Graph Neural Networks

Applied Machine Learning, KU

Daniel Murnane - May 8th, 2024

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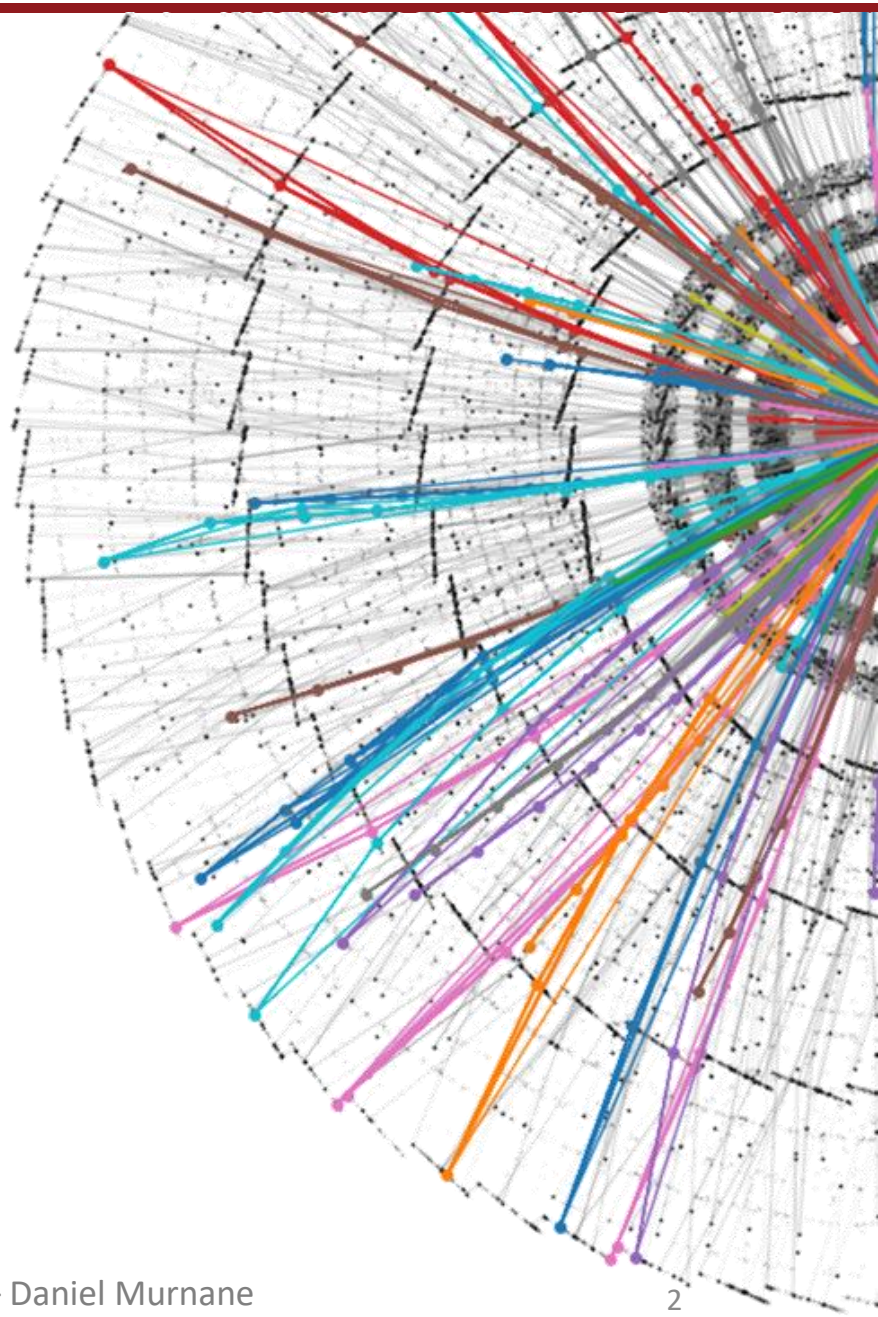
Introduction & Goals

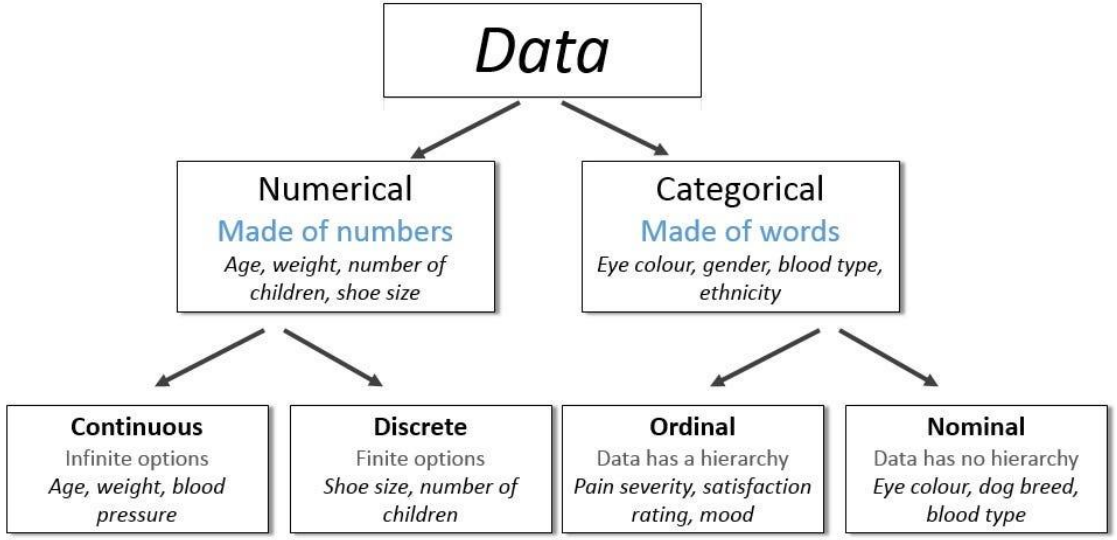
- Goals for today:
  - Understand point cloud structure
  - Understand graph structure
  - Look at some real data that is represented as a graph
  - Understand how to generalize from grid (image) to a graph
  - Think about some choices of GNN architectures
  - Zoom in to the Transformer as a kind of GNN
- Have borrowed content from Troels' slides from last year!



How can we represent data

Data types

- Let's tidy up our language: There are data types, and data structures
- A data type is an input to our neural network, it falls into one of the following types



Data structures

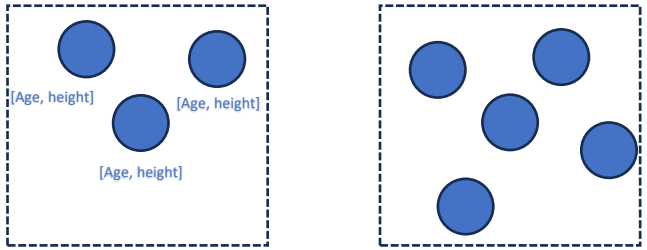
- Let’s tidy up our language: There are data types, and data structures
- A data type is an input to our neural network, it falls into one of the following types
- A data structure defines how each component of our dataset is related
- There are many data structures…

Data structures

- Tabular: Each sample has one entry

Data structures

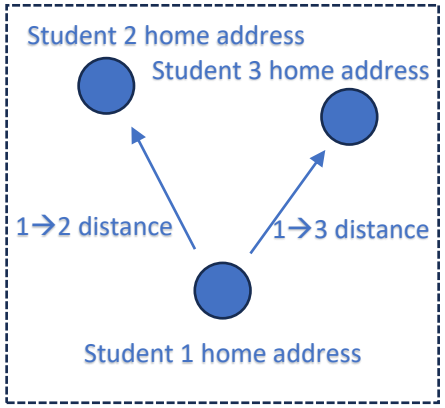
- **Tabular:** Each sample has one entry
- **Set:** Each sample has a variable number of entries



Class 1 Class 2

Data structures

- **Tabular:** Each sample has one entry
- **Set:** Each sample has a variable number of entries
- **Point Cloud:** Each sample has a variable number of entries, with some notion of distance



Class 1

Data structures

- Tabular: Each sample has one entry
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- Point Cloud: Each sample has a variable number of entries, with some notion of distance
- Grid: Each sample has a fixed number of entries, binned into a grid, with a natural distance

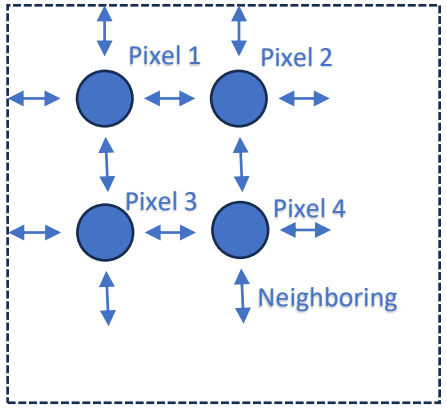

Image 1

Data structures

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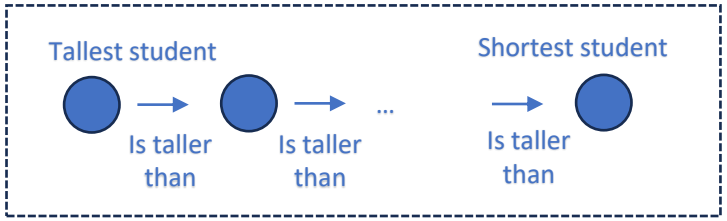
- Sequence: Each sample has an ordered list of variable number of entries



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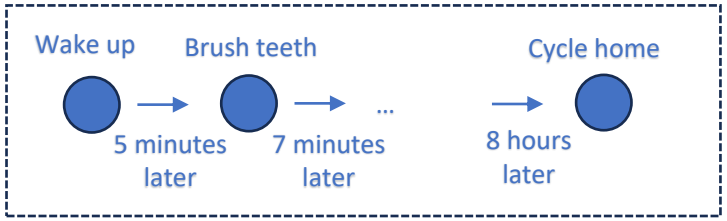
- Time series: Each sample has an ordered list of variable number of entries, with a neighbor distance given by time



Day 1

Data structures

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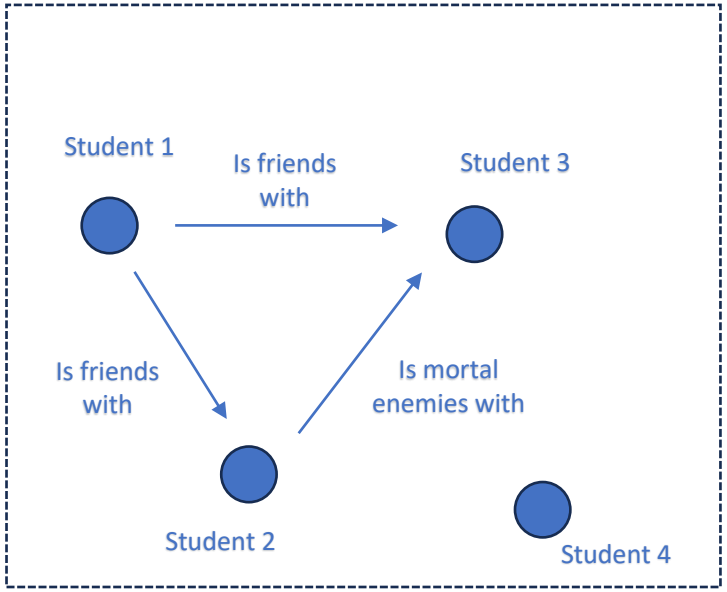
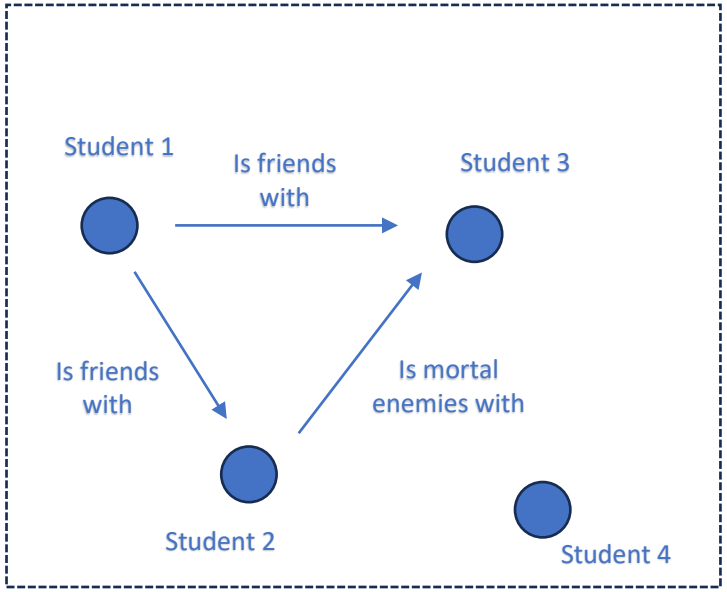
- Time series: Each sample has an ordered list of variable number of entries, with a neighbor distance given by time
- Graph: Each sample has a variable number of entries, with neighborhoods given by explicit pairwise relationships



Class 1

Data structures

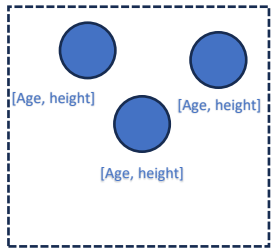
- Graph: Each sample has a variable number of entries, with neighborhoods given by explicit pairwise relationships
- A graph is a collection of *nodes* (objects or entries) and *edges* (relationships between each object)
- Nodes can have features, edges can have features
- A graph may also have graph-level or "global" properties, e.g. `class_1["topic"] = "applied ML"`



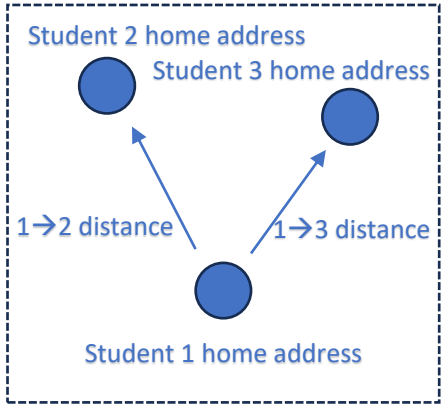
Class 1 = Applied ML

Data structures

- I encourage you to look at all data structures through the eyes of a graph



Class 1



Class 1

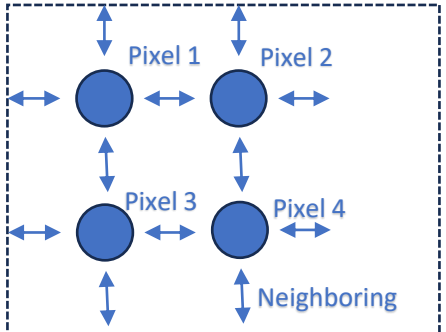
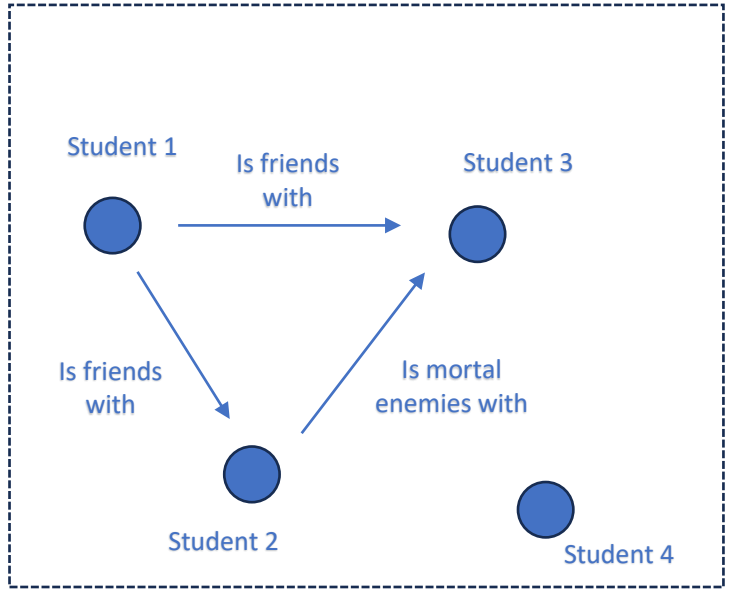


Image 1



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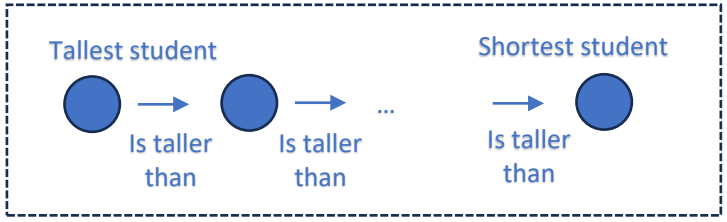
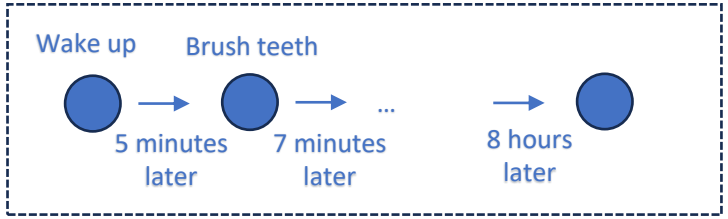


Class 1



Day 1

Graph Data

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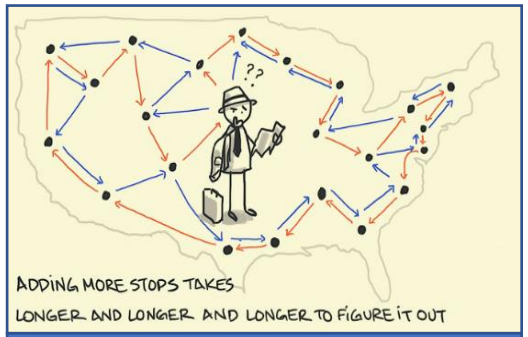
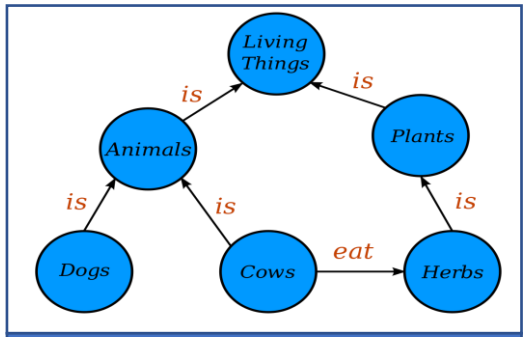
Classic Problems with Graphs



Travelling Salesman Problem



Knowledge Graph Comprehension

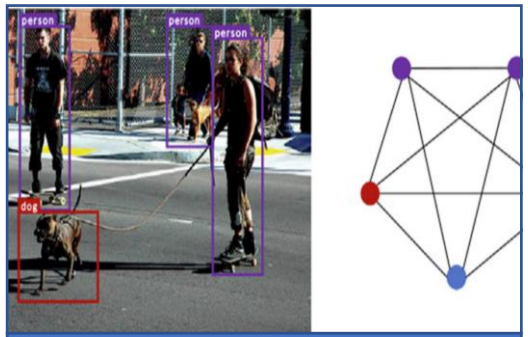
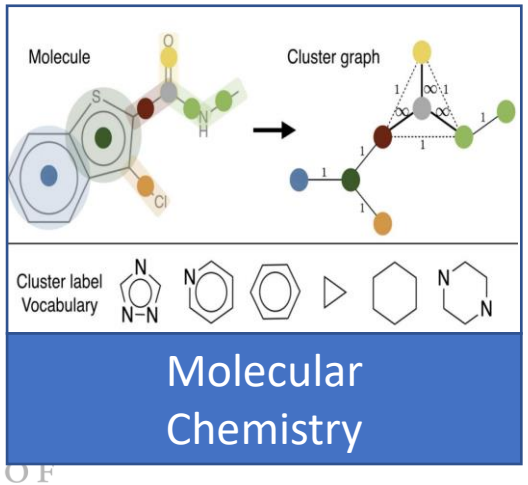
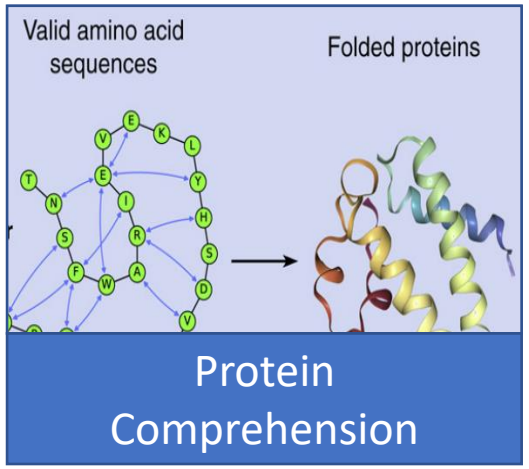


Image Comprehension



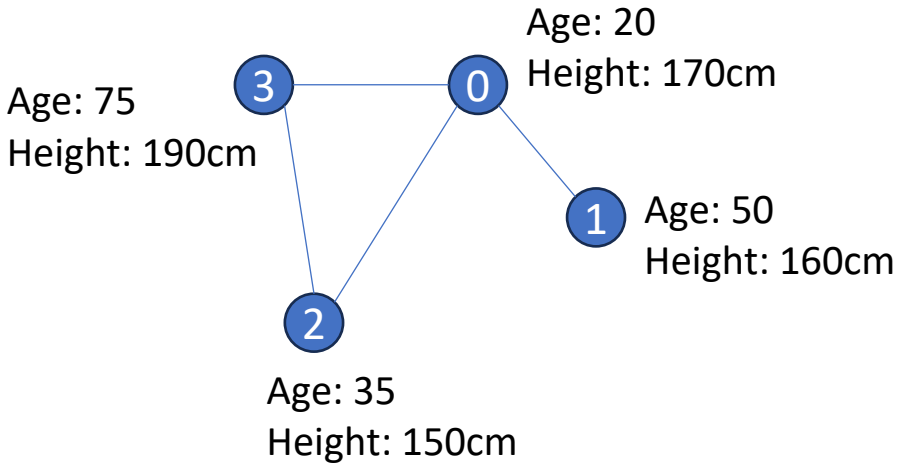
Molecular Chemistry



Protein Comprehension

Representing a Graph

- Nodes – a list of node vectors n_i^k, where $i = 0, \ldots, N_n$ up to number of nodes, $k = 0, \ldots, N_f$ up to number of features
- Edges – an adjacency matrix A_{ij}, where $A_{ij} = 1$ when there is an edge between node i and node j, and 0 otherwise
- In practice, A_{ij} is mostly 0s, so let's represent it with a more efficient structure: E_{ij}, which is a list of *pairs* of node indices



$$n_i^k = \begin{bmatrix} 20 & 170 \\ 50 & 160 \\ 35 & 150 \\ 75 & 190 \end{bmatrix} \quad A_{ij} = \begin{bmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{bmatrix}$$

$$E_{ij} = \begin{bmatrix} 0 & 0 & 0 & 2 & 1 & 2 & 3 & 3 \\ 1 & 2 & 3 & 3 & 0 & 0 & 0 & 2 \end{bmatrix}$$

Removing the Grid

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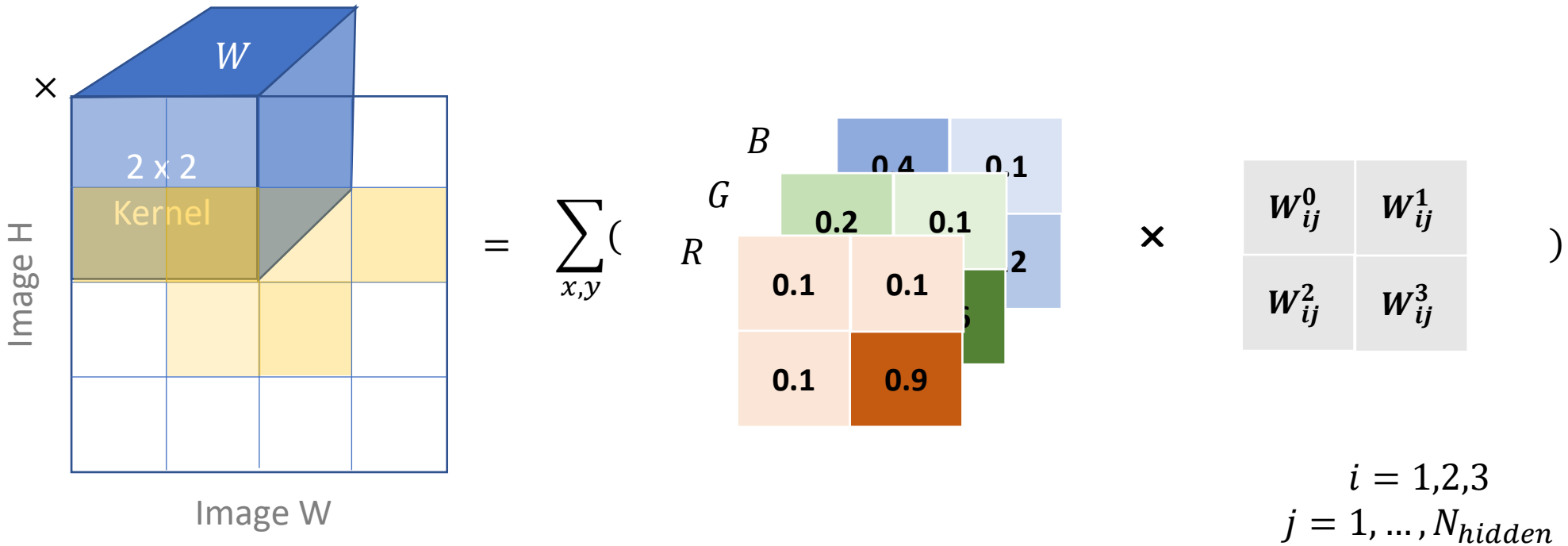
Recall the CNN

- Remember how the image convolution worked:

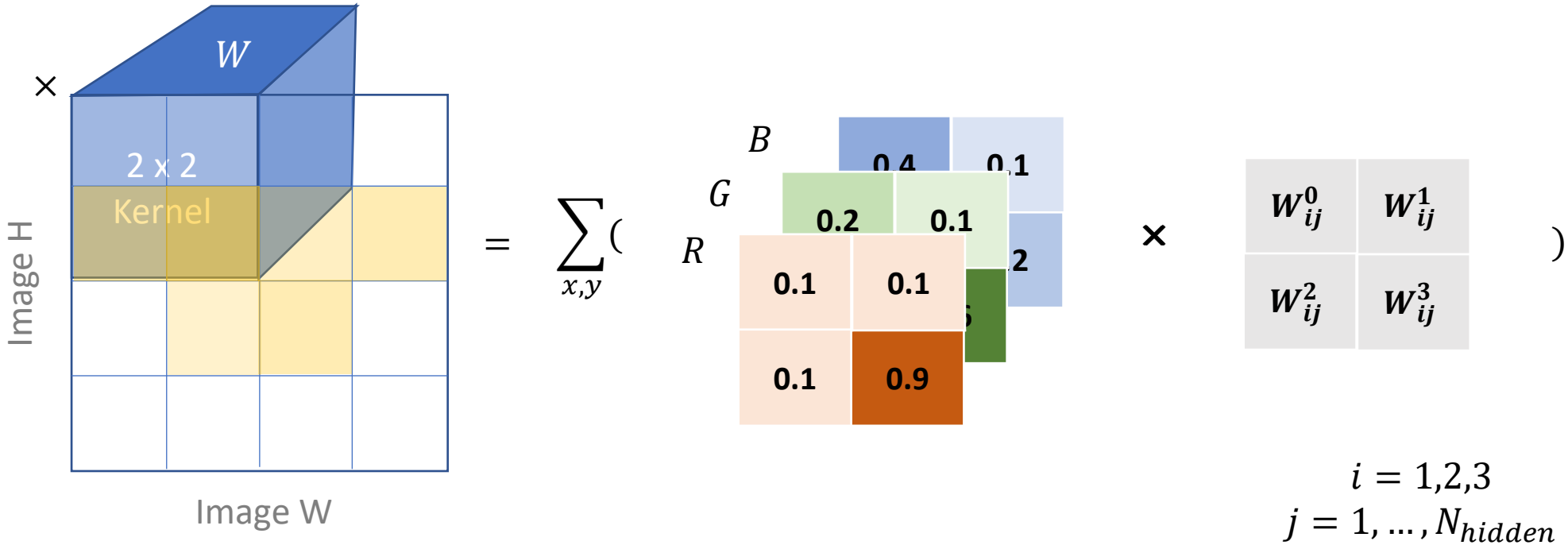


$i = 1,2,3$

$j = 1, \ldots, N_{hidden}$

Recall the CNN

- Let's rewrite this big tensor multiplication into smaller pieces…



$i = 1,2,3$

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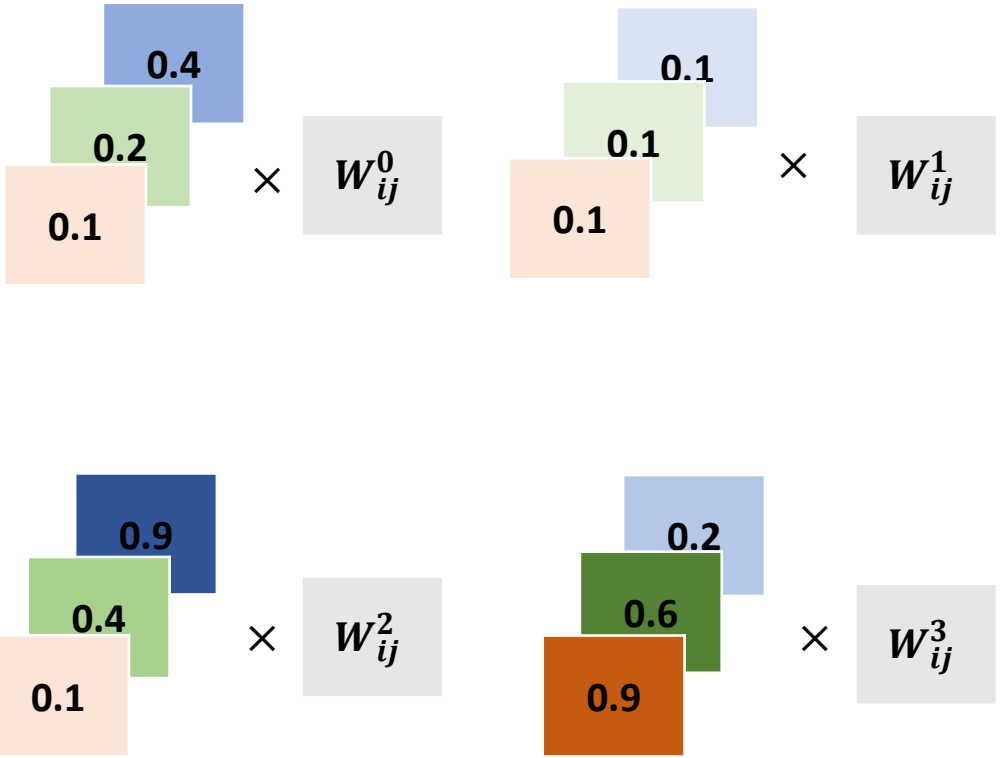
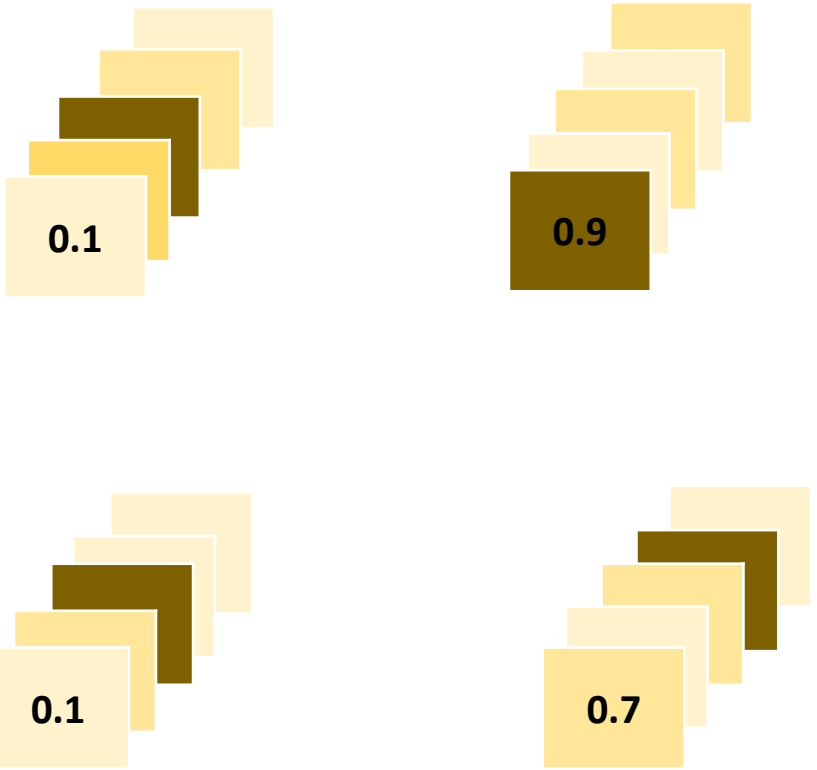
Recall the CNN

- Now this looks like each pixel in the window is passed through a simple linear layer of a feedforward NN



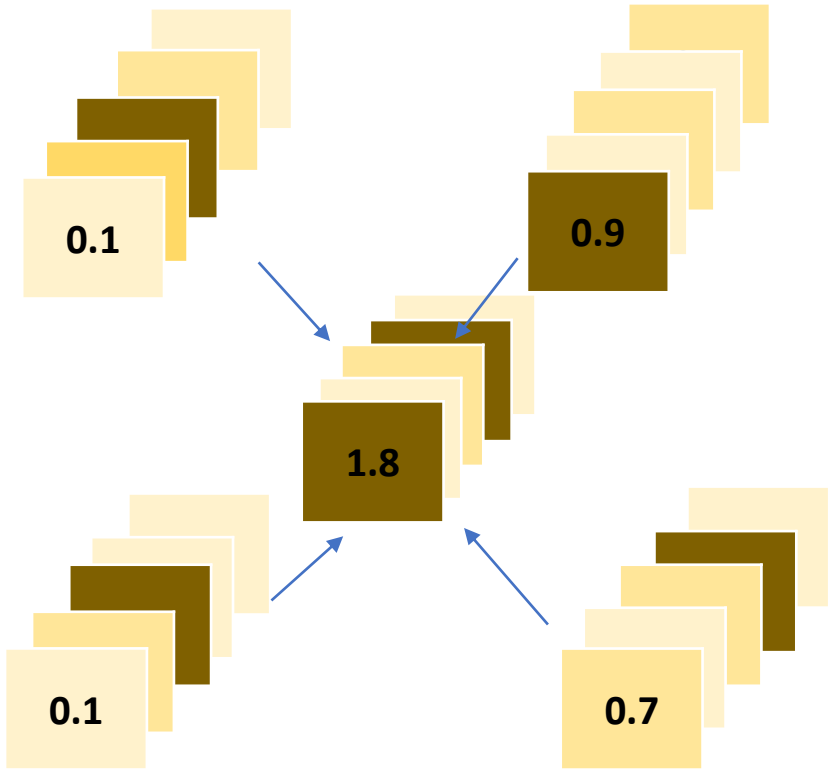
Recall the CNN

- Now this looks like each pixel in the window is passed through a simple linear layer of a feedforward NN
- Once we have passed each pixel through, we aggregate (in this case sum) the updated pixels



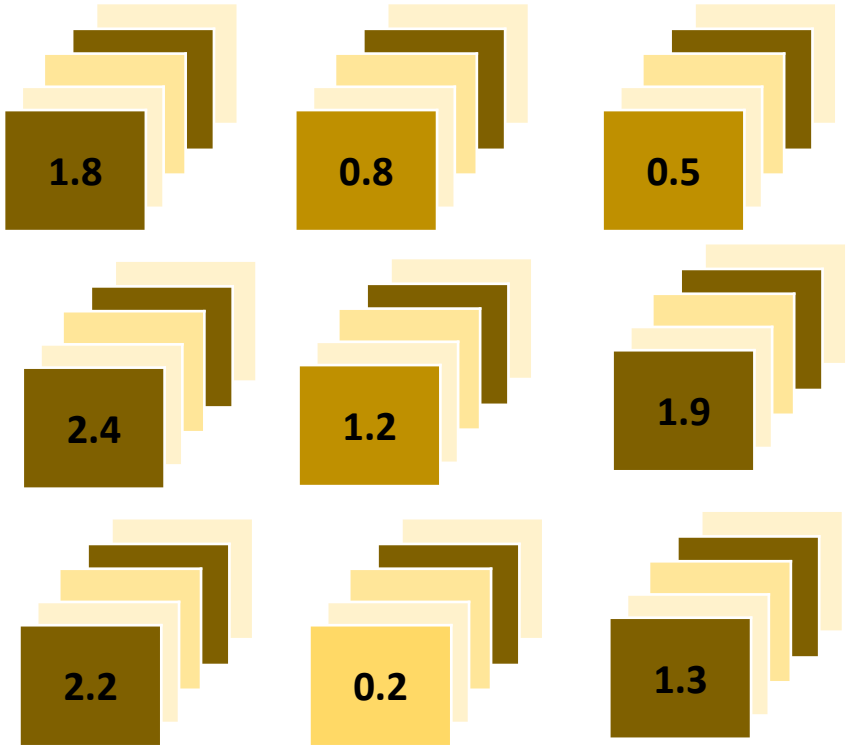
Recall the CNN

- Now this looks like each pixel in the window is passed through a simple linear layer of a feedforward NN
- Once we have passed each pixel through, we aggregate (in this case sum) the updated pixels
- The “center” of our 2x2 neighborhood is updated with the convolution outputs



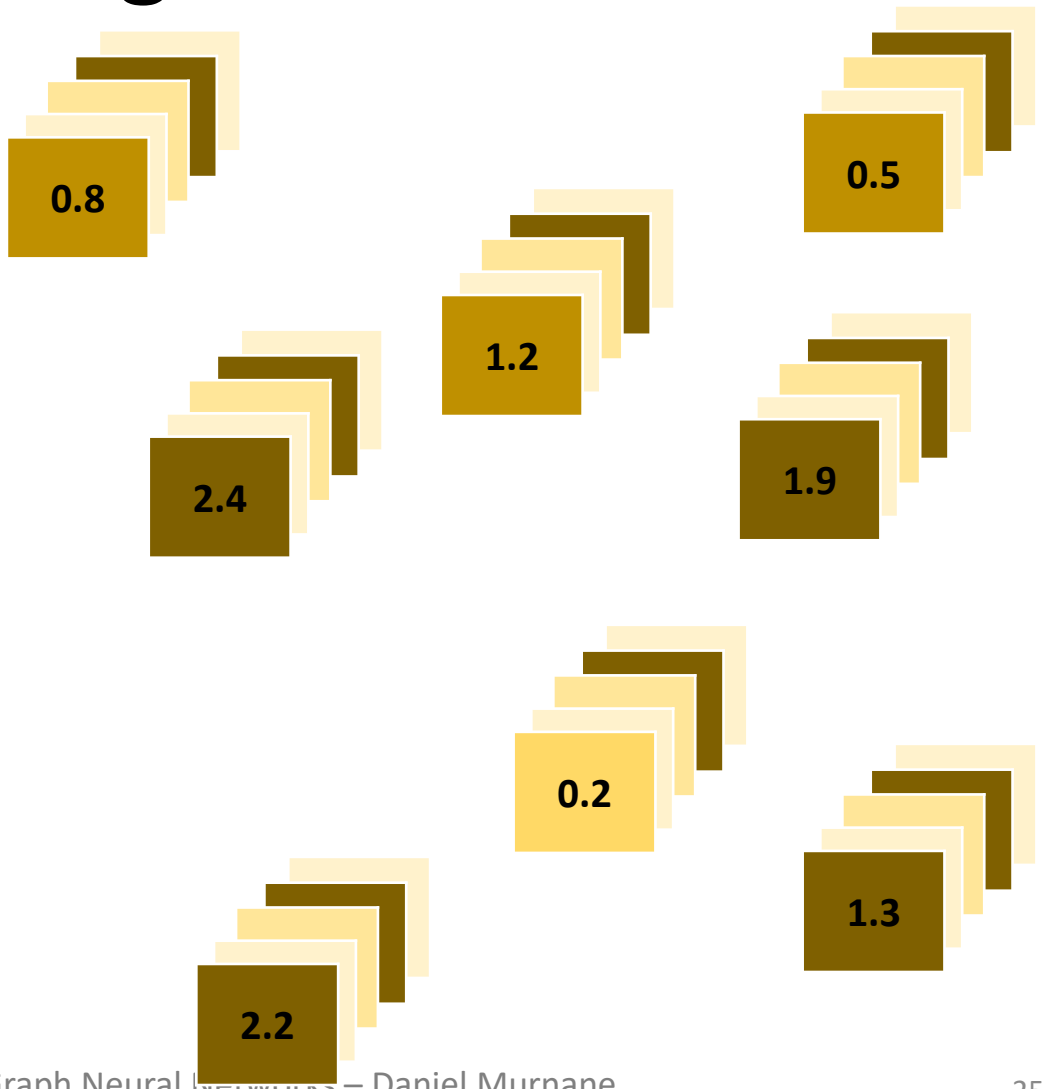
Recall the CNN

- The “center” of our 2x2 neighborhood is updated with the convolution outputs
- These centers form the inputs for the *next* convolution, which again happens in an $k \times k$ grid neighborhood



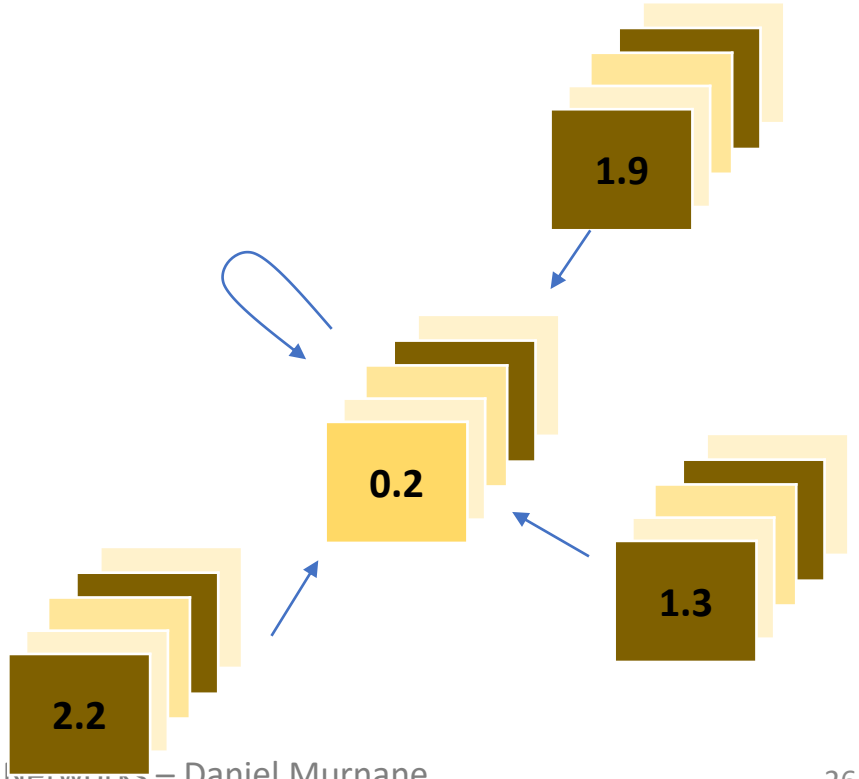
Now, let's throw away the grid structure

- Grids are convenient for images, but the world is not a grid
- Instead of "pixels", let's call each hidden vector now a "node"



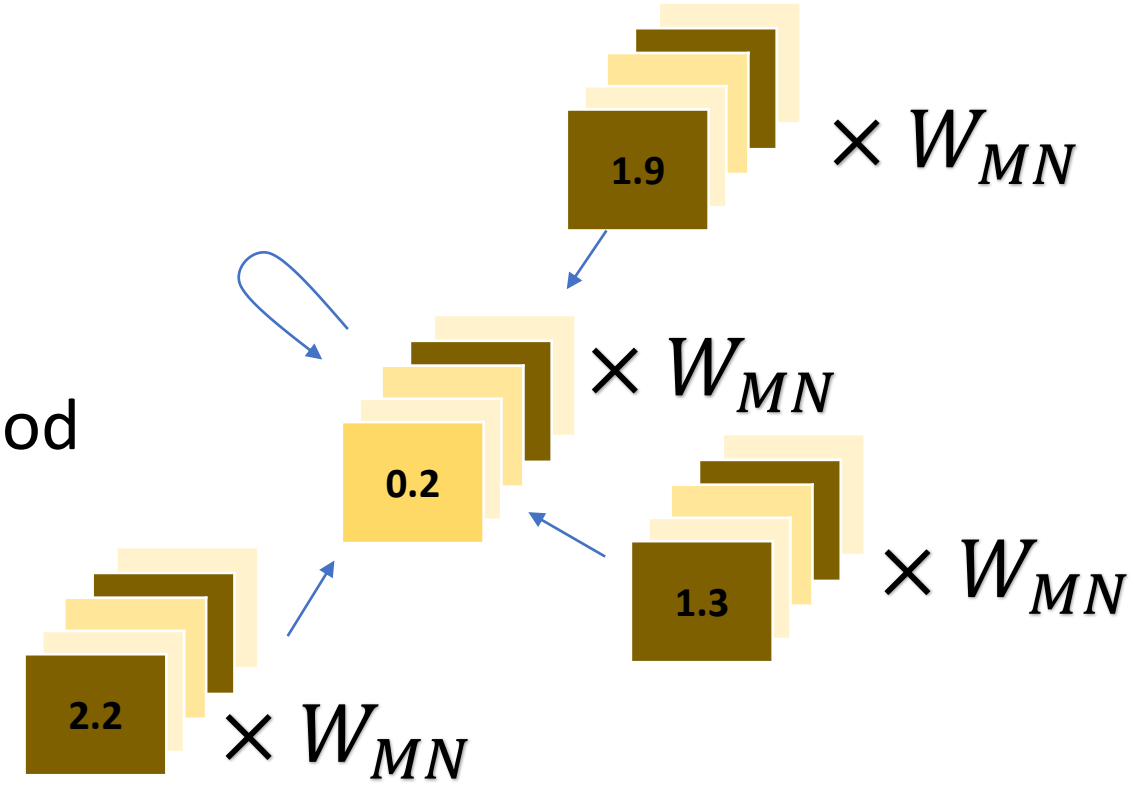
Now, let's throw away the grid structure

- Grids are convenient for images, but the world is not a grid
- Instead of "pixels", let's call each hidden vector now a "node"
- Let's also make each node the center of its own neighborhood
- And let's do our convolution over nearby nodes
- E.g. this would be one such neighborhood:



One final tweak!

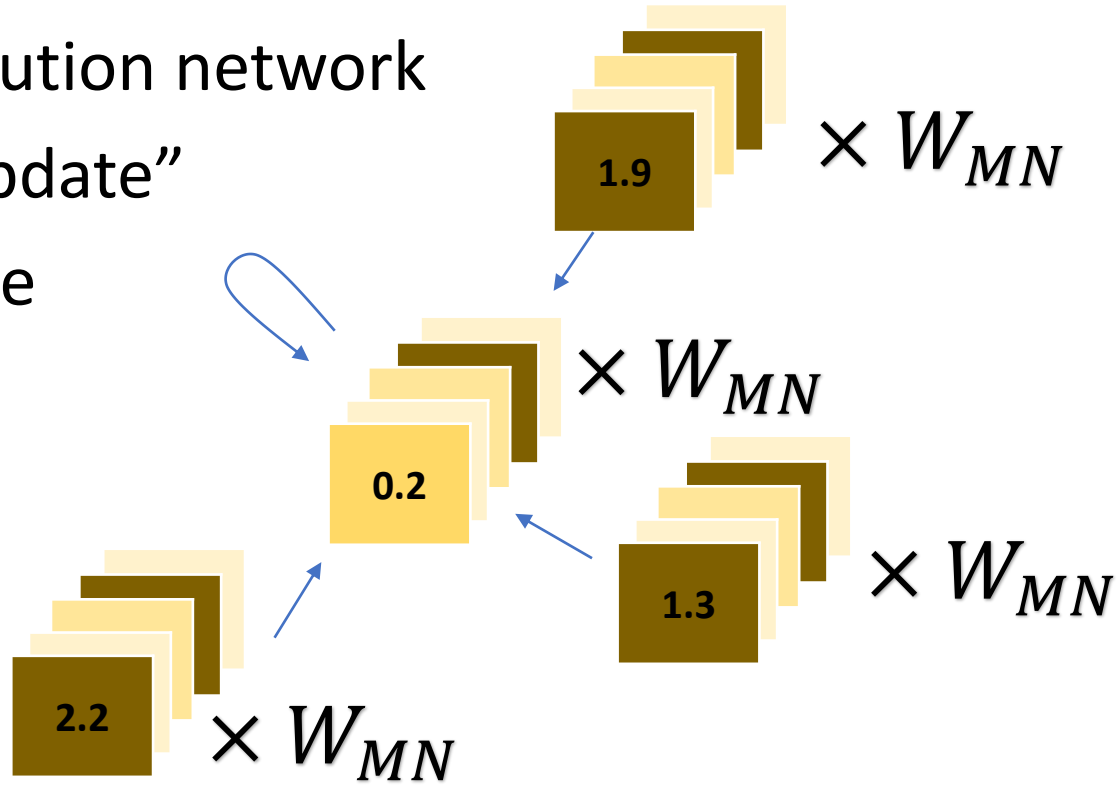
- Let's also make each node the center of its own neighborhood
- And let's do our convolution over nearby nodes
- E.g. this would be one such neighborhood
- In the CNN, each pixel had its own dedicated W. This was easy, because every neighborhood had a fixed number of pixels



- Now there are arbitrary number of nodes in each neighborhood, let's be even simpler and use the same W_{MN} for every node multiplication

This is a GNN!

- It's a simple one – a graph convolution network
- The $h_M \times W_{MN}$ step is a "node update"
- Passing these node features to the center node is called "message passing"
- Summing all the features is called "aggregation"
- Node update, message passing and aggregation are the building blocks for basically all graph neural networks



GNN Architectures

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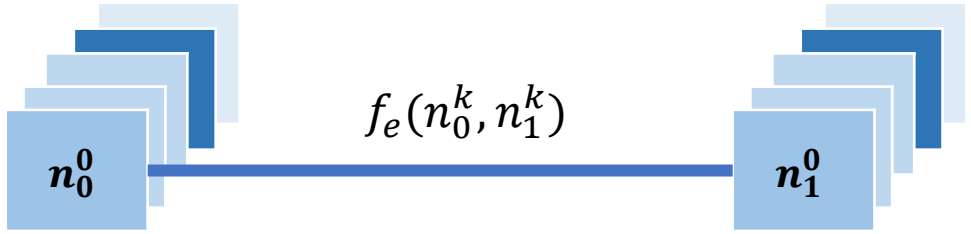
Message passing

- We can create a language for convolutions that will work for almost **every other** ML model
- It's called "message passing", and it has two parts: **calculate the message** between pairs of objects, then **aggregate** the messages coming into each object's neighborhood
- For a graph, a message is the features that are passed along an edge – a learnable function that takes in the two nodes on either side of that edge

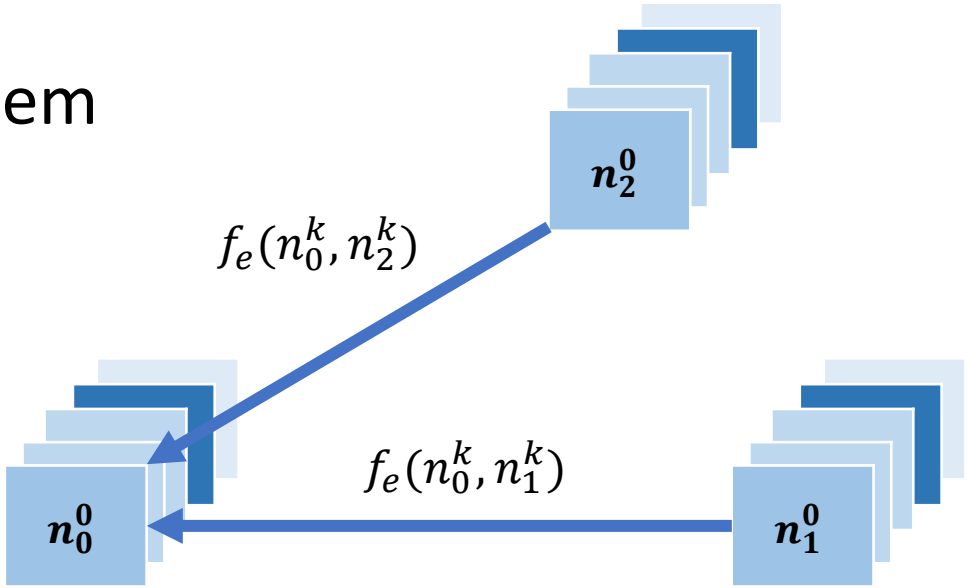


- f_e is a learnable function (feed-forward neural network)
- n_i^k are the N_k hidden channels of the N_i nodes in the graph

Aggregation & Permutation Invariance

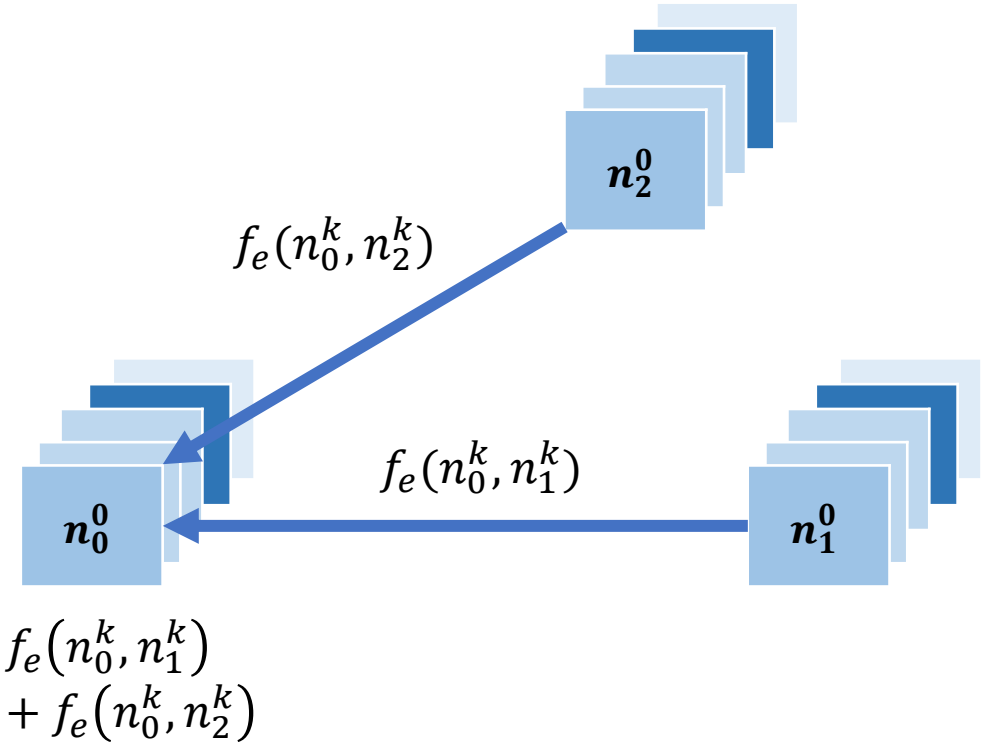
- We have a message function $m_{ij} = f_e(n_i^k, n_j^k)$, so how do we combine these messages around each node?
- We could stack them together and pass them through a FFNN? E.g. $f([m_{01}, m_{02}])$
- Two problems:

1. A FFNN has a fixed size, but we might have any number of incoming messages
2. If we switch the order that we receive the messages (which is meaningless), the output of the FFNN will be different!



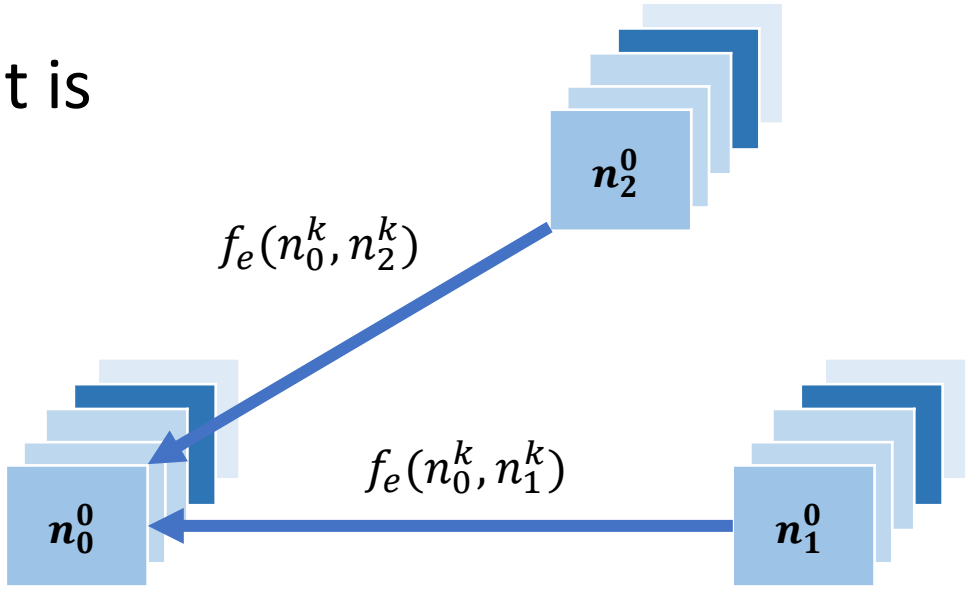
Aggregation & Permutation Invariance

- What we are looking for is a “permutation invariant” way to combine any number of incoming messages
- There are a few ways to do this, but the simplest is to take the sum (or mean/max/min)
- The choice of aggregation function is a hyperparameter (like the CNN pooling step)



Node update

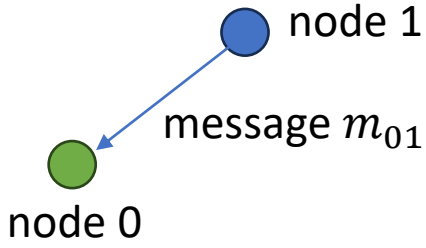
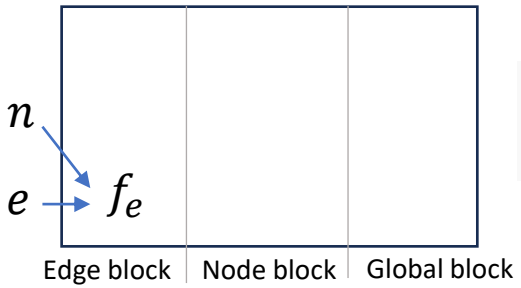
- The final step is to pass this aggregated information through a node FFNN
- The f_e is an edge-wise function/network, it is the same for every edge
- The f_n is a node function/network, it is the same for every node
- Note that even though the function is the same across all nodes or edges, the *outputs* of the function depend on the node or edge features



$$n_0'^k = f_n(f_e(n_0^k, n_1^k) + f_e(n_0^k, n_2^k))$$

Let's put it all together…

	Equations	Pictures	GNN Blocks	Code

1. Calculate messages	$m_{ij}^{l} = f_e(n_i^k, n_j^k)$, where there are edges between $i \rightarrow j$			`def message_passing(self, x, start, end):`
				`  edge_features = torch.cat([x[start], x[end]], dim=1)`
				`  e = self.edge_network(edge_features)`
				`  return e`

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Equations

Pictures

GNN Blocks

Code

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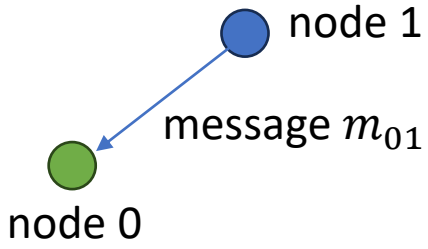

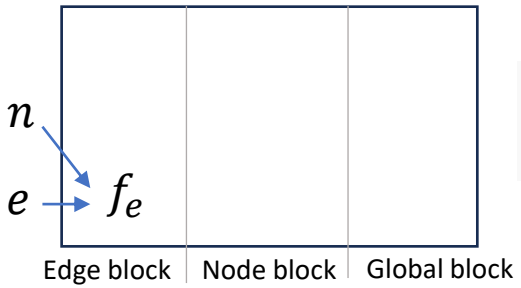


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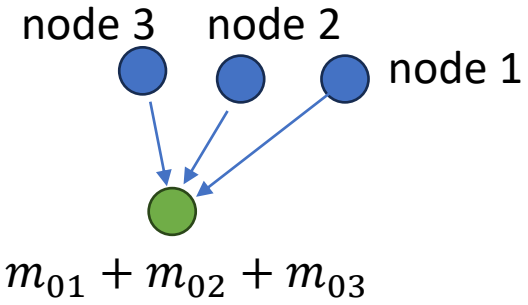
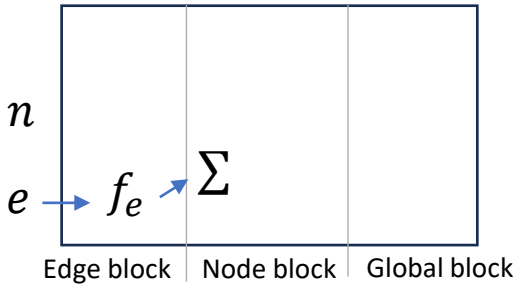
    edge_features = torch.cat([x[start], x[end]], dim=1)
    e = self.edge_network(edge_features)
    return e
```

2. Aggregate messages

$$a_i^l = \sum_j (m_{ij}^l)$$

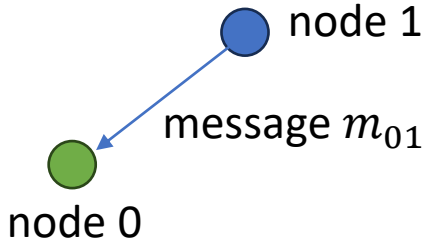
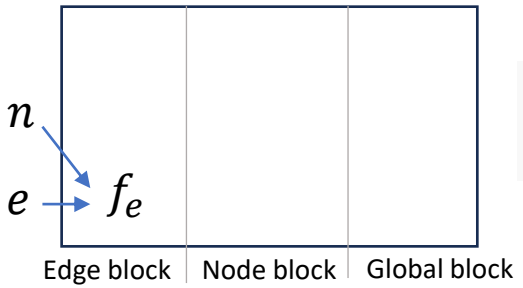


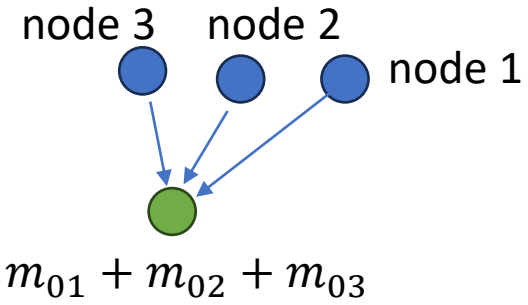
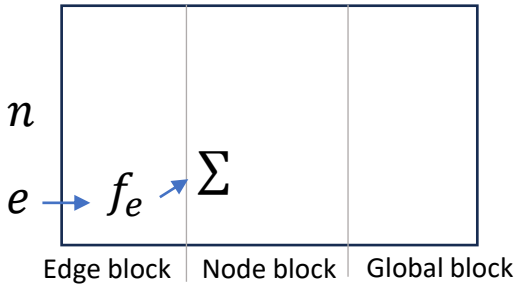
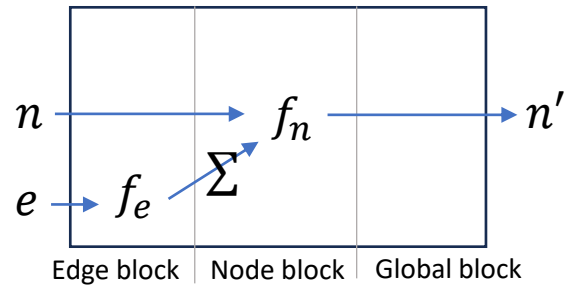



```
x = scatter_add(e, end)
```

Let's put it all together…

	Equations	Pictures	GNN Blocks	Code

1. Calculate messages	$m_{ij}^l = f_e(n_i^k, n_j^k)$, where there are edges between $i \rightarrow j$			`def message_passing(self, x, start, end):`
				`edge_features = torch.cat([x[start], x[end]], dim=1)`
				`e = self.edge_network(edge_features)`
				`return e`

2. Aggregate messages	$a_i^l = \sum_j (m_{ij}^l)$			`x = scatter_add(e, end)`
3. Update nodes	$n'^k_i = f_n(a_i^l, n_i^k)$			`x = self.node_network(x)`

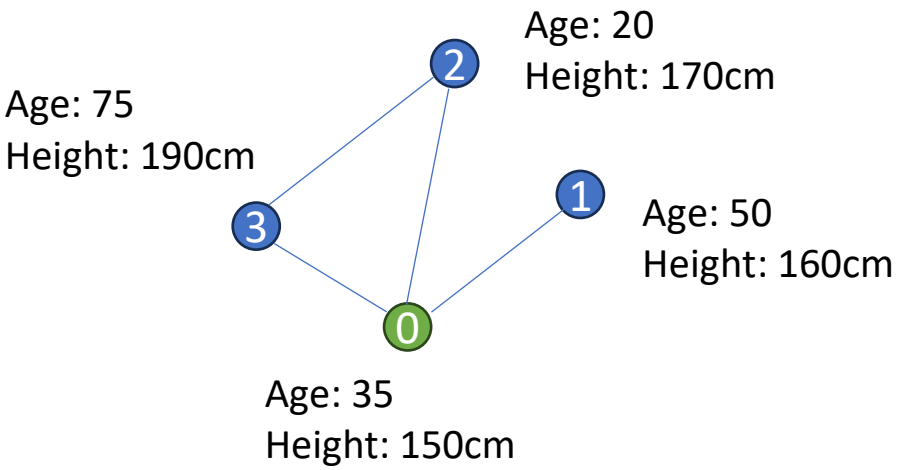
Let's put it all together… with an example!

Let's assume our "learned" message function is just:

$$f_e(n_i^k, n_j^k) = n_i^k - n_j^k$$

and our "learned" node update function is just:

$$f_n(a_i^k, n_i^k) = \frac{1}{2}(a_i^k + n_i^k)$$



$$n_i^k = \begin{bmatrix} 20 & 170 \\ 50 & 160 \\ 35 & 150 \\ 75 & 190 \end{bmatrix}$$

$$E_{ij} = \begin{bmatrix} 0 & 0 & 0 & 2 & 1 & 2 & 3 & 3 \\ 1 & 2 & 3 & 3 & 0 & 0 & 0 & 2 \end{bmatrix}$$

1. Calculate messages

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$$m_{01}^l = [20 - 50, 170 - 160] = [-30, 10]$$

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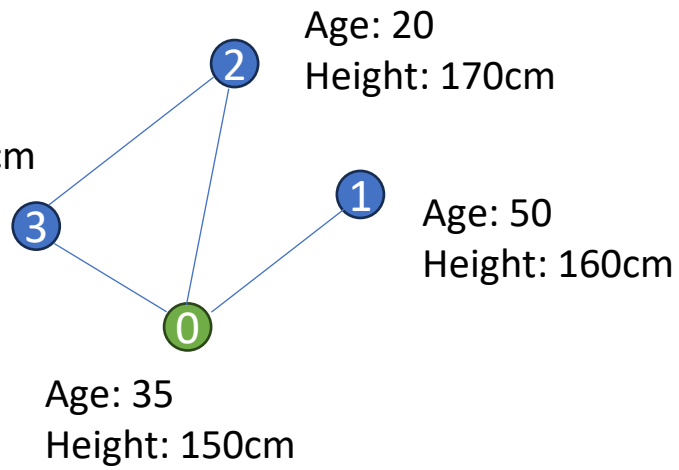

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$$m_{ij}^l = \left[\begin{bmatrix} -30 \\ 10 \end{bmatrix}, \begin{bmatrix} -15 \\ 20 \end{bmatrix}, \begin{bmatrix} -55 \\ -20 \end{bmatrix}, \begin{bmatrix} -40 \\ -40 \end{bmatrix}, \begin{bmatrix} 30 \\ -10 \end{bmatrix}, \begin{bmatrix} 15 \\ 20 \end{bmatrix}, \begin{bmatrix} 55 \\ 20 \end{bmatrix}, \begin{bmatrix} 40 \\ 40 \end{bmatrix}\right]$$

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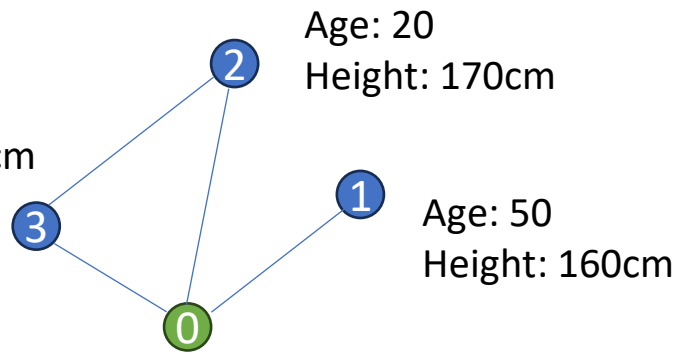

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2. Aggregate messages

$$a_i^l = \sum_j (m_{ij}^l)$$

$$\begin{aligned} a_0^l &= m_{01}^l + m_{02}^l + m_{03}^l \\ &= \begin{bmatrix} -30 \\ 10 \end{bmatrix} + \begin{bmatrix} -15 \\ 20 \end{bmatrix} + \begin{bmatrix} -55 \\ -20 \end{bmatrix} \\ &= \begin{bmatrix} -100 \\ 10 \end{bmatrix} \end{aligned}$$

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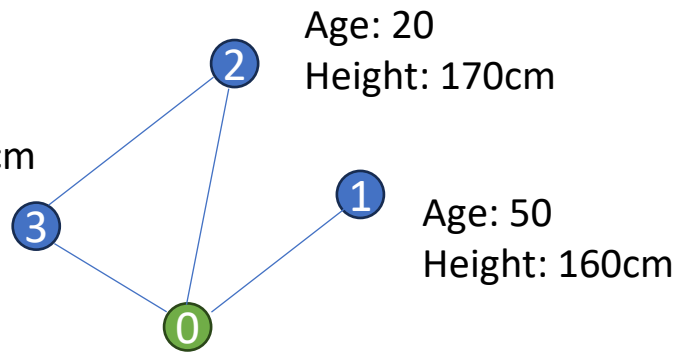

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2. Aggregate messages

$$a_i^l = \sum_j (m_{ij}^l)$$

$$a_i^l = [\begin{bmatrix} -100 \\ 10 \end{bmatrix}, \begin{bmatrix} 30 \\ -10 \end{bmatrix}, \begin{bmatrix} -25 \\ -20 \end{bmatrix}, \begin{bmatrix} 95 \\ 60 \end{bmatrix}]$$

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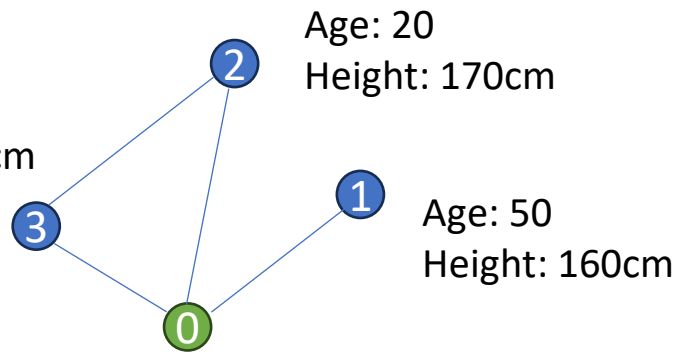

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3. Update nodes

$$n'^k_i = f_n(a_i^l, n_i^k)$$

$$n'^k_0 = f_n(a_0^l, n_0^k) = \frac{1}{2}(\begin{bmatrix} -100 \\ 10 \end{bmatrix} + \begin{bmatrix} 20 \\ 170 \end{bmatrix}) = \begin{bmatrix} -40 \\ 90 \end{bmatrix}$$

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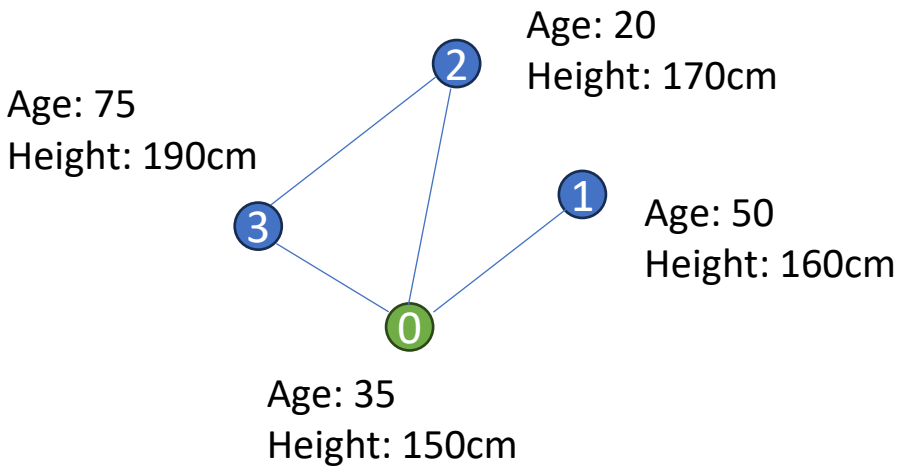

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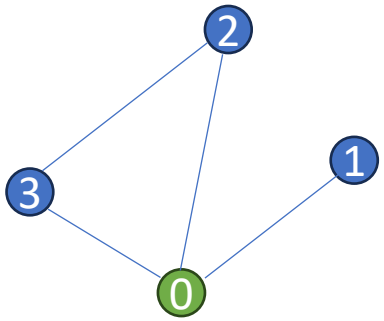
3. Update nodes

$$n'^k_i = f_n(a_i^l, n_i^k)$$

$$n'^k_i = \begin{bmatrix} -40 & 90 \\ 40 & 75 \\ 5 & 65 \\ 85 & 125 \end{bmatrix}$$

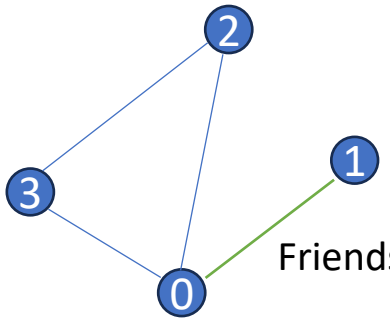
GNN tasks vs. architectures

- Just like with the CNN, the choice of GNN convolution is usually separate from the final training task
- Any GNN convolution that does message passing, and updates hidden node features, allows us to predict:



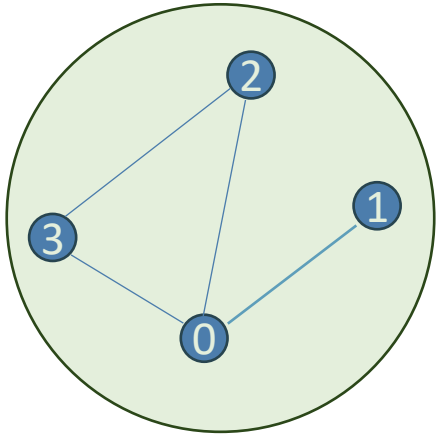
Age: ?
Height: ?

Node features



Friendship status?

Edge features



Class topic?

Global features

The Transformer as a GNN

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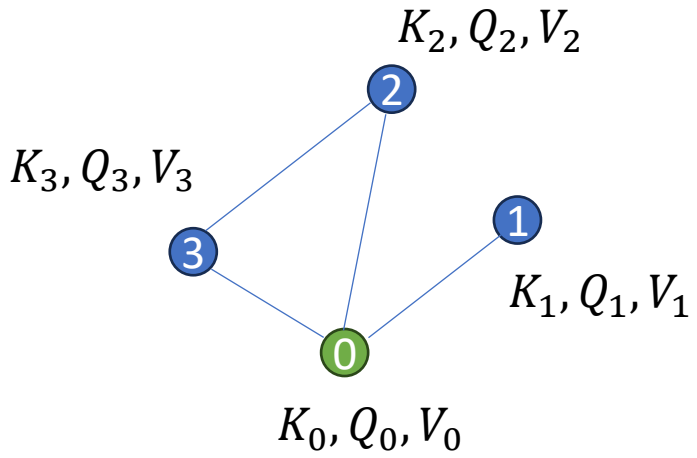
Let's build a ***very*** specific graph convolution…

- For each node, attach *three* sets of hidden features: K, Q, V



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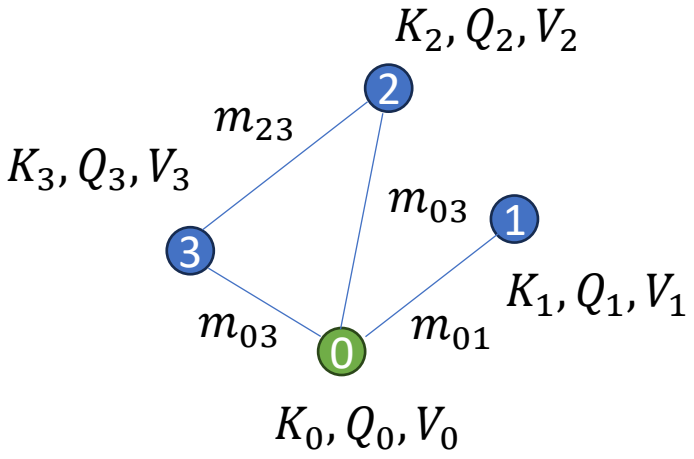
- For each node, attach *three* sets of hidden features: K, Q, V
- Define a message function on each edge:

$$m_{ij} = f_e\left(K_i^k, Q_j^k\right) = softmax\left(\sum_k K_i^k Q_j^k\right)$$



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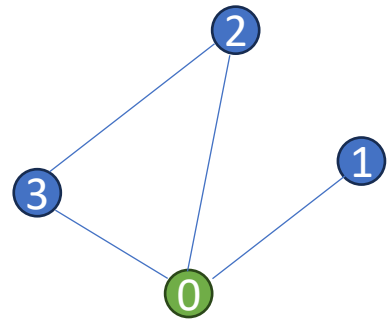
- Define an aggregation function around each node:

$a_i^k = \sum_j m_{ij} V_j^k$, this is just a weighted sum



$V_0 m_{01} + V_0 m_{02} + V_0 m_{03}$

Let's build a ***very*** specific graph convolution…

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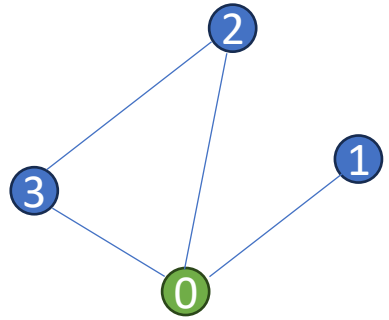

$f_n^K(a_i), f_n^Q(a_i), f_n^V(a_i)$

- Define an aggregation function around each node:

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- The node update is just FFNNs to get the next K', Q', V'

Let's build a ***very*** specific graph convolution…

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THIS IS A TRANSFORMER

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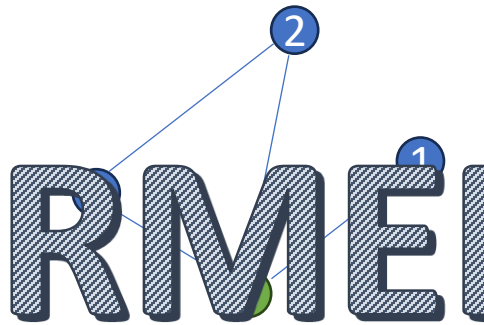
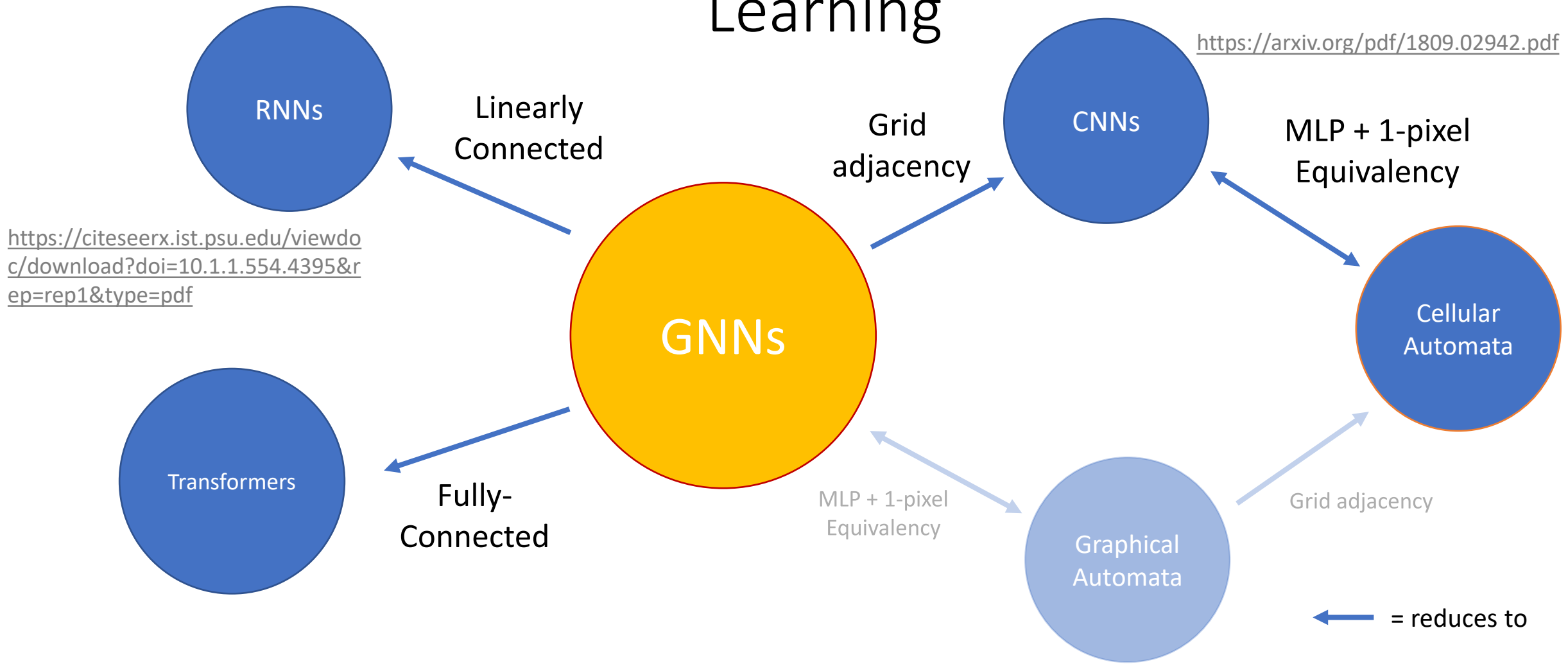


The Landscape of Geometric Deep Learning



https://github.com/murnanedaniel/GNN-as-Transformer-as-GNN/blob/main/0-Transformer_vs_GNN_Annotated.ipynb
https://arxiv.org/pdf/2012.09699.pdf

Case Studies

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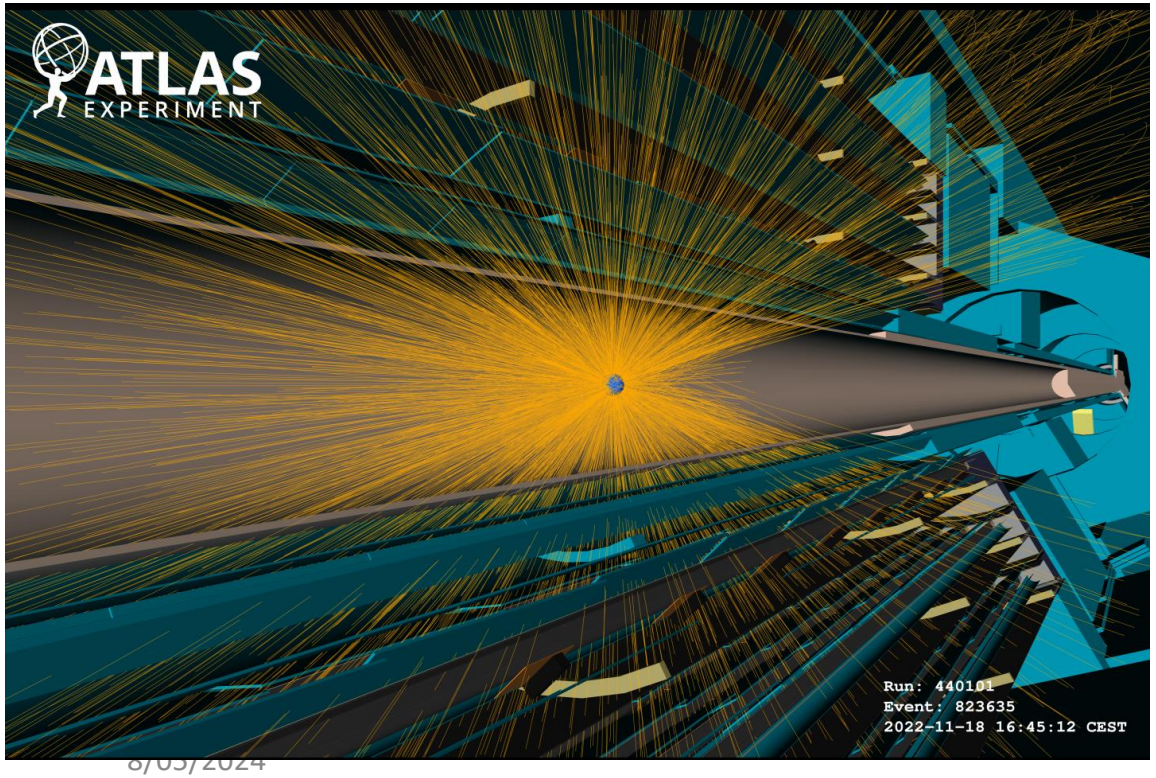
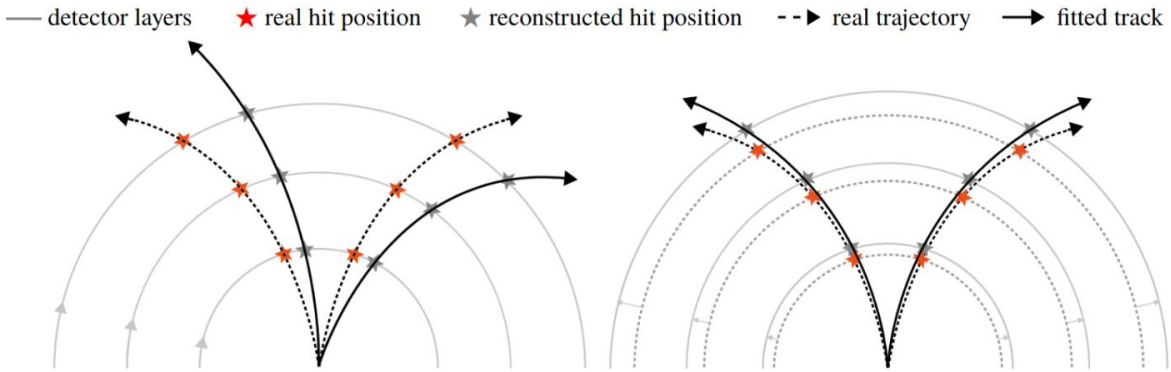
Google Maps

- DeepMind worked with Google Maps developers to apply a GNN to estimate travel time
- Improved estimates by up to 50% in large cities
- Maps are *really* hard to optimize on, as they exhibit combinatorial behavior
- GNNs can give fast, approximate solutions to map problems

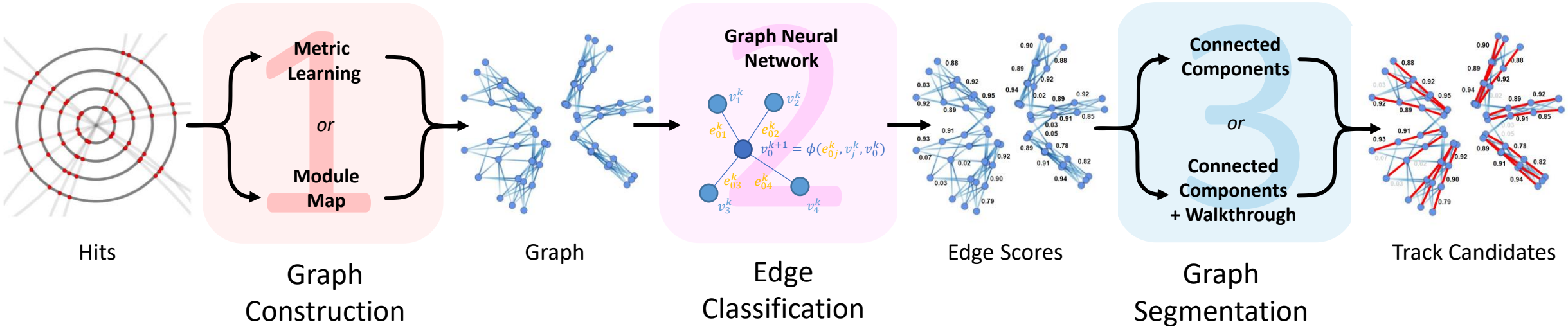
Edge Classification for Particle Tracking

- In the ATLAS experiment, we need to connect points in the detector to reconstruct particle tracks
- It's a massive connect-the-dots game, with 300,000 dots to connect, every 25 nanoseconds





Edge Classification for Particle Tracking



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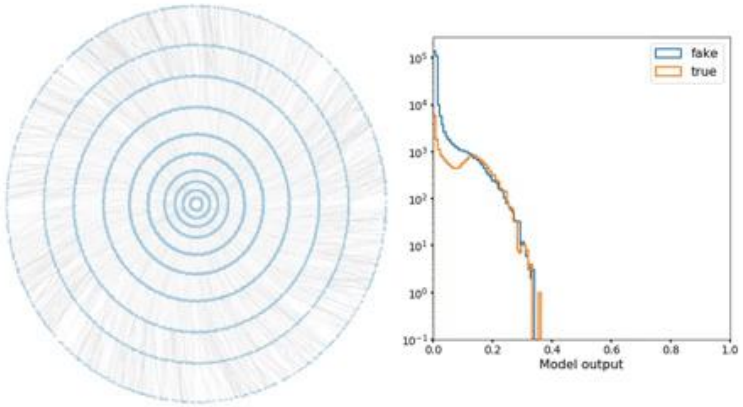

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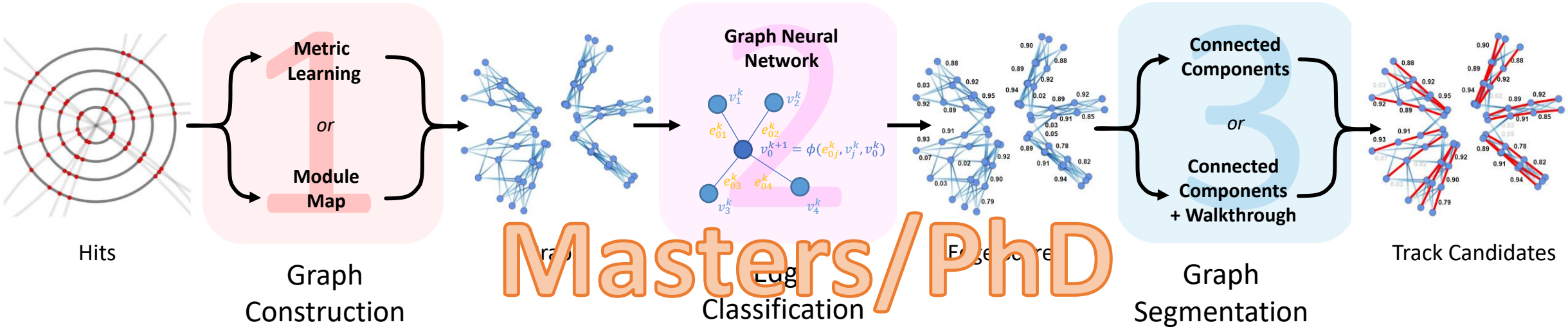

Masters/PhD projects available!

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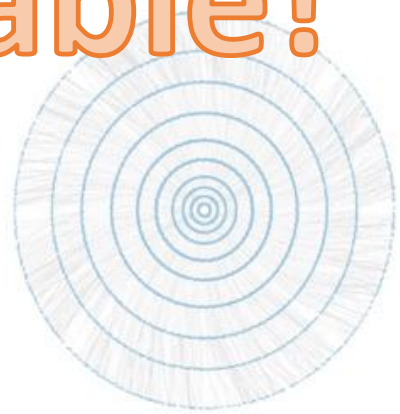
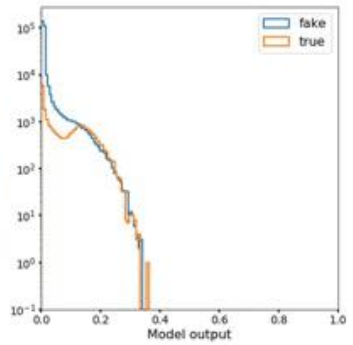
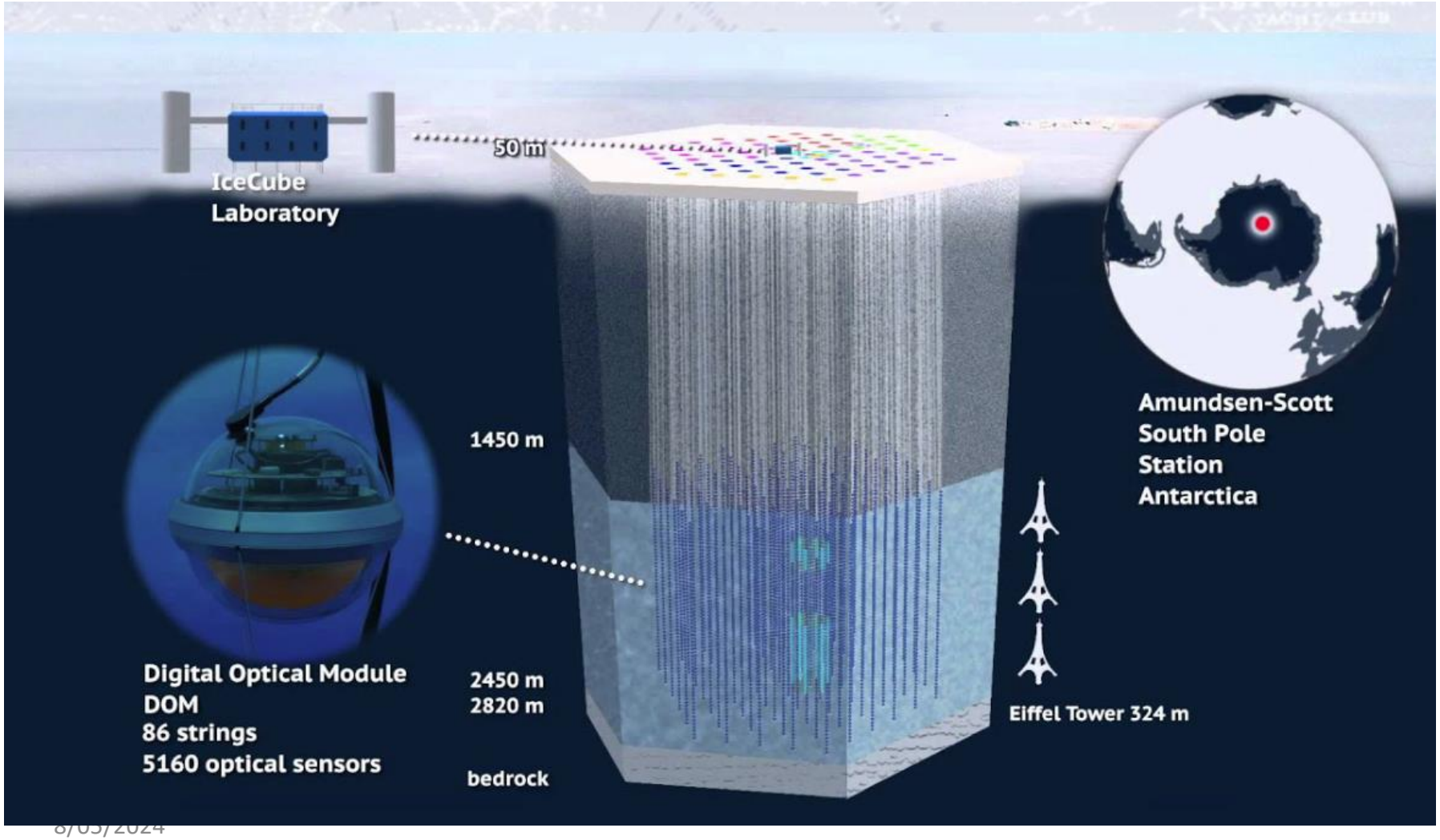


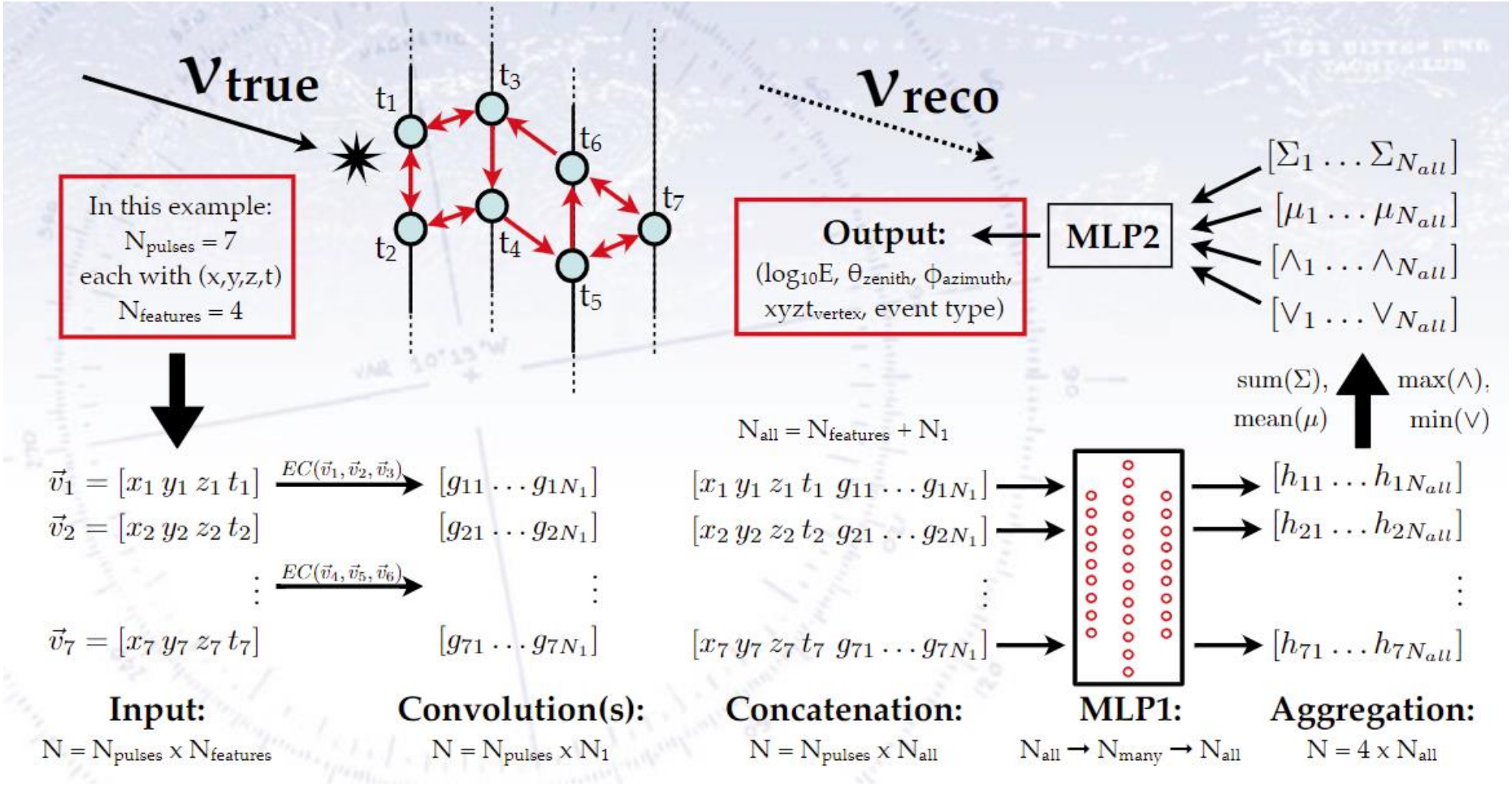


Ice Cube neutrino prediction



- Neutrino observatory inside the ice of Antarctica
- Goal is to detect neutrinos and measure precisely the direction they came from, their energy, what type of neutrino they are, etc.

Ice Cube neutrino prediction



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