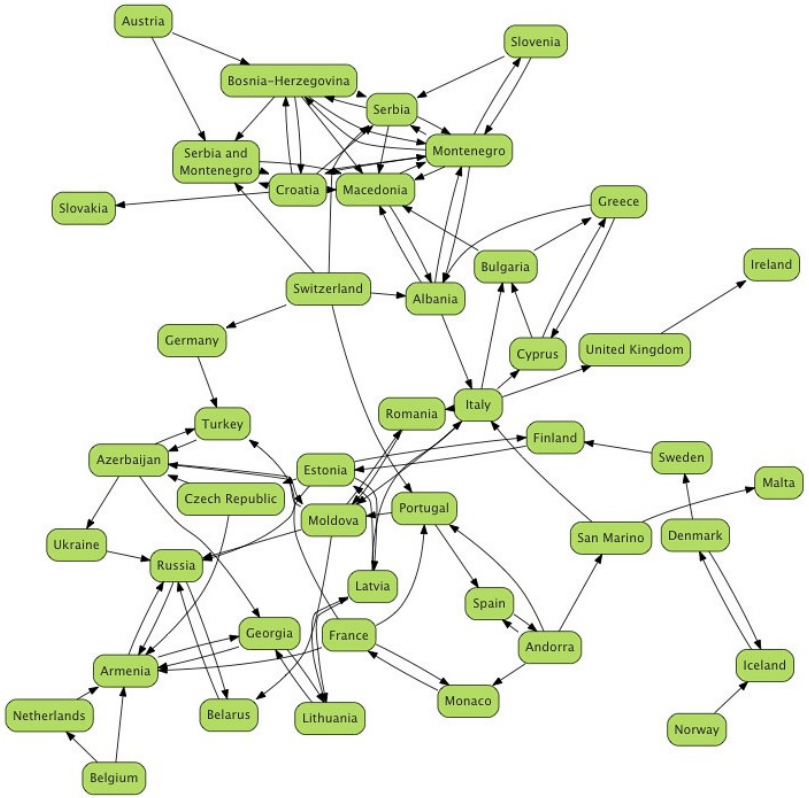


Social networks. >1B nodes; >10B edges

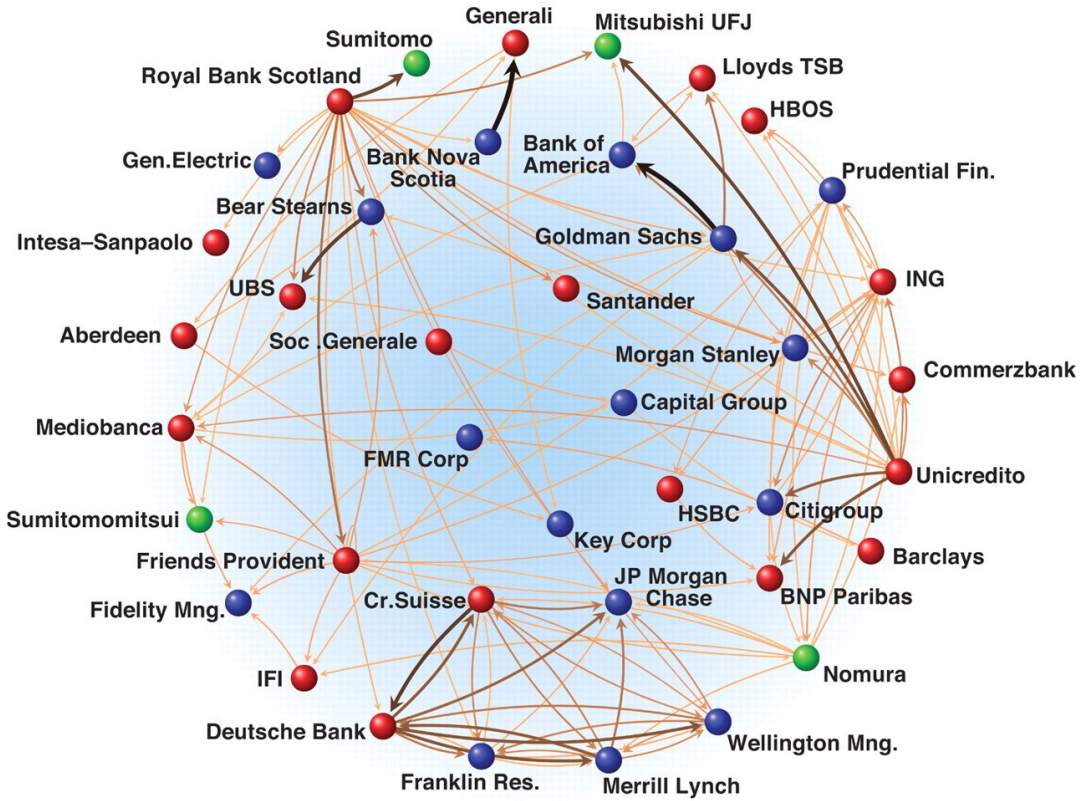


Biological systems

WHERE DO WE FIND/USE GRAPHS?



Eurovision song contest



Economics

AN IMAGE IS A GRAPH WITH REGULAR STRUCTURE

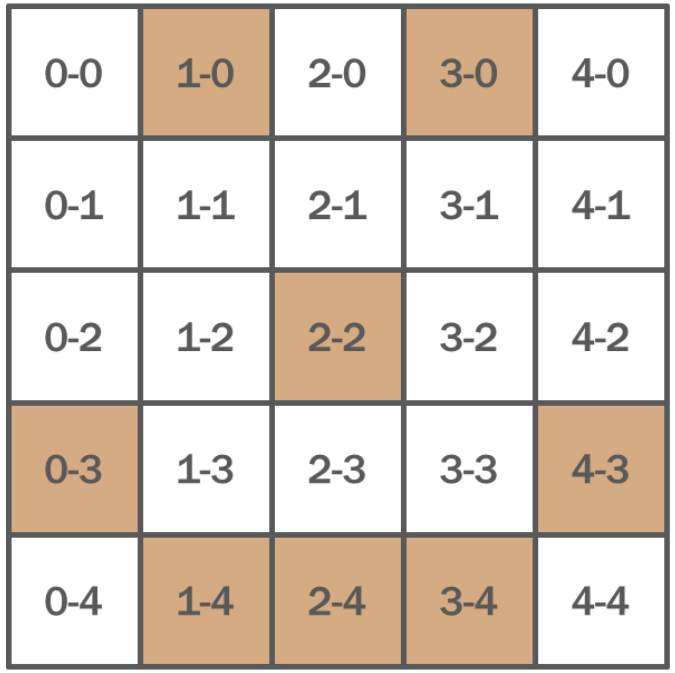
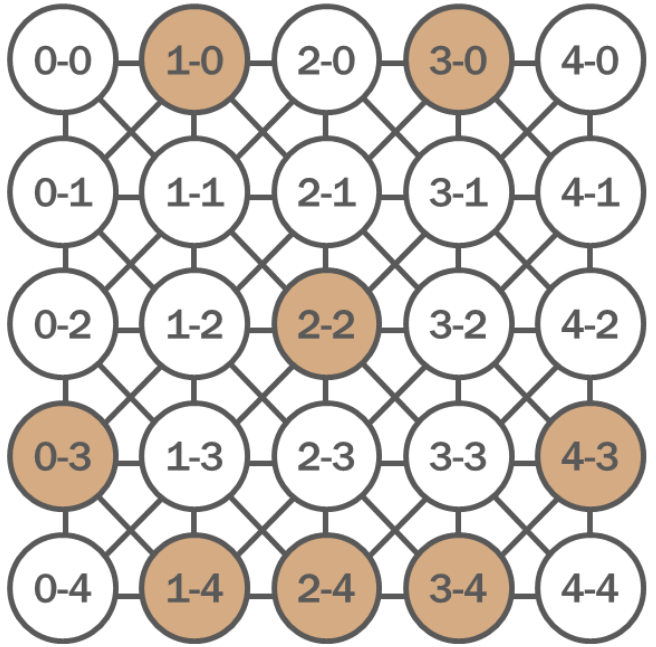
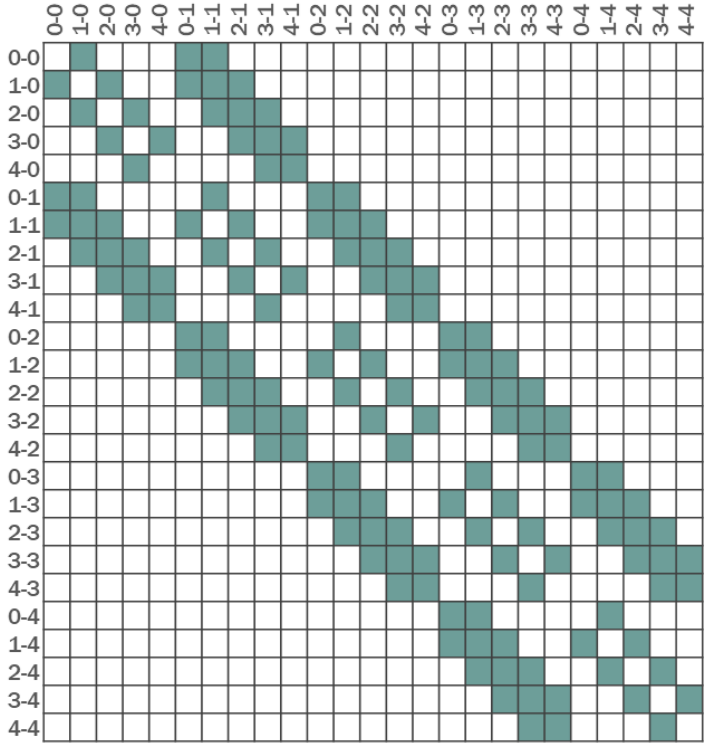


Image pixels

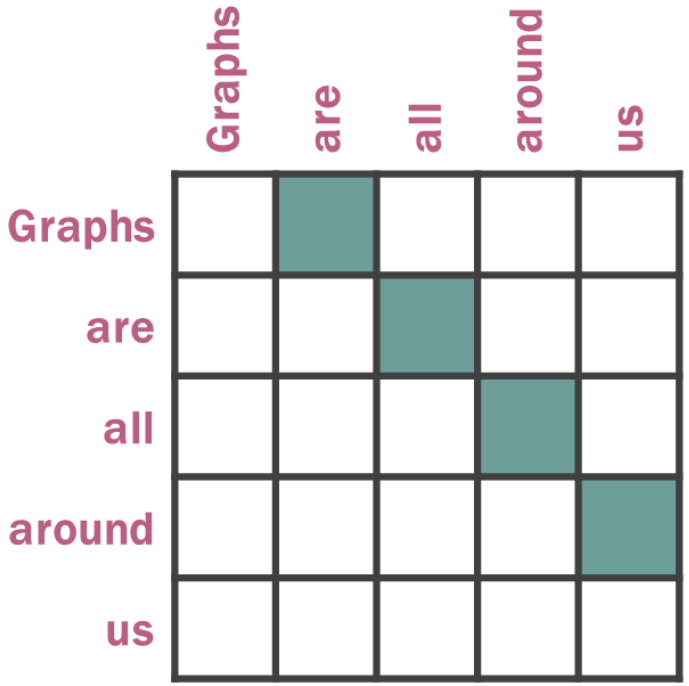


Graph structure

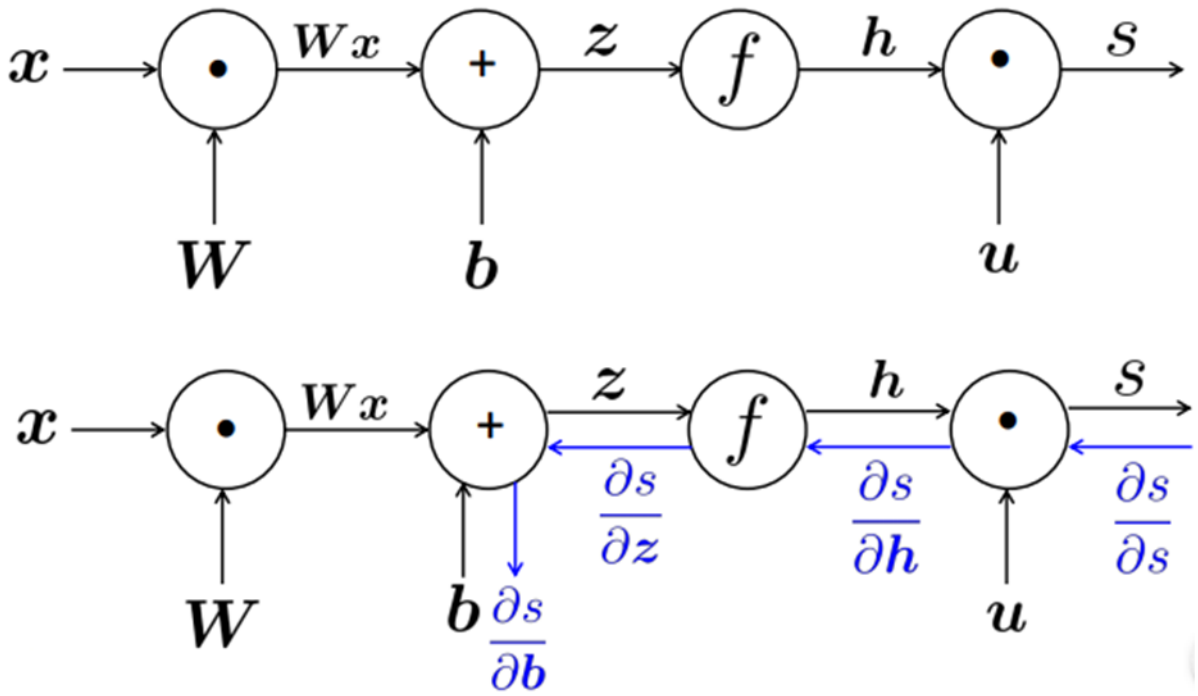


Adjacency matrix

A SENTENCE CAN BE A DIRECTED GRAPH



A NEURAL NETWORK IS A GRAPH



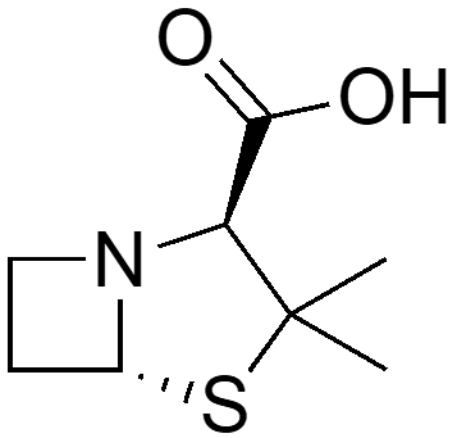
$$s = \boldsymbol{u}^T \boldsymbol{h}$$

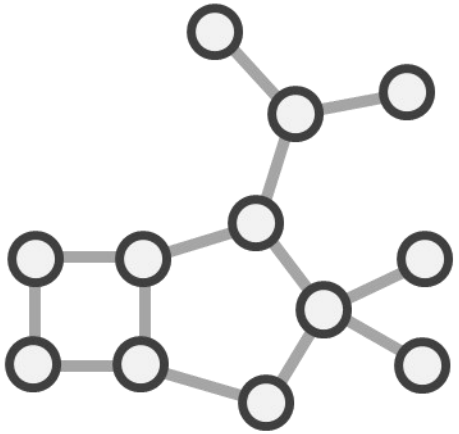
$$\boldsymbol{h} = f(\boldsymbol{z})$$

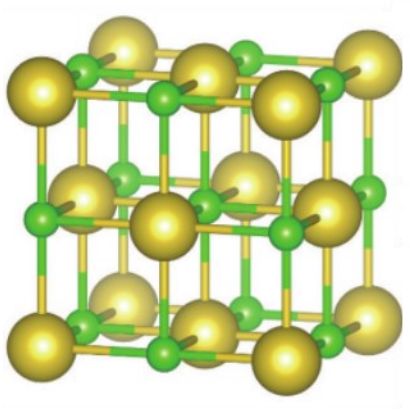
$$\boldsymbol{z} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}$$

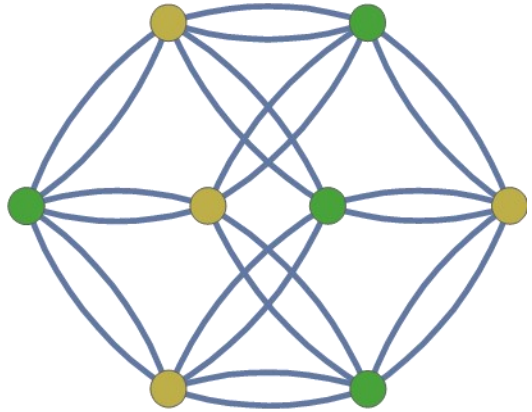
$\boldsymbol{x}$ (input)

GRAPHS ARE A NATURAL REPRESENTATION FOR CHEMISTRY

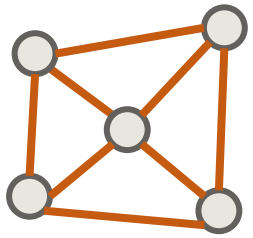




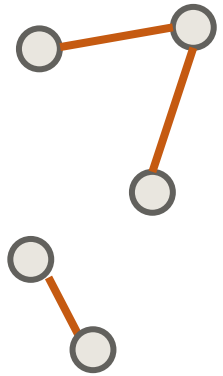




ALL GRAPHS ARE NOT ALIKE



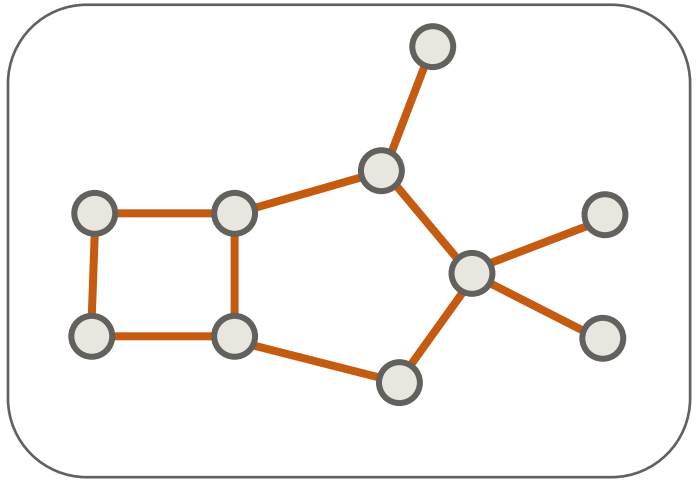
Fully connected



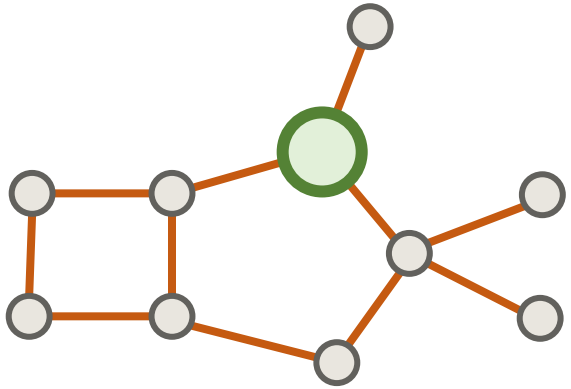
Sparse

Dataset	Graphs	Nodes	Edges
Fully con.	1	5	20
Sparse	2	<4	<3
Wikipedia	1	12M	378M
qm9	134k	<9	<26
Cora	1	23k	91k

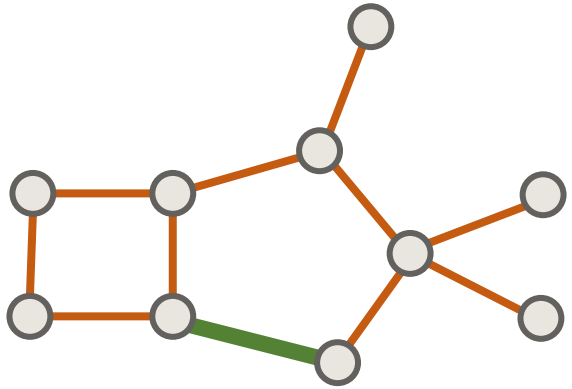
TYPES OF PROPERTIES CALCULATED ON GRAPHS



Graph level e.g. total energy

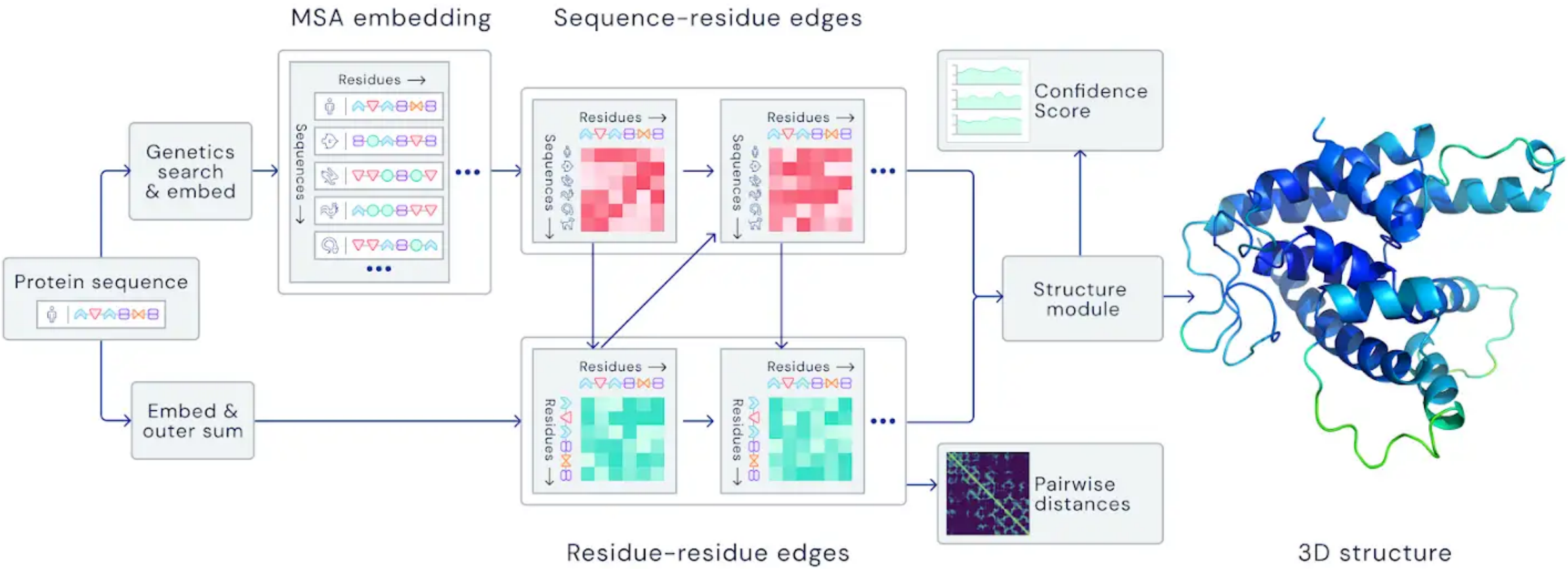


Node level e.g. forces



Edge level e.g. bond order

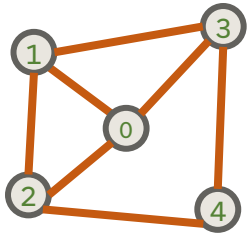
GNNS JUST HELPED WIN A NOBEL PRIZE

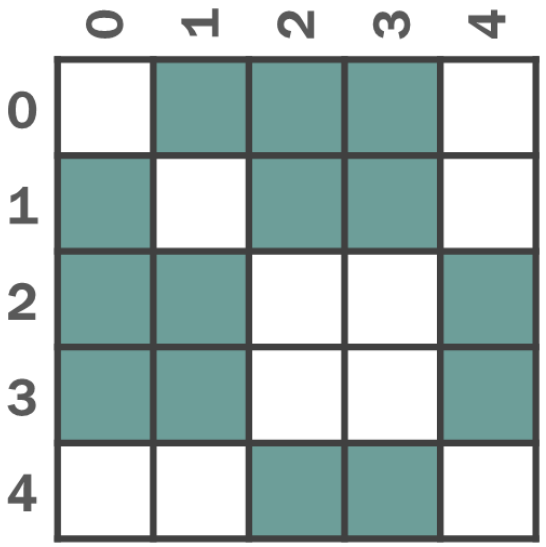


Represent the protein as a graph of amino acids

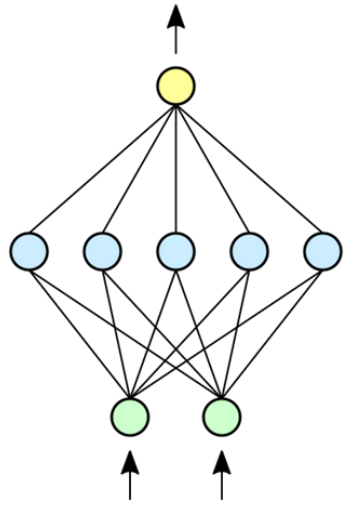
INCLUDING GRAPHS IN DEEP LEARNING

Could directly use the adjacency matrix





$$\begin{bmatrix} 0 & 1 & 1 & 1 & 0 \\ 1 & 0 & 1 & 1 & 0 \\ 1 & 1 & 0 & 0 & 1 \\ 1 & 1 & 0 & 0 & 1 \\ 0 & 0 & 1 & 1 & 0 \end{bmatrix}$$



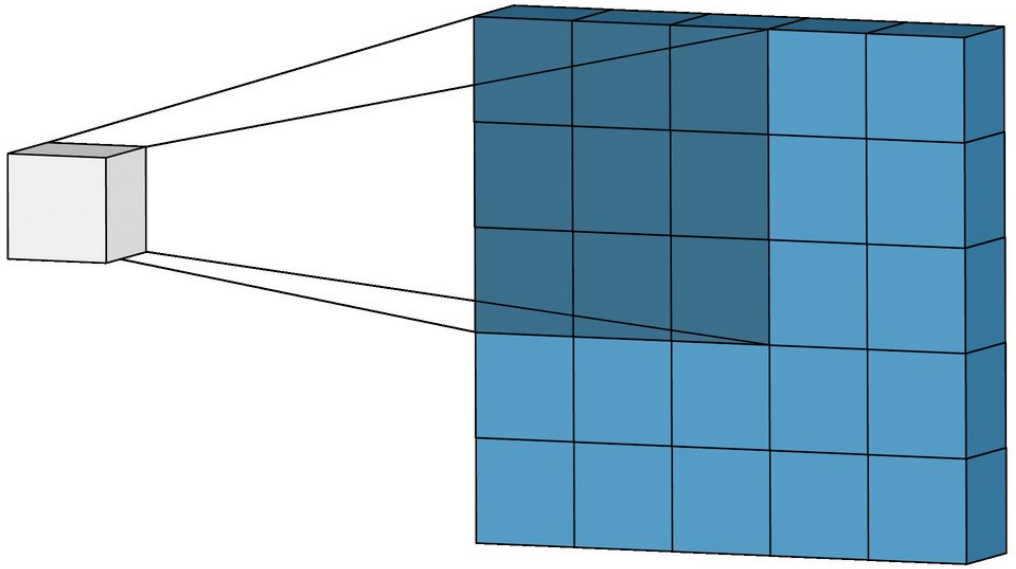
Issues: variable size and order dependency

CONVOLUTIONS FOR GRAPHS

A convolutional neural network (CNN) filter transforms and combines information from neighbouring pixels in an image

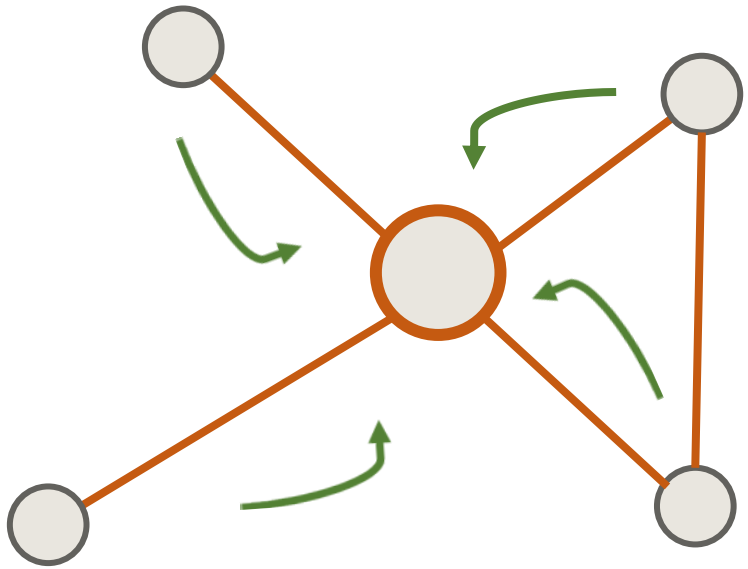
0	−1	0
−1	4	−1
0	−1	0

Convolution filter
learned during training to extract higher level features e.g., edges



CONVOLUTIONS FOR GRAPHS

Images can be seen as a regular graph;
can we extend the concept of convolutions?

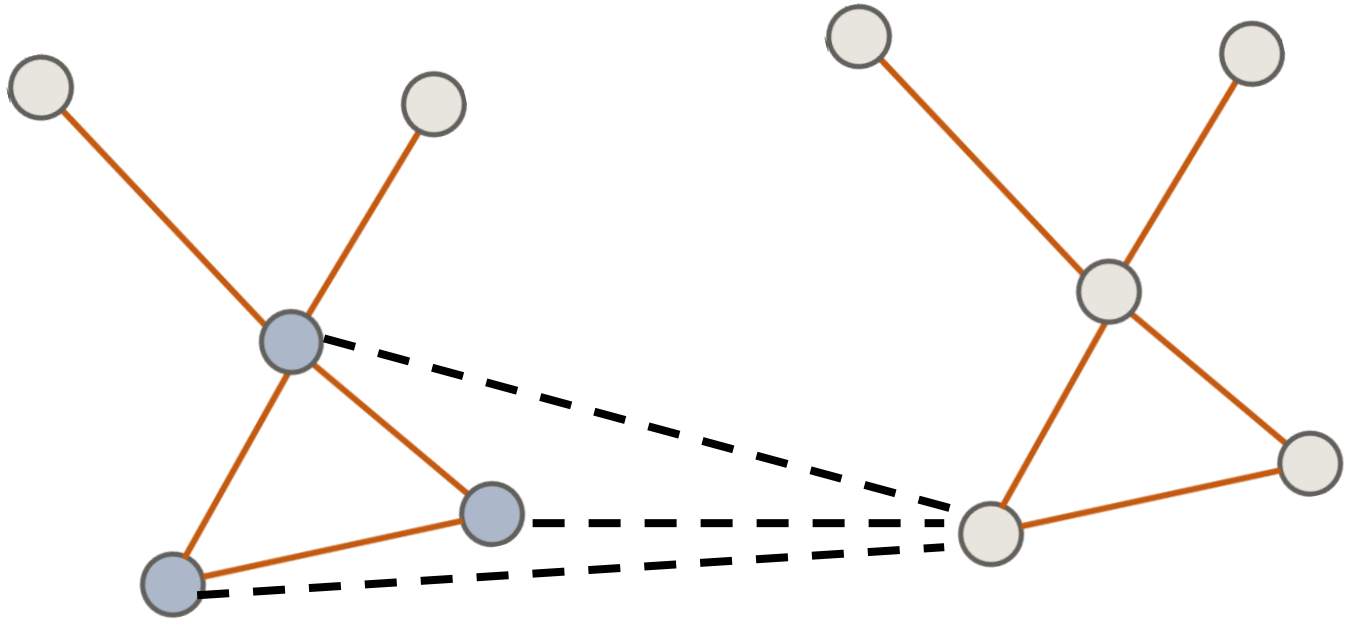


Convolution from neighbour nodes

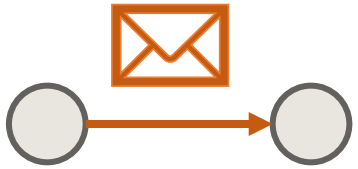
Convolution to centre nodes

CONVOLUTIONS FOR GRAPHS

By iterating over the entire graph each node receives information from its neighbours



WHERE DO NEURAL NETWORKS COME IN?

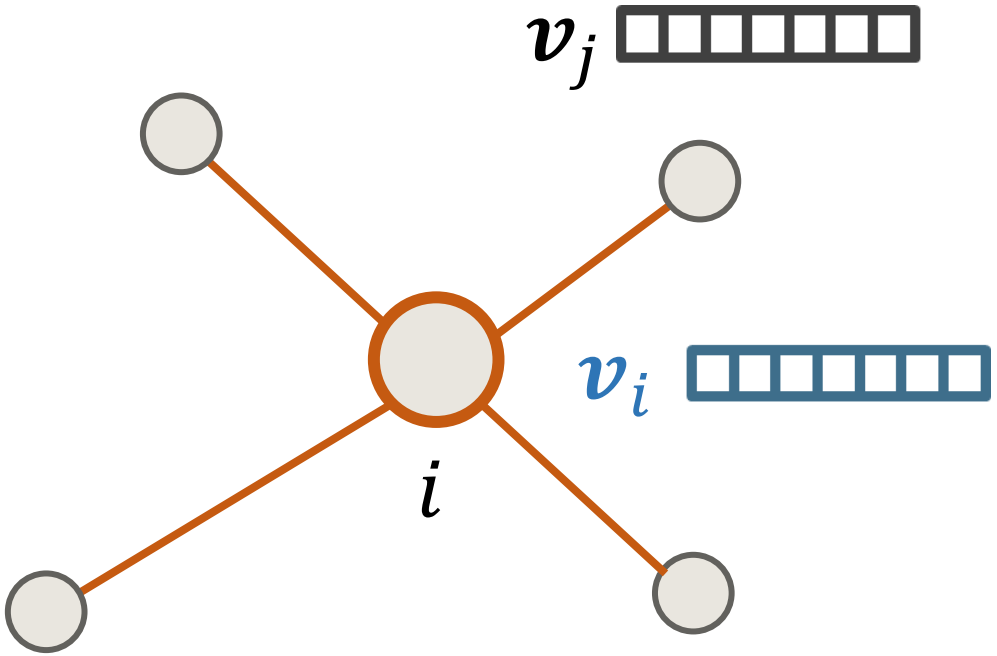


Message passing
What information flows from one node to the next

Message pooling
How neighbouring information is added together

Node updates
How the received information changes the node

HOW THE MESSAGE GETS PASSED



Message passing function

$$m_i = \bigoplus_{j \in \mathcal{N}(i)} M_t(v_i, v_j)$$

Message pooling function

Node update function

$$v_i' = U_t(v_i, m_i)$$

THE FIRST GRAPH CONVOLUTIONAL NETWORKS

SEMI-SUPERVISED CLASSIFICATION WITH GRAPH CONVOLUTIONAL NETWORKS

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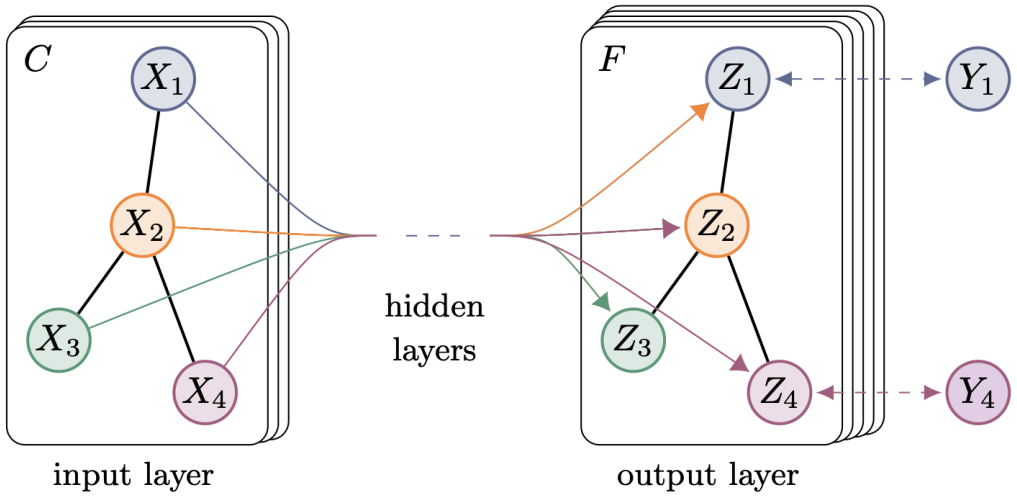
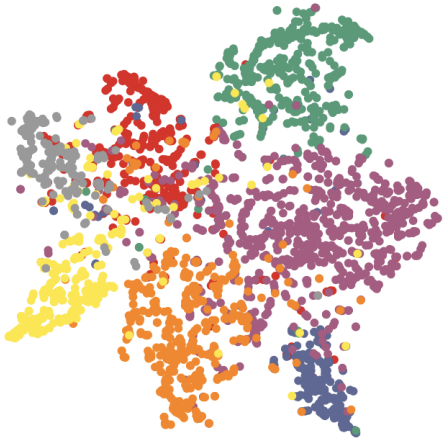


(a) Graph Convolutional Network



(b) Hidden layer activations

IMPLEMENTATION OF A GNN

Message

$$\boldsymbol{v}_j$$

No processing, node vector

Message pooling

$$\boldsymbol{m}_i = \sum_{j \in \mathcal{N}(i)} \frac{\boldsymbol{v}_j}{|\mathcal{N}(i)|}$$

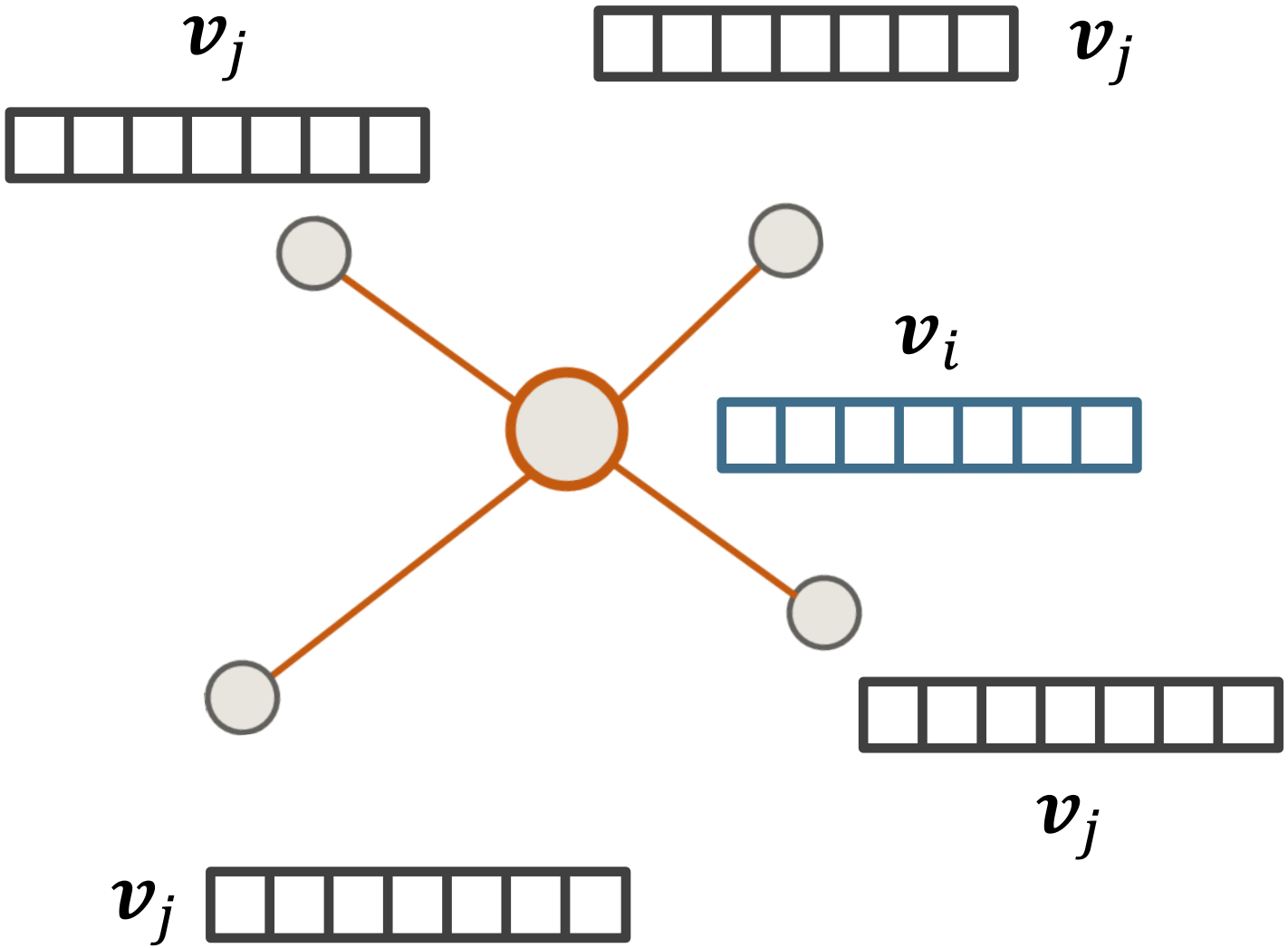
Mean pool across all neighbours

Node update

$$\boldsymbol{v}_i' = \sigma(\mathbf{W}\boldsymbol{m}_i + \mathbf{B}\boldsymbol{v}_i)$$

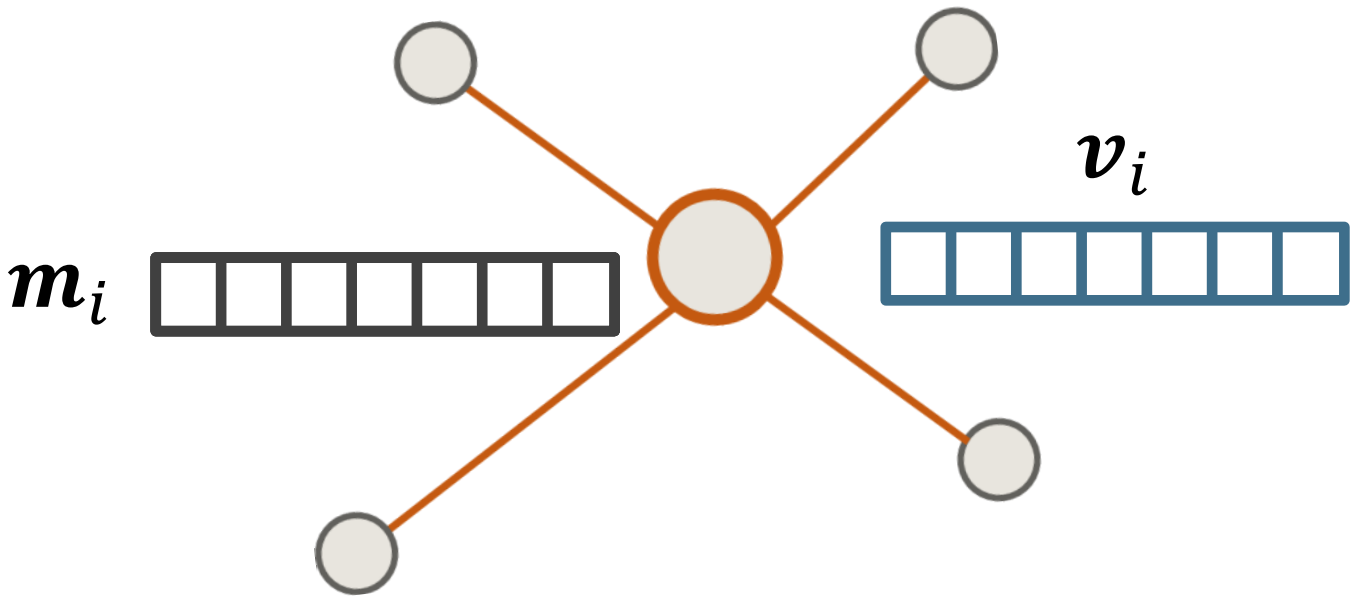
Parameterized lernable function - MLP

VISUALISATION OF A GNN CONVOLUTION



1. Prepare messages

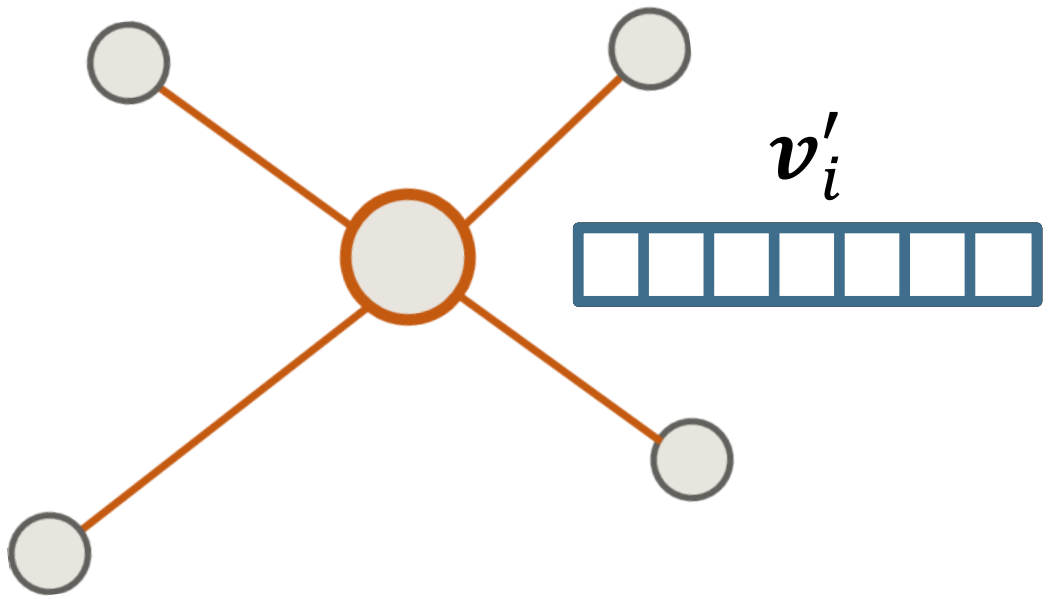
VISUALISATION OF A GNN CONVOLUTION



1. Prepare messages

2. Pool messages

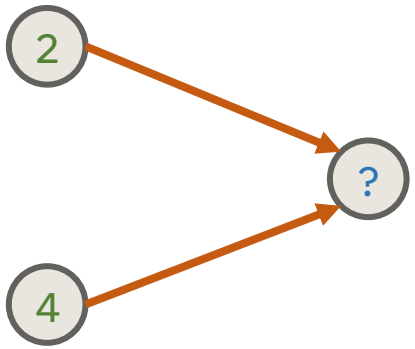
VISUALISATION OF A GNN CONVOLUTION



1. Prepare messages
2. Pool messages
3. Update embedding

PROPERTIES OF THE POOLING FUNCTION

The pooling function must be invariant to node ordering
and the number of nodes



Function	Node value
Max	4
Mean	3
Sum	6

TRAINING A GNN

$$\boldsymbol{v}_i' = \sigma\left(\mathbf{W}\sum_{j\in\mathcal{N}(i)}\frac{\boldsymbol{v}_j}{|\mathcal{N}(i)|} + \mathbf{B}\boldsymbol{v}_i\right)$$

Feed the final node embeddings to a loss function

Run an optimiser to train the weight parameters

$\mathbf{W}$ and $\mathbf{B}$ are shared across all nodes

EFFICIENCY AND INDUCTIVE CAPABILITY

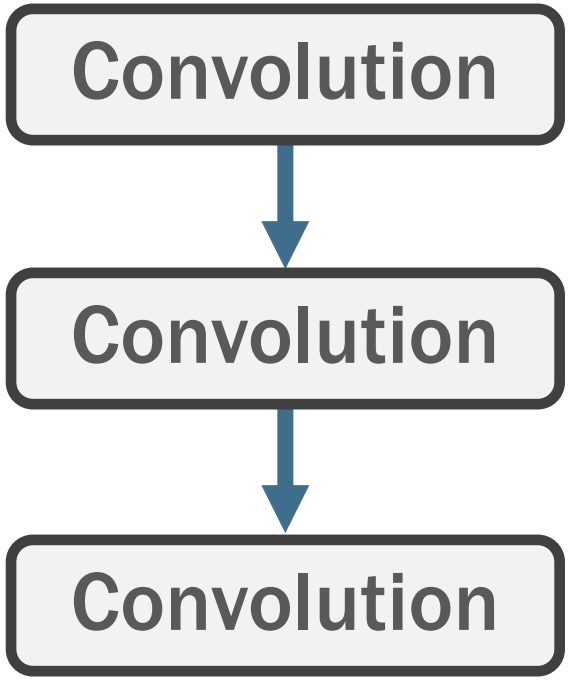
Each node has its own network due to its connectivity

Message, pool, and update functions are shared for all nodes

Can increase number of nodes without increasing the number of parameters

Can introduce new unseen node structures and just plug in the same matrices

STACKING CONVOLUTIONS



$\boldsymbol{v}_i^{(0)}$

$\boldsymbol{v}_i^{(1)}$

$\boldsymbol{v}_i^{(2)}$

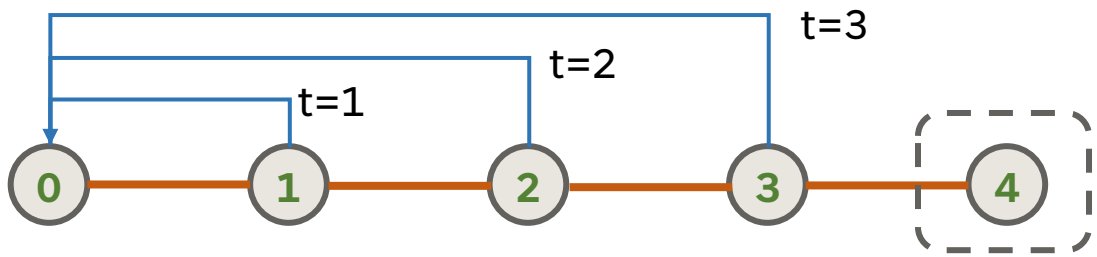
$\boldsymbol{v}_i^{(3)}$

$$\boldsymbol{v}_i^{(t+1)} = \sigma\left(\mathbf{W}^{(t)} \sum_{j \in \mathcal{N}(i)} \frac{\boldsymbol{v}_j^{(t)}}{|\mathcal{N}(i)|} + \mathbf{B}^{(t)} \boldsymbol{v}_i^{(t)}\right)$$

Weights are unique for each layer

THE ADVANTAGE OF MULTIPLE CONVOLUTIONS

Graphs are inherently local – they only get information up to t convolutions away

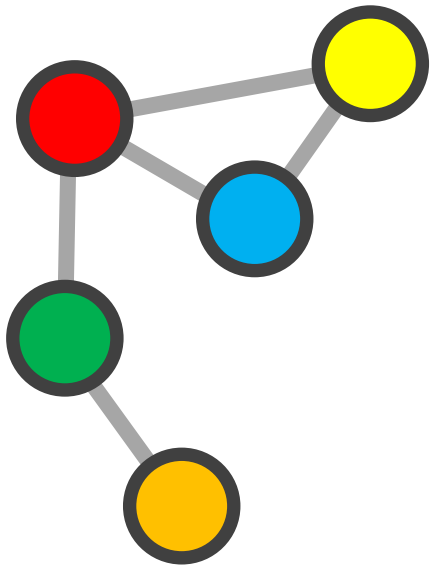


Node 4 is never seen by node 0

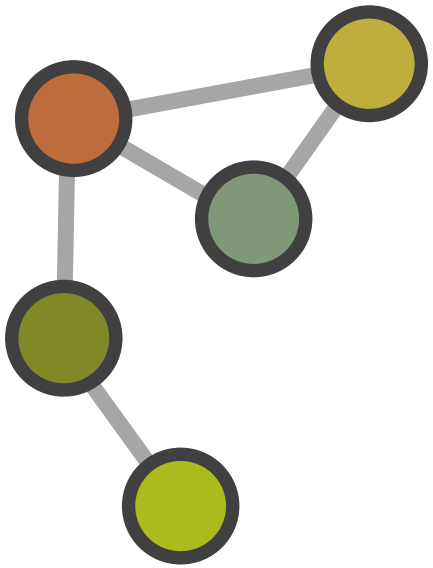
Stacking convolutions increases the receptive field of the graph

THE DRAWBACK OF MULTIPLE CONVOLUTIONS

However, too many convolutions causes over smoothing —
all node embeddings converge to the same value



t=0



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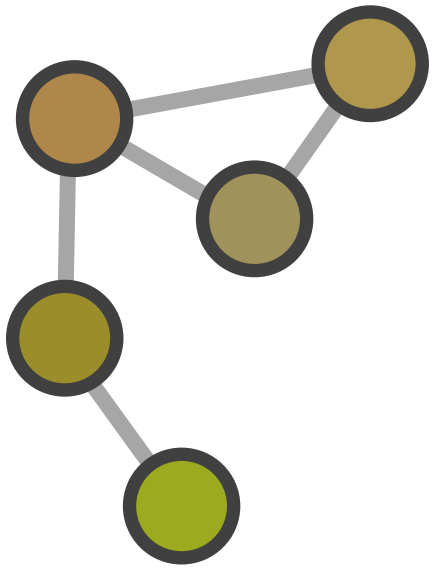

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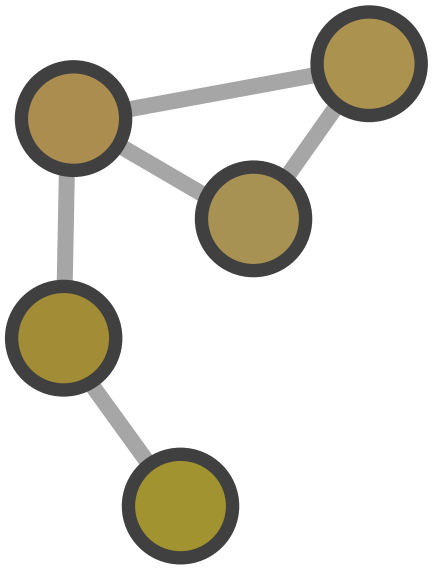
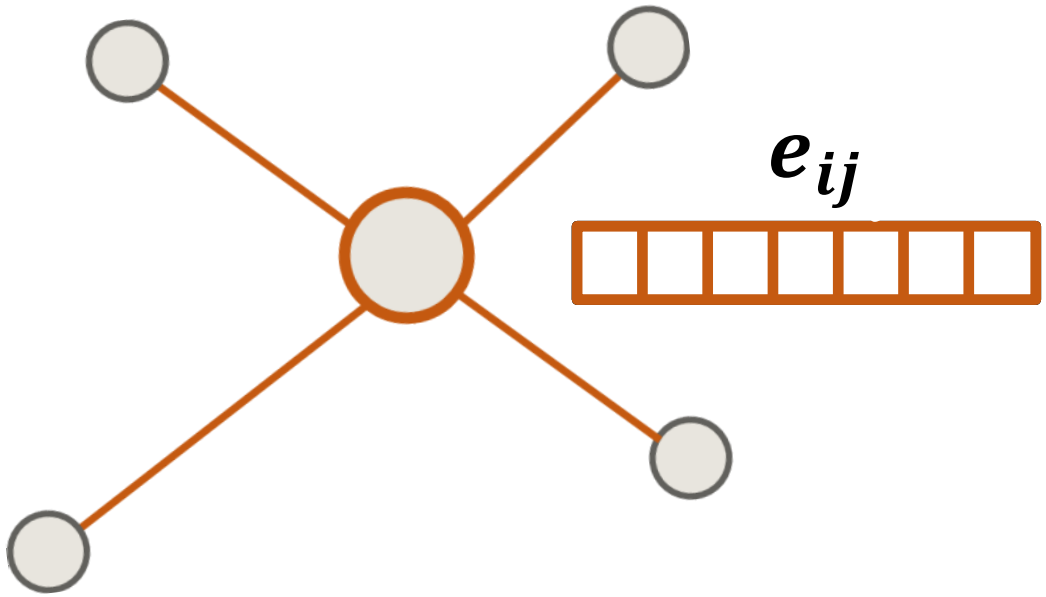


t=3

EDGE EMBEDDINGS



Edge embedding

$$m_i = \bigoplus_{j \in \mathcal{N}(i)} M_t(v_i, v_j, e_{ij})$$

$$v_i' = U_t(v_i, m_i)$$

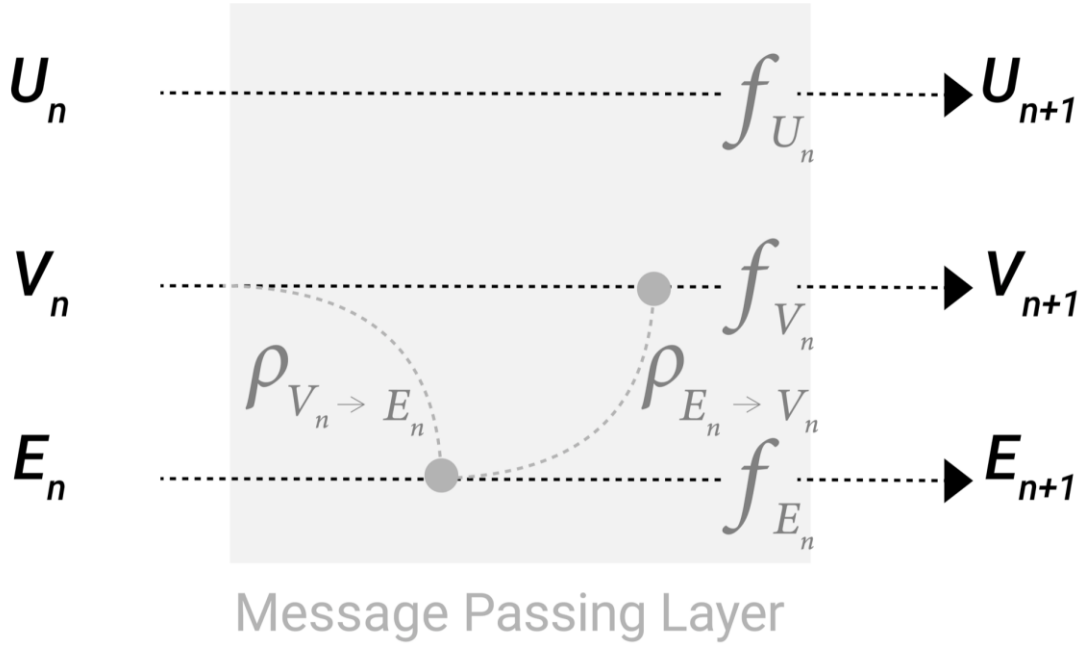
The update function stays the same

MESSAGE PASSING NETWORKS – SIGNIFICANT FLEXIBILITY

Many options for how to treat edges in the pooling function

Edge embeddings may have different dimensionality to node embeddings

An option is to pool all edges and concatenate them at the end

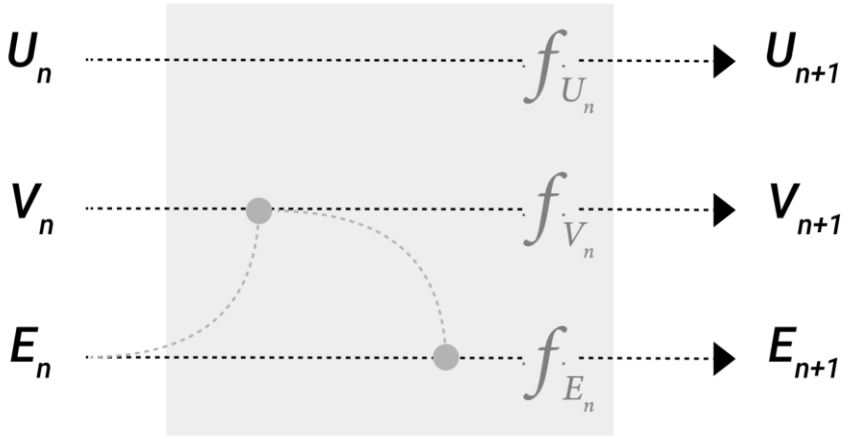


MESSAGE PASSING NETWORKS – SIGNIFICANT FLEXIBILITY

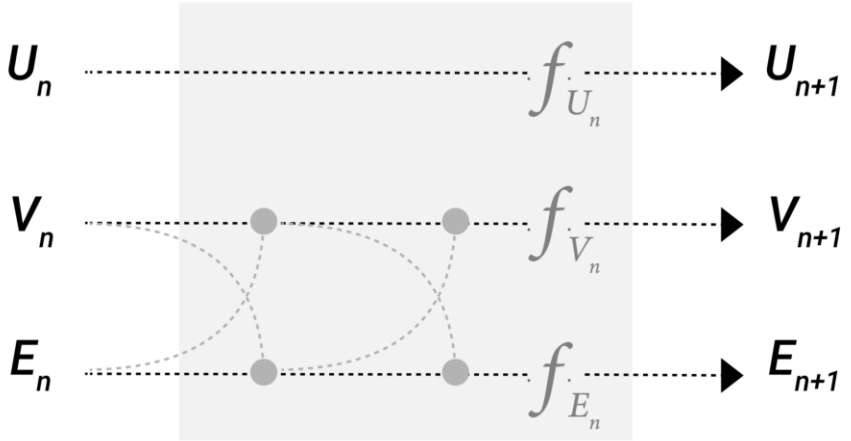
Can update nodes before edges or vice versa

Or have a weave design to pass messages back and forth

All flexible design choices in message passing networks



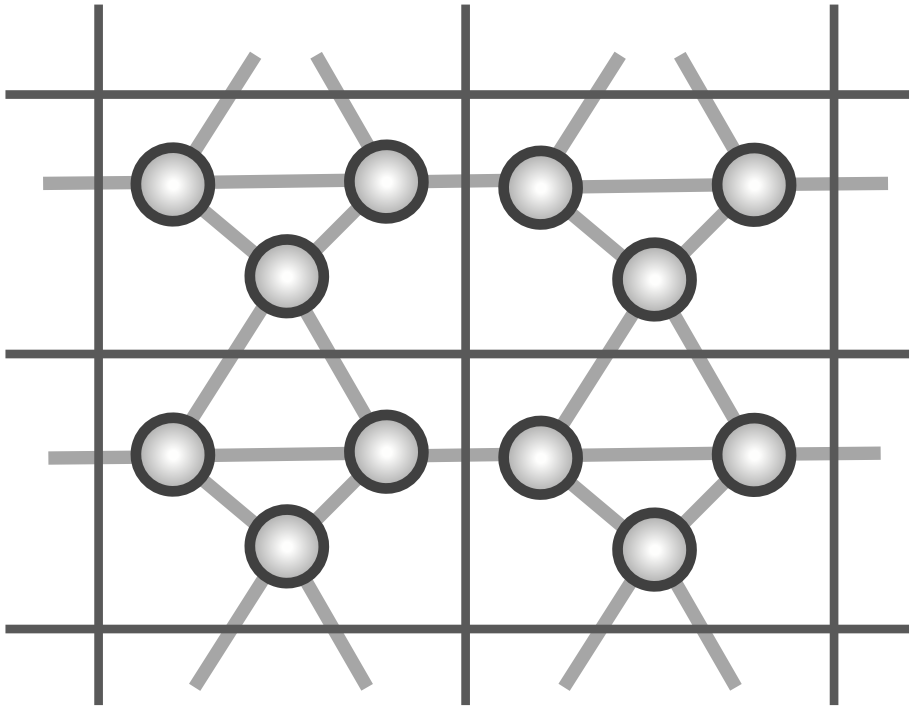
Node Then Edge Learning



Weave Layer

CONVOLUTIONAL GRAPH NETWORKS FOR CRYSTALS

Graphs are a natural representation for crystals and but we have extra design constraints

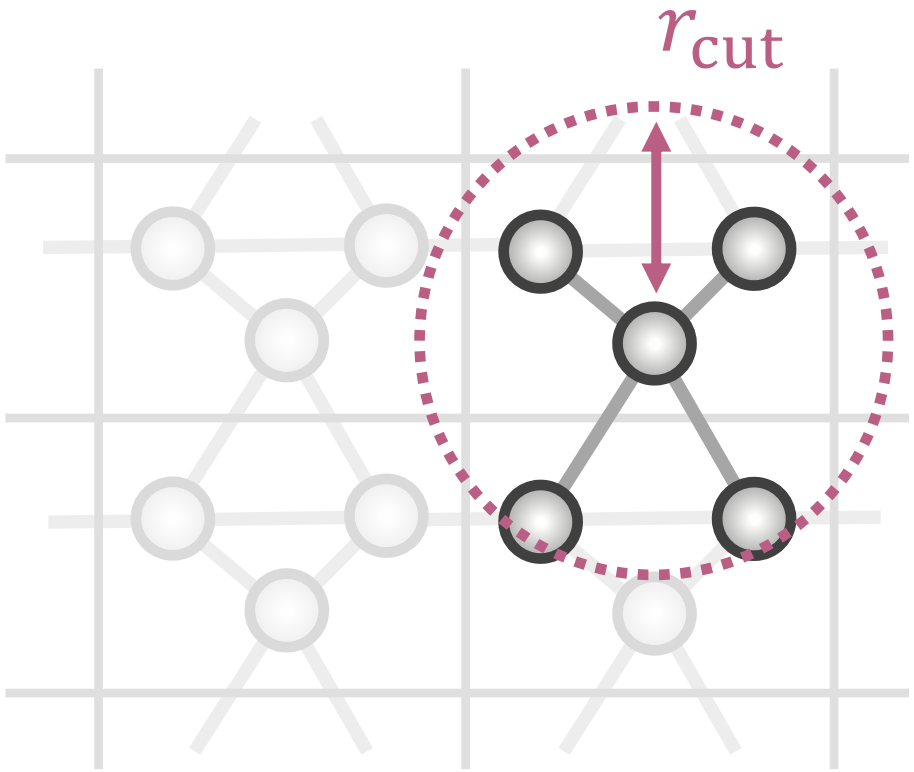


Networks should be permutation and translation invariant

Properties depend on atom types and coordinates not just connectivity

CONSTRUCTING THE GRAPH FROM A CRYSTAL STRUCTURE

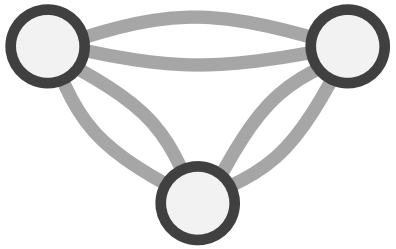
Include all atoms within a certain cut-off as neighbours



Must consider periodic boundaries

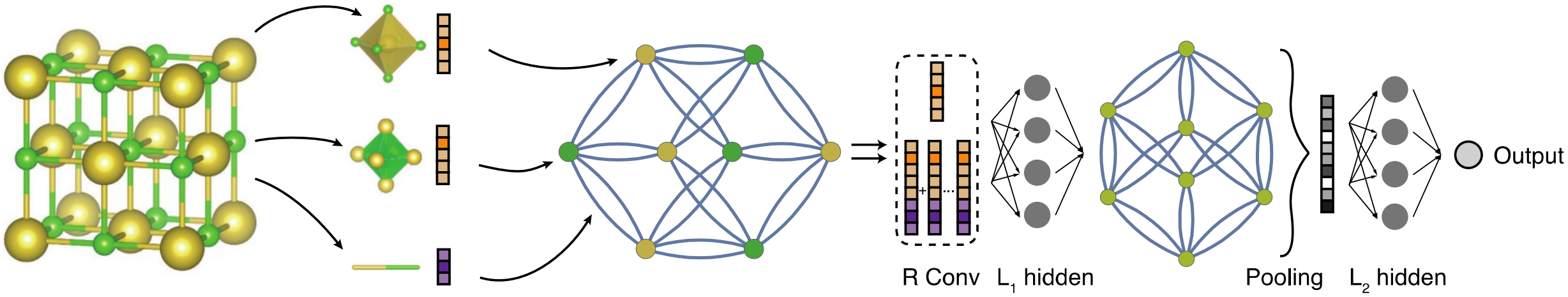
Perform the procedure for each atom in the unit cell

Nodes can share multiple edges to the same neighbour due to PBC



CRYSTAL GRAPH CONVOLUTIONAL NEURAL NETWORKS (CGCNN)

CGCNN was the first time graph convolutions were applied to crystals



Xie and Grossman Phys. Rev. Lett. 120, 145301 (2018)

IMPLEMENTATION OF CGCNN

Message function:

$$\boldsymbol{m}_i^{(t)} = \boldsymbol{v}_i^{(t)} \oplus \boldsymbol{v}_j^{(t)} \oplus \boldsymbol{e}_{i,j}$$

Update function:

$$\boldsymbol{v}_i^{(t+1)} = \boldsymbol{v}_i^{(t)} + \sum_{j \in \mathcal{N}(i)} \sigma\left(\mathbf{W}_f^{(t)} \boldsymbol{m}_i^{(t)} + \boldsymbol{b}_f^{(t)}\right) \odot g\left(\mathbf{W}_s^{(t)} \boldsymbol{m}_i^{(t)} + \boldsymbol{b}_s^{(t)}\right)$$

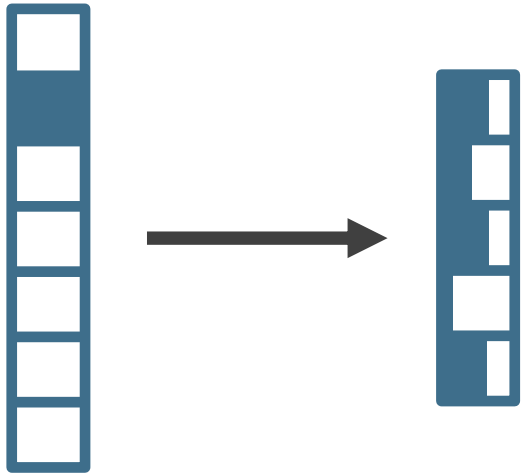
sigmoid

"gate"

softplus

INITIALISATION — NODE AND EDGE EMBEDDINGS

What to do for the initial node and edge embeddings?



Nodes

The element type is one-hot encoded (dimension of 119) and passed through an MLP

Edges

The bond distance is projected onto a Gaussian basis (40 basis functions)

READOUT — CALCULATING THE FINAL PREDICTION

CGCNN generates *graph level* predictions, how are these generated from the final node embeddings?

Final pooling of all nodes

$$\boldsymbol{u}_c = \sum_{i \in \mathcal{G}} \frac{\boldsymbol{v}_i^{(T)}}{|\mathcal{G}|}$$

num atoms

SLP readout

$$E = \sigma(\mathbf{W}_r \mathbf{u}_c + \boldsymbol{b}_r)$$

Property predicted

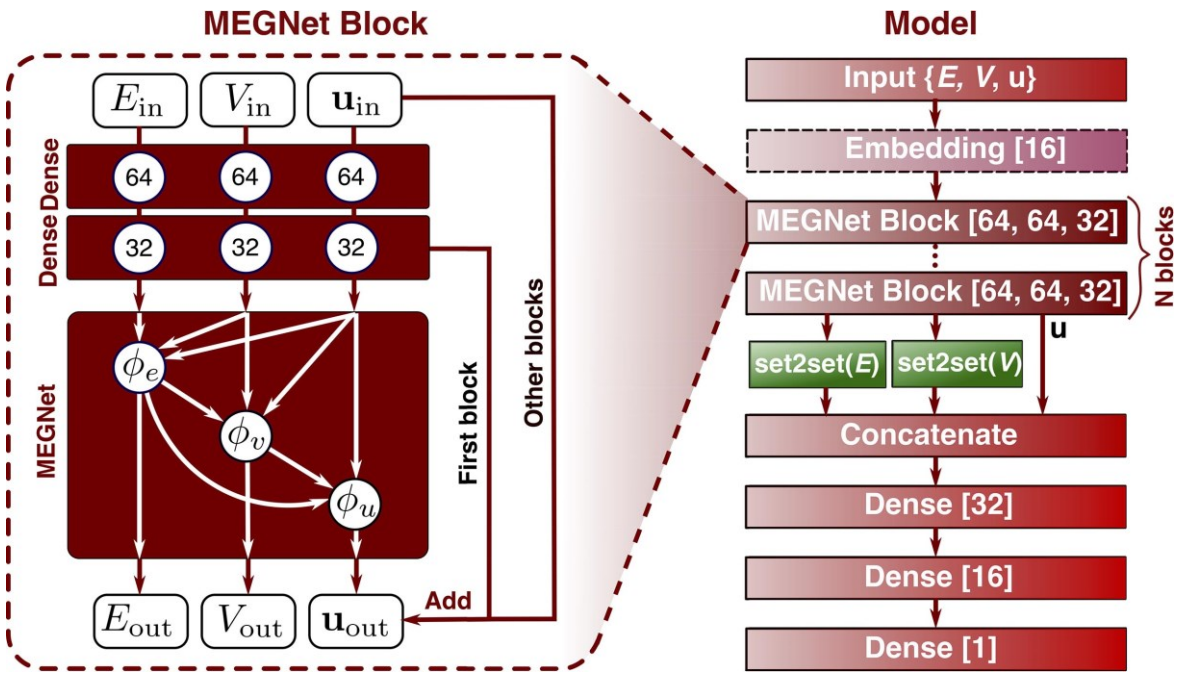
CGCNN PERFORMANCE

CGCNN shows good accuracy for such a simple model but errors are still too large for reliable science

Property	# of train data	Unit	MAE_{model}	MAE_{DFT}
Formation energy	28 046	eV/atom	0.039	0.081–0.136 [28]
Absolute energy	28 046	eV/atom	0.072	···
Band gap	16 458	eV	0.388	0.6 [32]
Fermi energy	28 046	eV	0.363	···
Bulk moduli	2041	log(GPa)	0.054	0.050 [13]
Shear moduli	2041	log(GPa)	0.087	0.069 [13]
Poisson ratio	2041	···	0.030	···

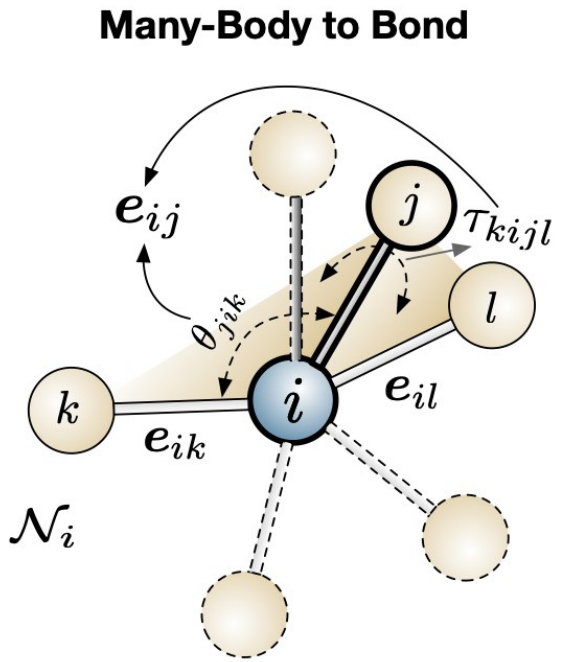
ADVANCED MESSAGE PASSING NETWORKS

CGCNN only uses bond lengths as features. More advanced networks show improved performance



MEGNet

Crystal features and set2set pooling

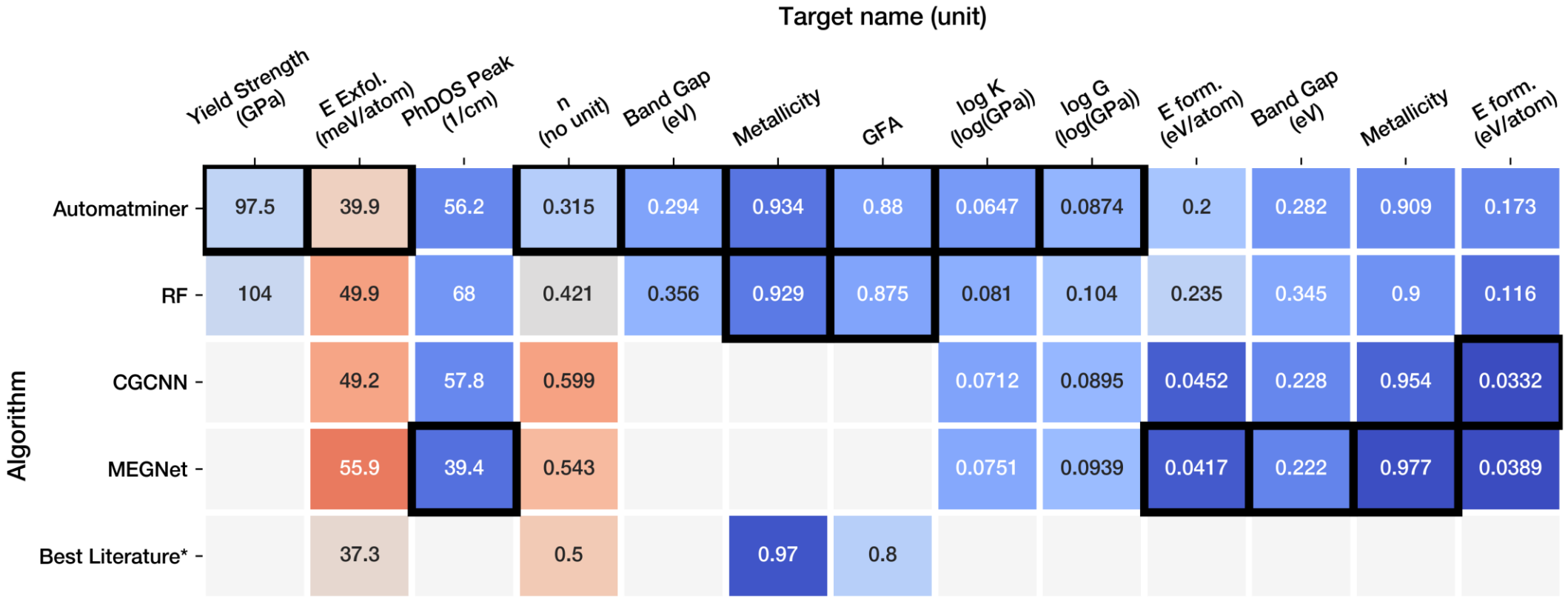


M3GNet

Bond angles and dihedrals

GRAPH NETWORKS AND THE MATBENCH DATASET

Graph neural networks are widely used for property predictions in chemistry but excel on larger datasets



npj Comput. Mater. **6**, 138 (2020)

USES OF GRAPH NETWORKS

GNNs take up most of the top spots on the current leader board

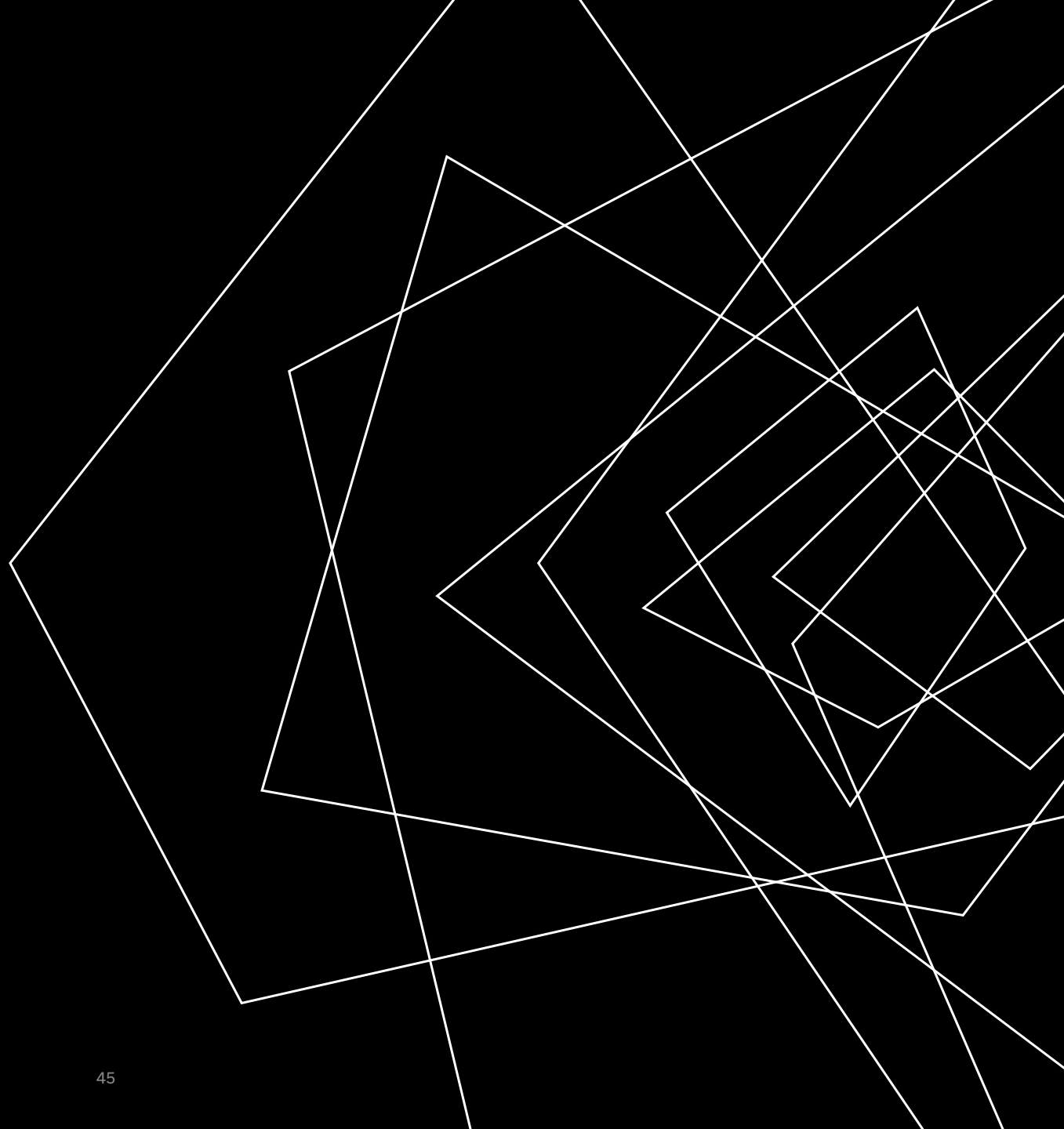
Many high-performance MLIPs use graphs (MACE, nequip, allegro)

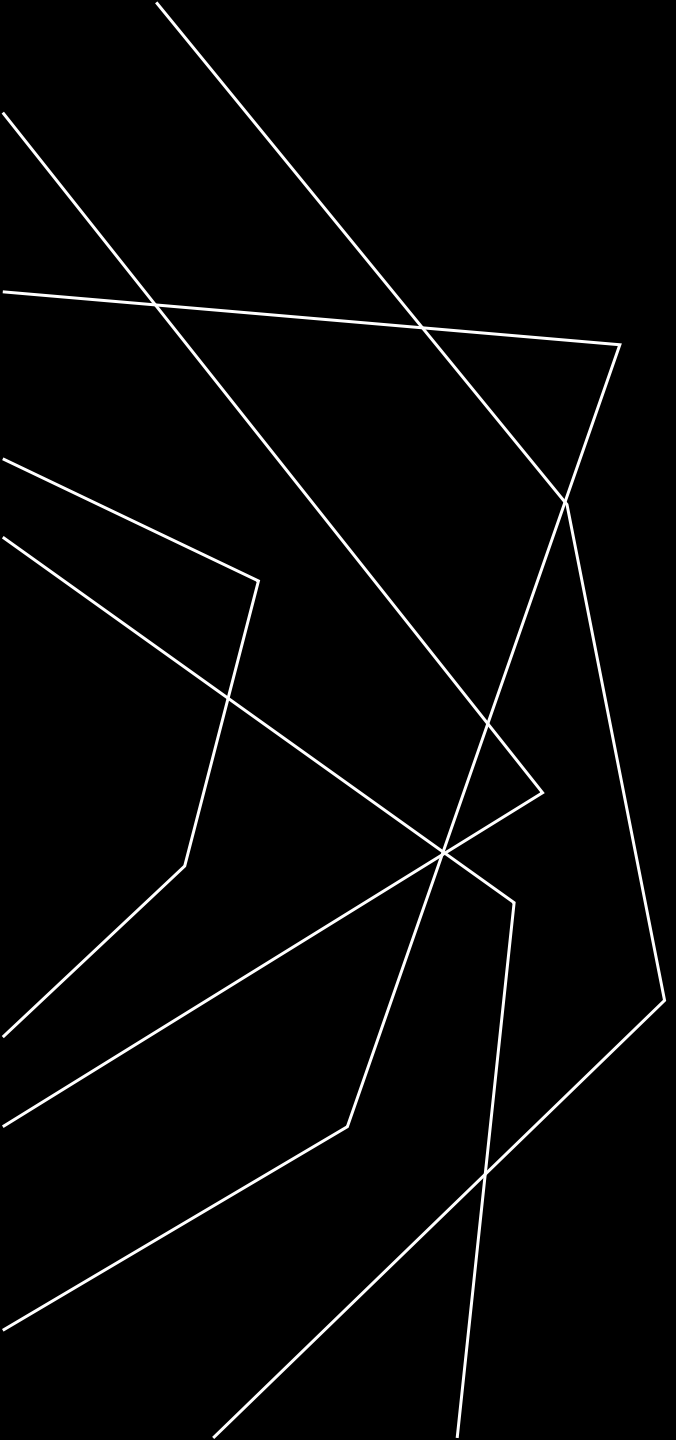
Task name	Samples	Algorithm	Verified MAE (unit) or ROCAUC	Notes
matbench_steels	312	MODNet (v0.1.12)	**87.7627 (MPa)**	
matbench_jdft2d	636	MODNet (v0.1.12)	**33.1918 (meV/atom)**	
matbench_phonons	1,265	MegNet (kgcnn v2.1.0)	**28.7606 (cm^-1)**	structure required
matbench_expt_gap	4,604	MODNet (v0.1.12)	**0.3327 (eV)**	
matbench_dielectric	4,764	MODNet (v0.1.12)	**0.2711 (unitless)**	
matbench_expt_is_metal	4,921	AMMExpress v2020	**0.9209**	
matbench_glass	5,680	MODNet (v0.1.12)	**0.9603**	
matbench_log_gvrh	10,987	coNGN	**0.0670 (log10(GPa))**	structure required
matbench_log_kvrh	10,987	coNGN	**0.0491 (log10(GPa))**	structure required
matbench_perovskites	18,928	coGN	**0.0269 (eV/unit cell)**	structure required
matbench_mp_gap	106,113	coGN	**0.1559 (eV)**	structure required
matbench_mp_is_metal	106,113	CGCNN v2019	**0.9520**	structure required
matbench_mp_e_form	132,752	coGN	**0.0170 (eV/atom)**	structure required

https://matbench.materialsproject.org

CONCEPT CHECKLIST

- Many datasets can be represented as graphs.
- GNNs work by i) building a graph and ii) propagating information between neighbours using NNs
- GNNs are scalable and can generalise well
- There are many possibilities for designing GNNs





THANK YOU

mdi-group.github.com