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Graph Neural Networks for Reconstruction in Liquid Argon Time Projection Chambers

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CLARIPHY meeting

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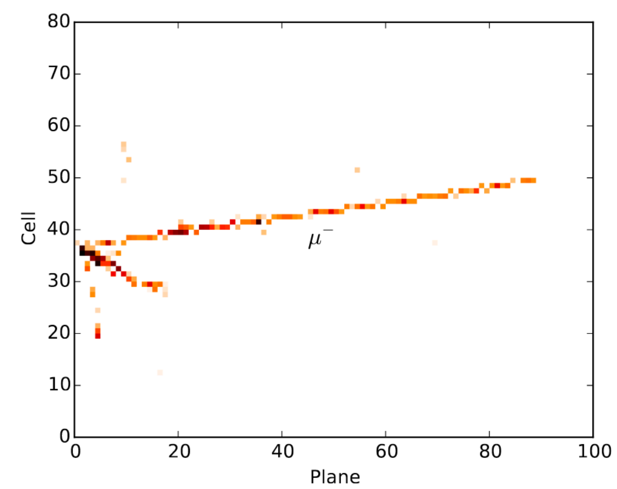
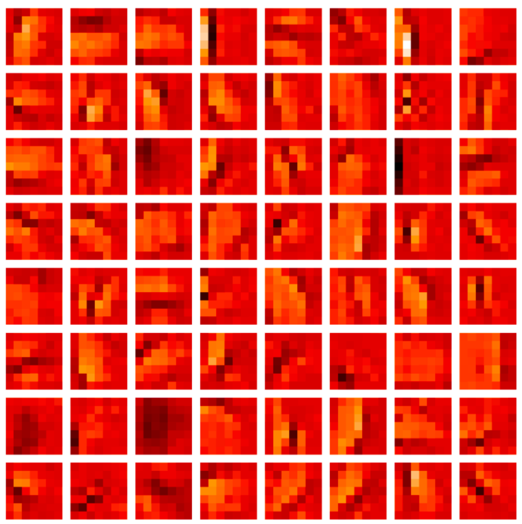
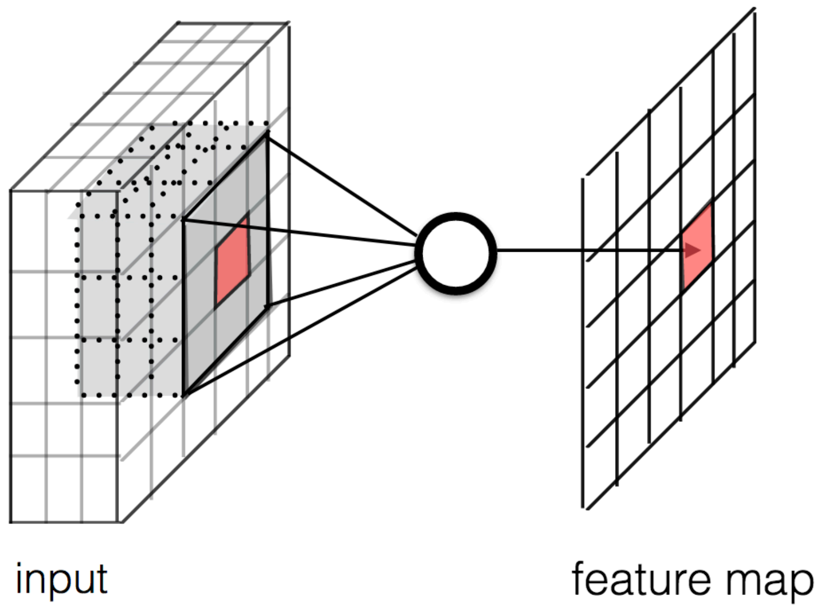
Neutrino physics

- Convolutional neural networks show great promise in image classification over the past decade.
- Most neutrino detector technologies naturally provide pixel maps which can be classified using CNNs.
- Examples: NOvA, MicroBooNE, DUNE.





arXiv:1604.01444

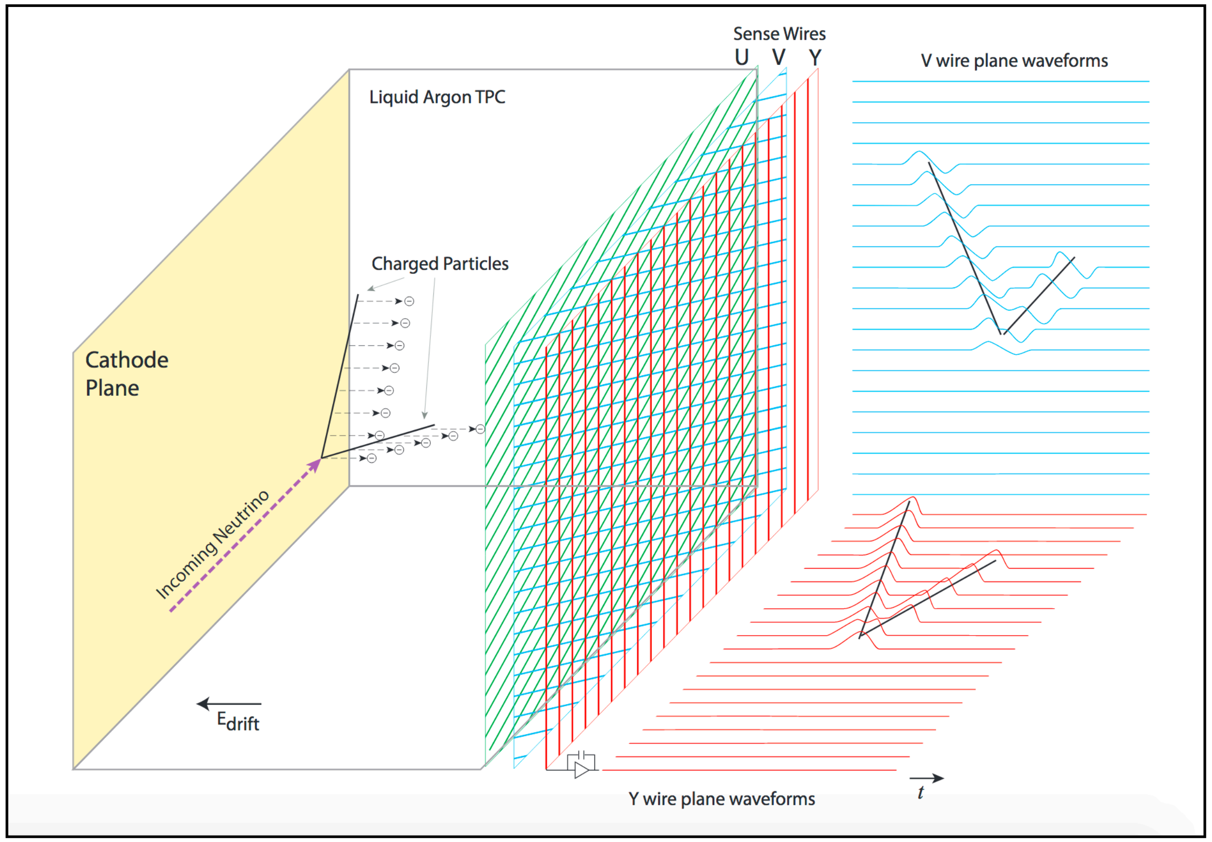


- Issues with this approach:
  - **Dense** representation of **sparse** data.
  - Operate over mostly empty space!
  - Need to transform 3D representation into voxels.
- GNNs can work with reconstructed spacepoints natively.

Liquid Argon Time Projection Chambers

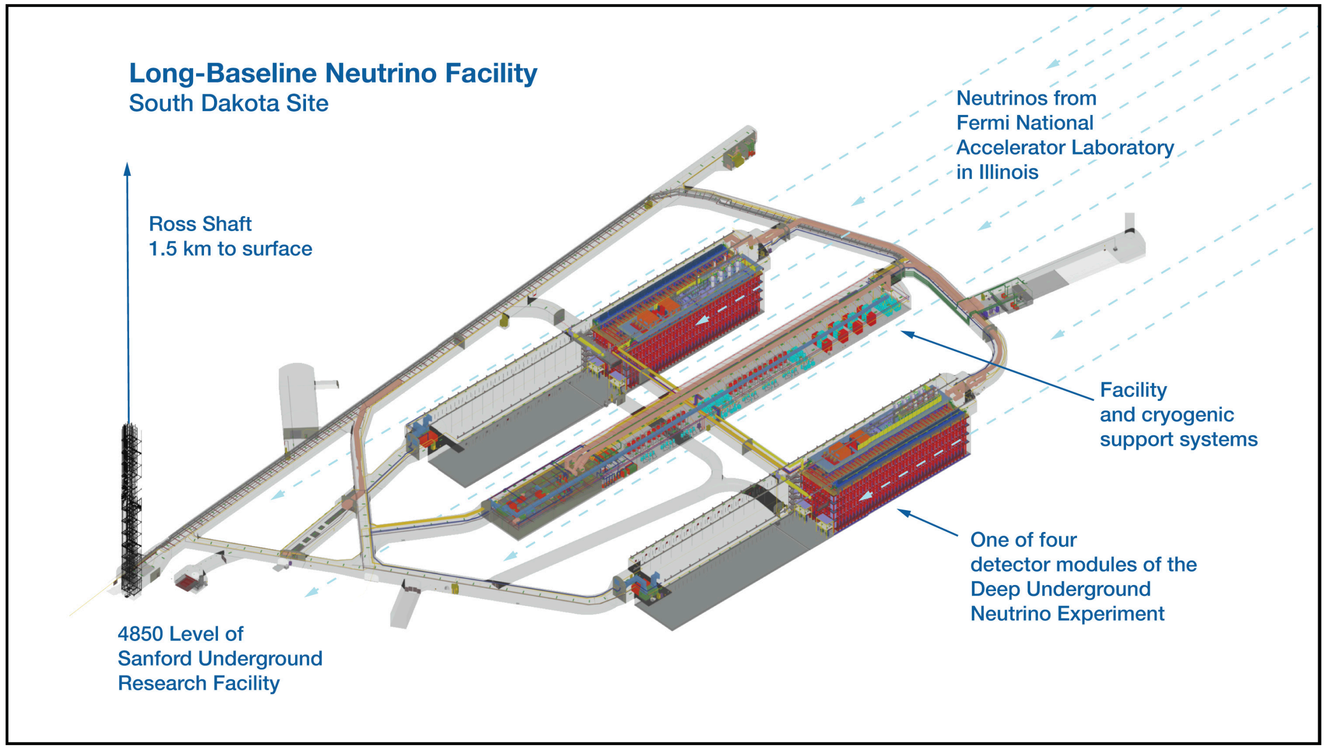
- Liquid Argon Time Projection Chambers (LArTPCs) are currently a very important detector technology for neutrino physics.
  - At FNAL: MicroBooNE, Icarus, SBND.
  - Future: DUNE (70kT LArTPC deep underground, plus near detector).

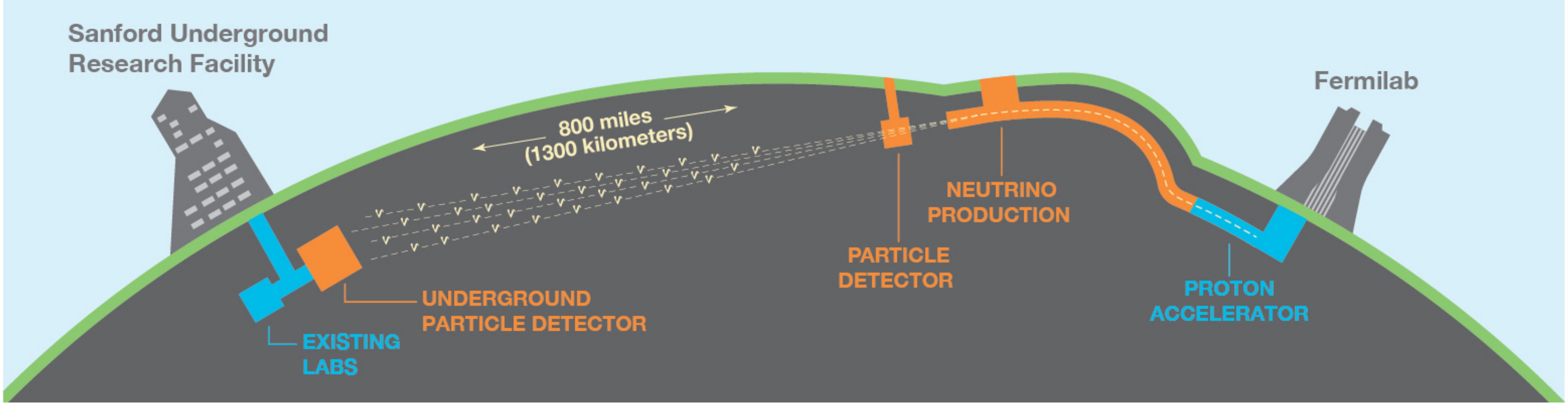
- Charged particles ionize liquid argon as they travel.
- Ionisation electrons drift due to HV electrode field, and are collected by anode wires.
- Wire spacing ~3mm – produce **high-resolution images**.



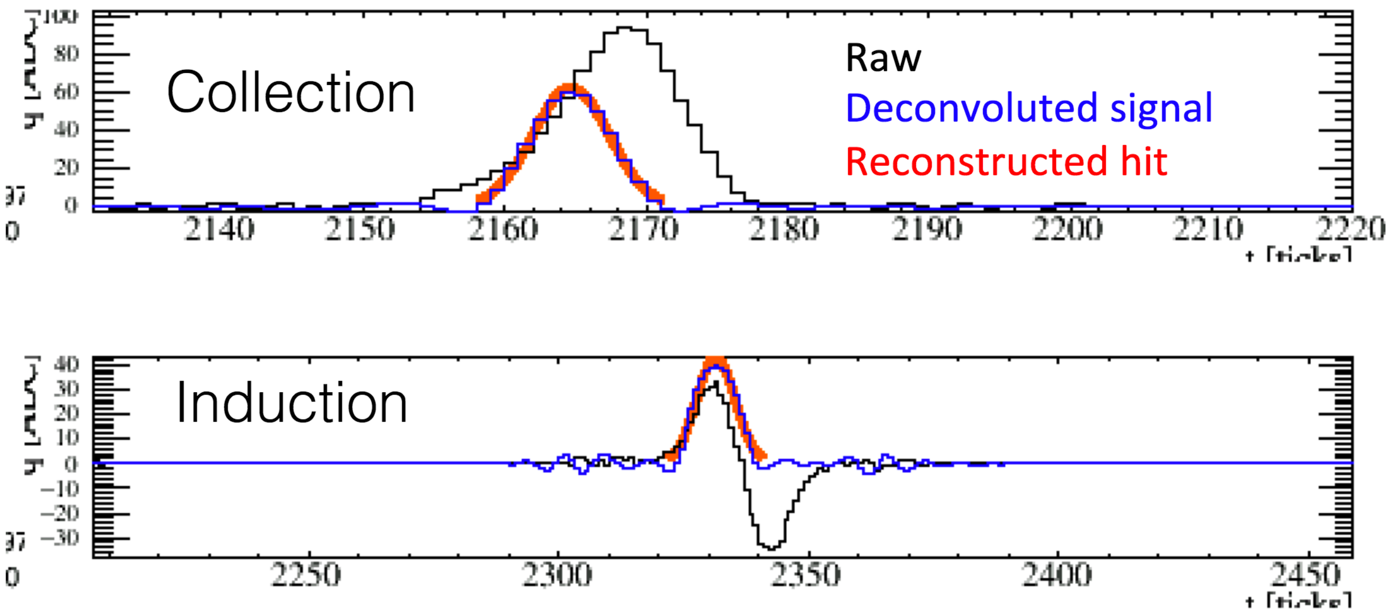
DUNE far detector

- **70 kt** LArTPC, **1.5km** underground.
- High exposure in low-background environment.
- **Modular design:**
  - Four large detector modules.
  - Each consists of 200 individual TPCs.
  - Transformations necessary to combine data across multiple modules in 2D.

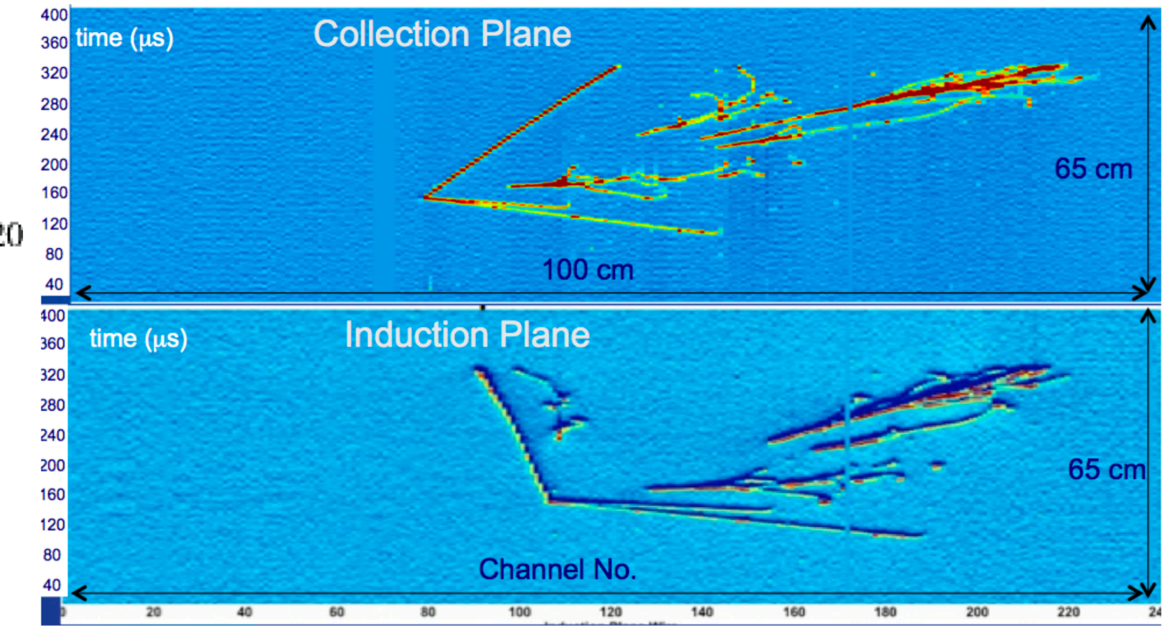




Standard reconstruction chain



T. Yang (ICHEP 2016)

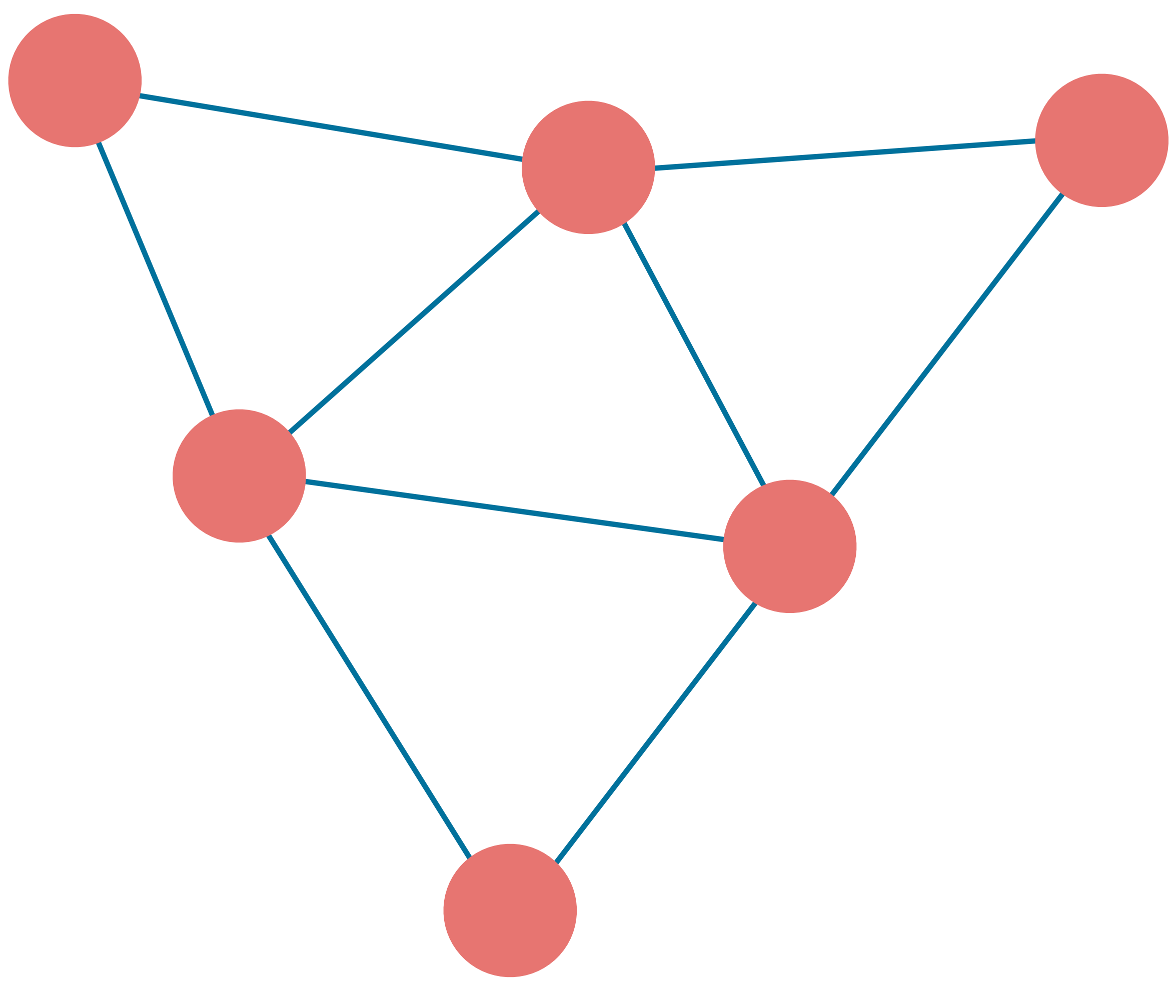


ArgoNeuT data event

- Raw TPC output is wire waveforms.
- Waveforms are then deconvolved and hit-finding is applied to produce Gaussian hits.
- Each wire plane forms a 2D image in the space of wire vs readout time.
- Three wire planes angled at -36°, 0°, 36° provide three 2D representations of the event.
- These 2D representations can be used to construct a 3D representation of the event.

Graph neural networks

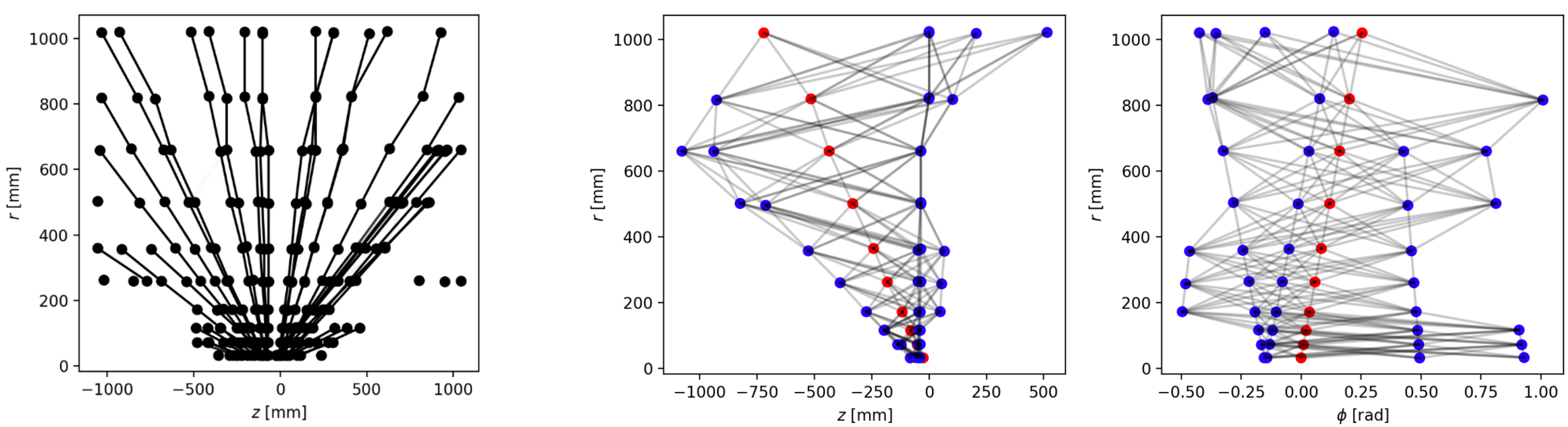
- Describe information structure as a **graph** represented by **nodes** and **edges**.



- **Nodes** are generalised as quantised objects with some arbitrary set of **features**.
- **Edges** describe the **relationships** between nodes.
- Perform convolutions on nodes and edges to learn relationships within the graph.
- Output is user-defined:
  - Classify nodes or edges.
  - Classify full graph.
  - Regression outputs.

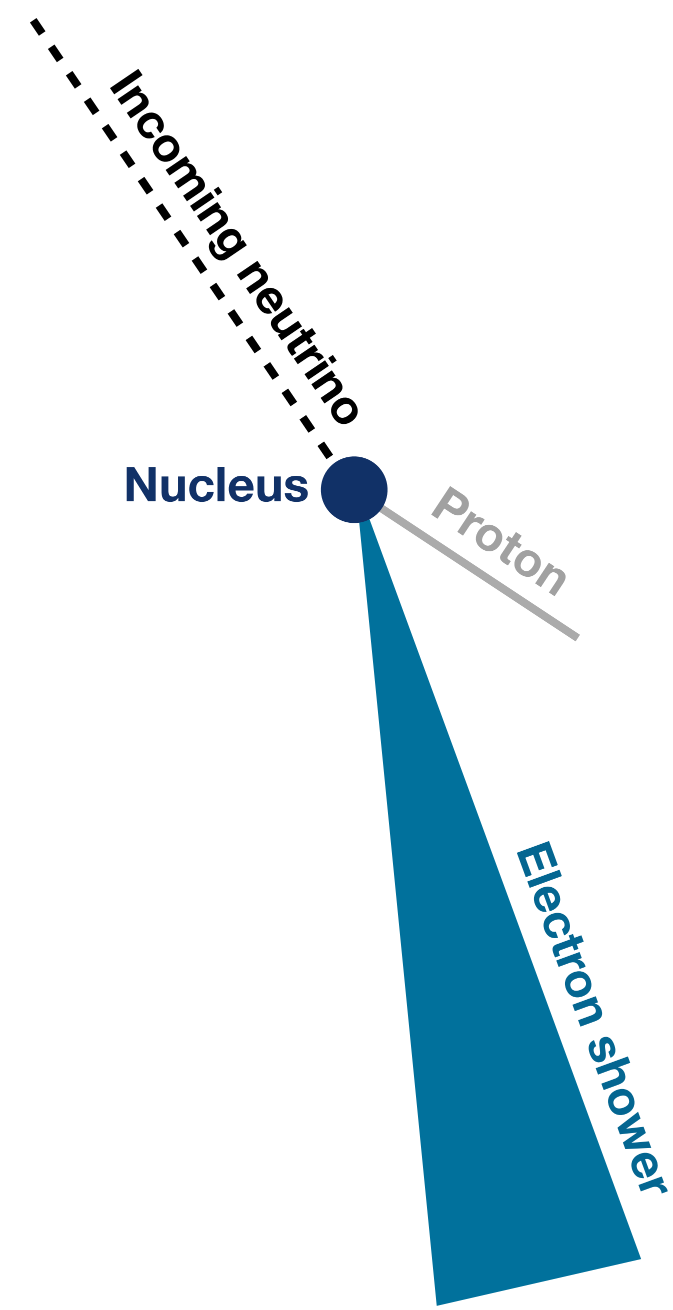
Graph networks in HEP

- Investigating the use of **Graph Neural Networks (GNNs)** as an alternative to Convolutional Neural Networks (CNNs).
- Building on promising results from the **HEP.TrkX** collaboration using such methods for track reconstruction in the LHC world.
- **Exa.TrkX** project building on these results to further develop techniques in HL-LHC, and branch out to explore other detector technologies like LArTPCs.

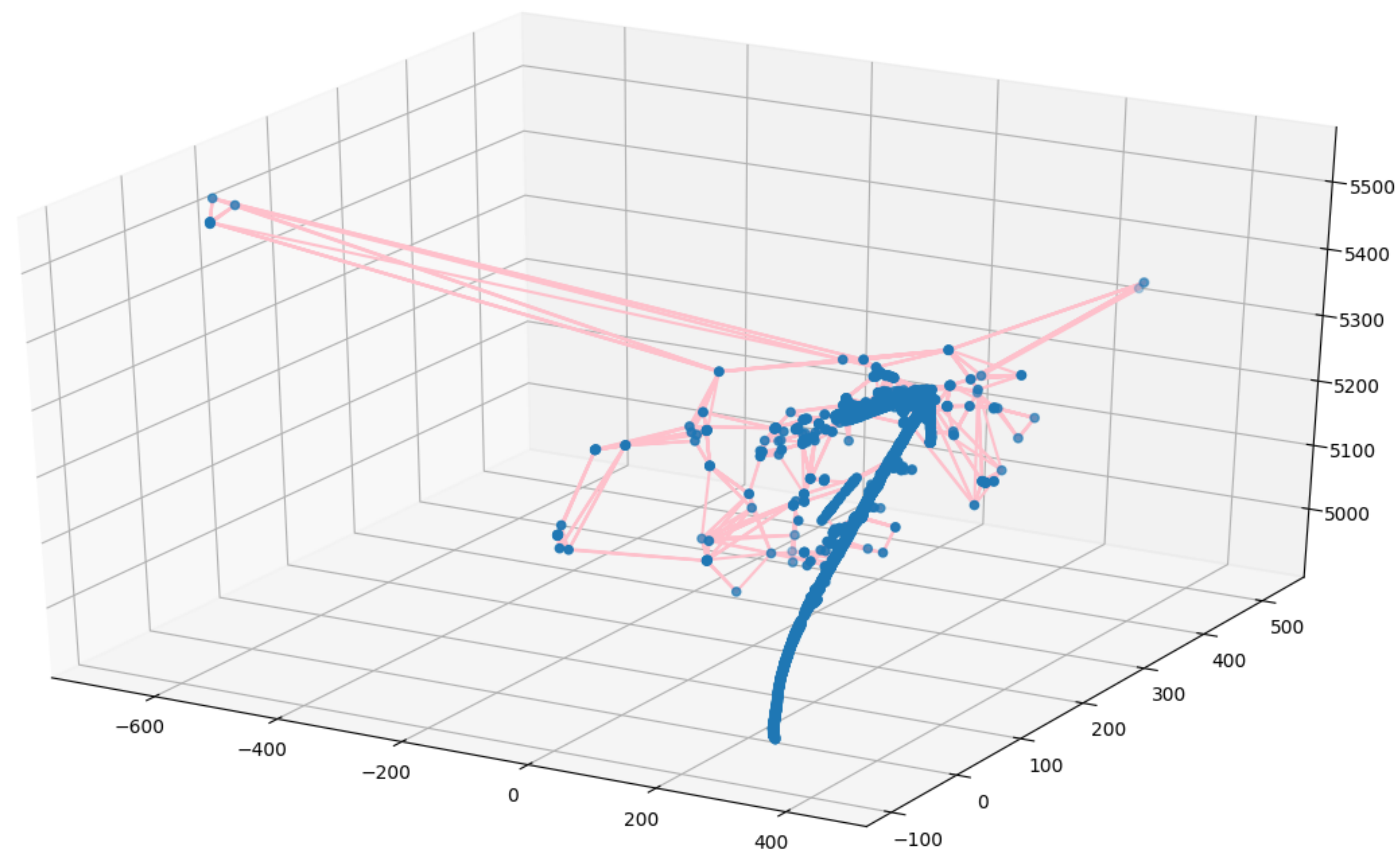


Simulation

- Utilising two sets of simulation for these studies:
  - **Atmospheric neutrino interactions**
    - Higher in primary neutrino energy (typically ~tens of GeV).
    - Broad angular distribution.
    - Higher occupancy events.
  - **CCQE beam neutrino interactions**
    - Few-GeV energy.
    - Neutrinos travel along beam direction.
    - Typically “clean” interactions – primary lepton (e,μ) and minimal hadronic activity.

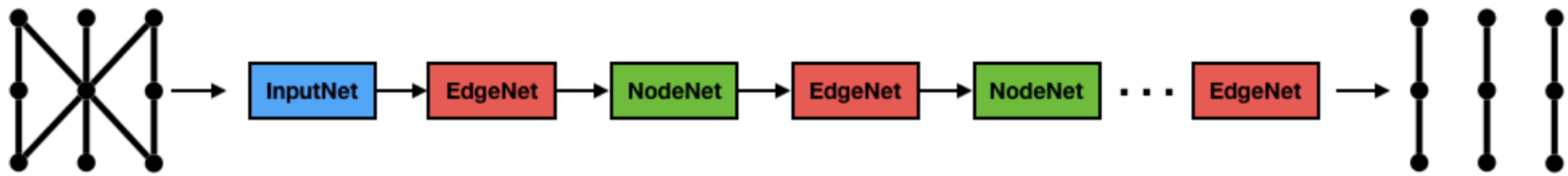


Clustering



- First approach: cluster reconstructed spacepoints in 3D.
- Draw potential connections between 3D spacepoints.
- Classify edges as true or false based on whether the same underlying simulated particle was responsible for producing them.

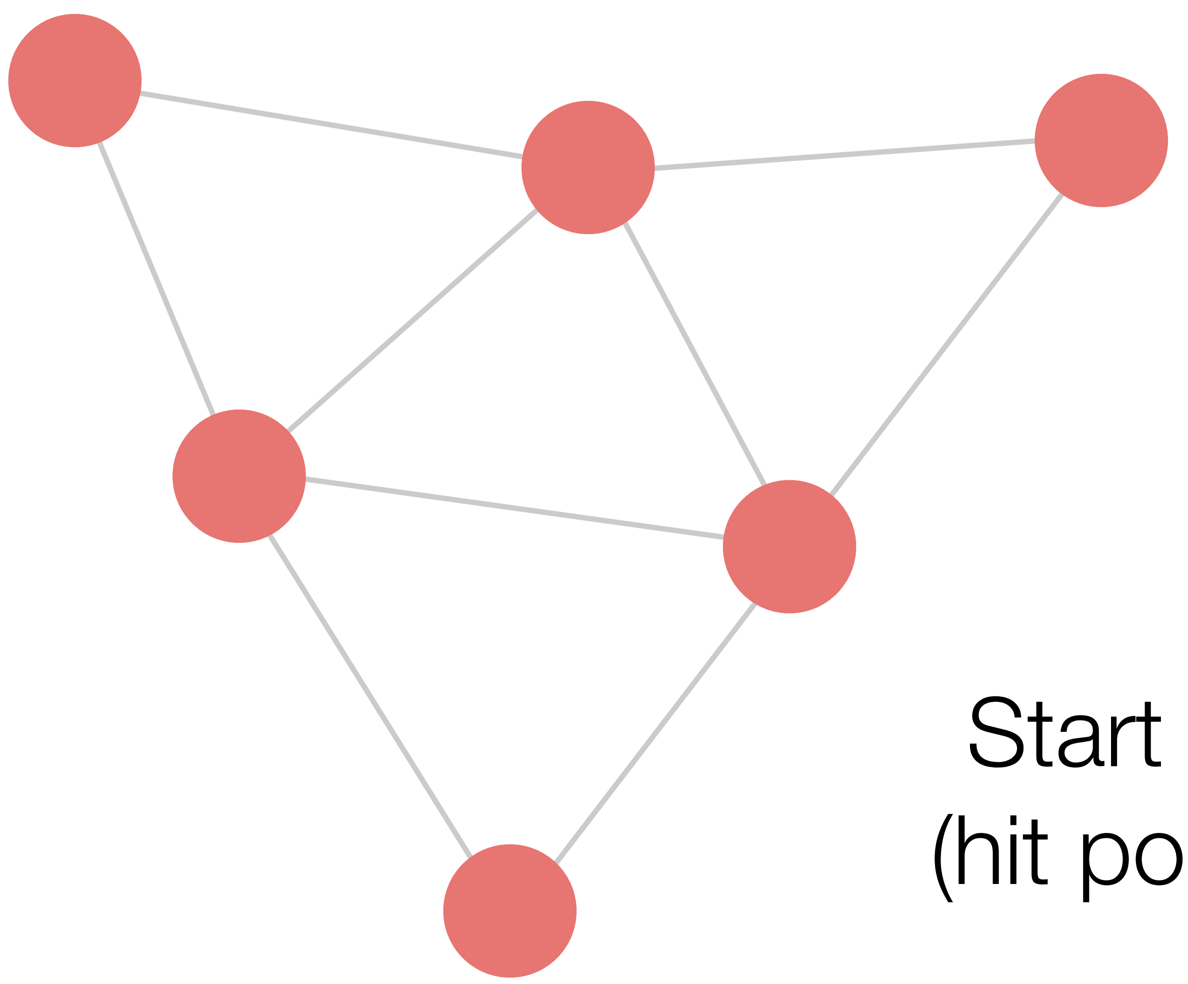
Message-passing networks



arxiv:1810.06111

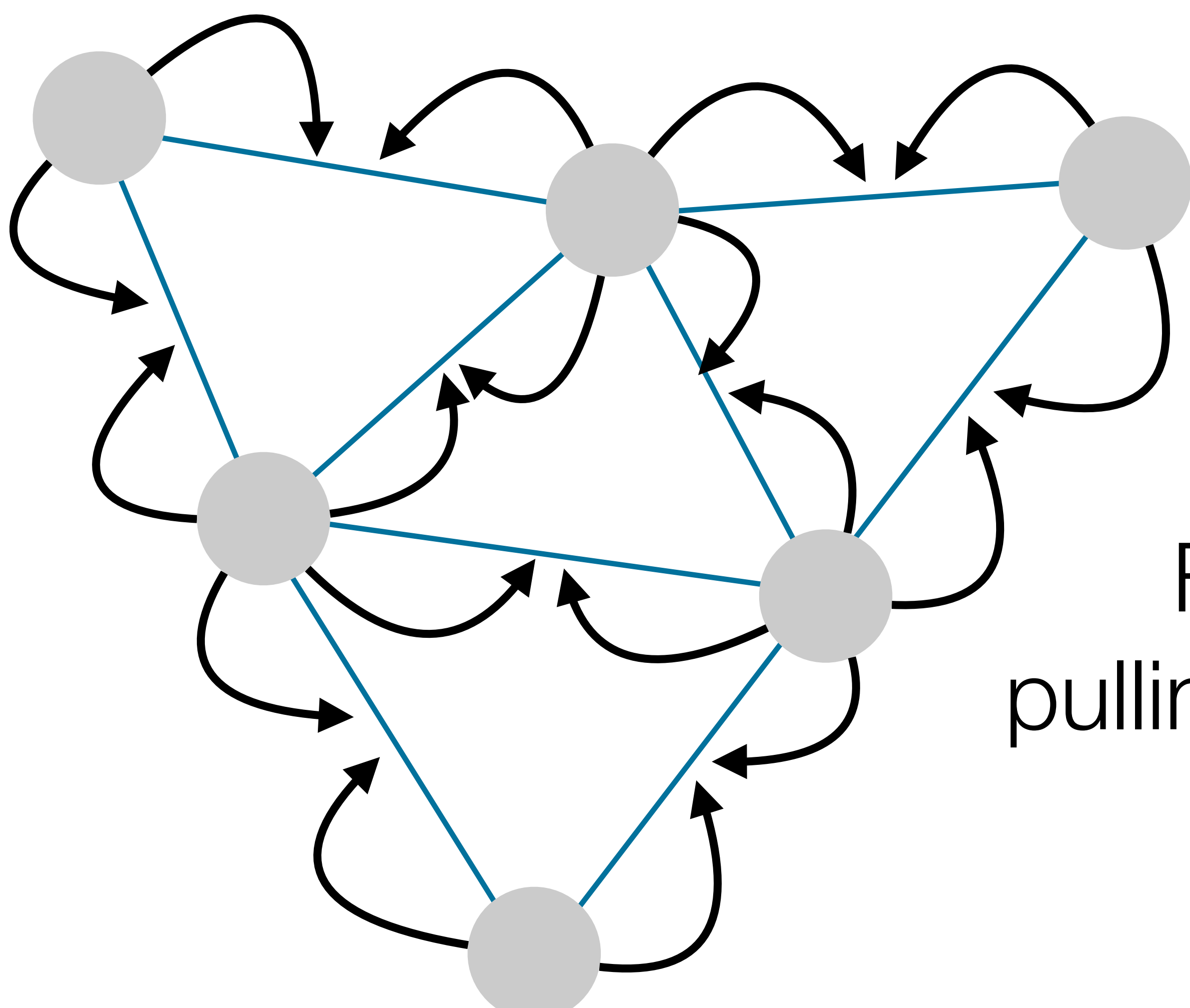
- Message-passing network aggregates information from neighbouring nodes across edges to form new features on each node, utilising an attention mechanism to weight up useful edges.
- Repeat the same network multiple times in order for information to travel further across the graph over multiple iterations (the "message passing").
- **Edge classifier:**
    - Input for each node is the features of incoming and outgoing nodes.
    - Two multi-layer perceptrons, using Tanh and sigmoid activations.
    - Outputs sigmoid score on each edge.
- **Node classifier:**
    - Uses edge score to aggregate each node's features with incoming & outgoing edges as input.
    - Two multi-layer perceptrons with Tanh activation.
    - Produces new features for each node.

Message-passing network



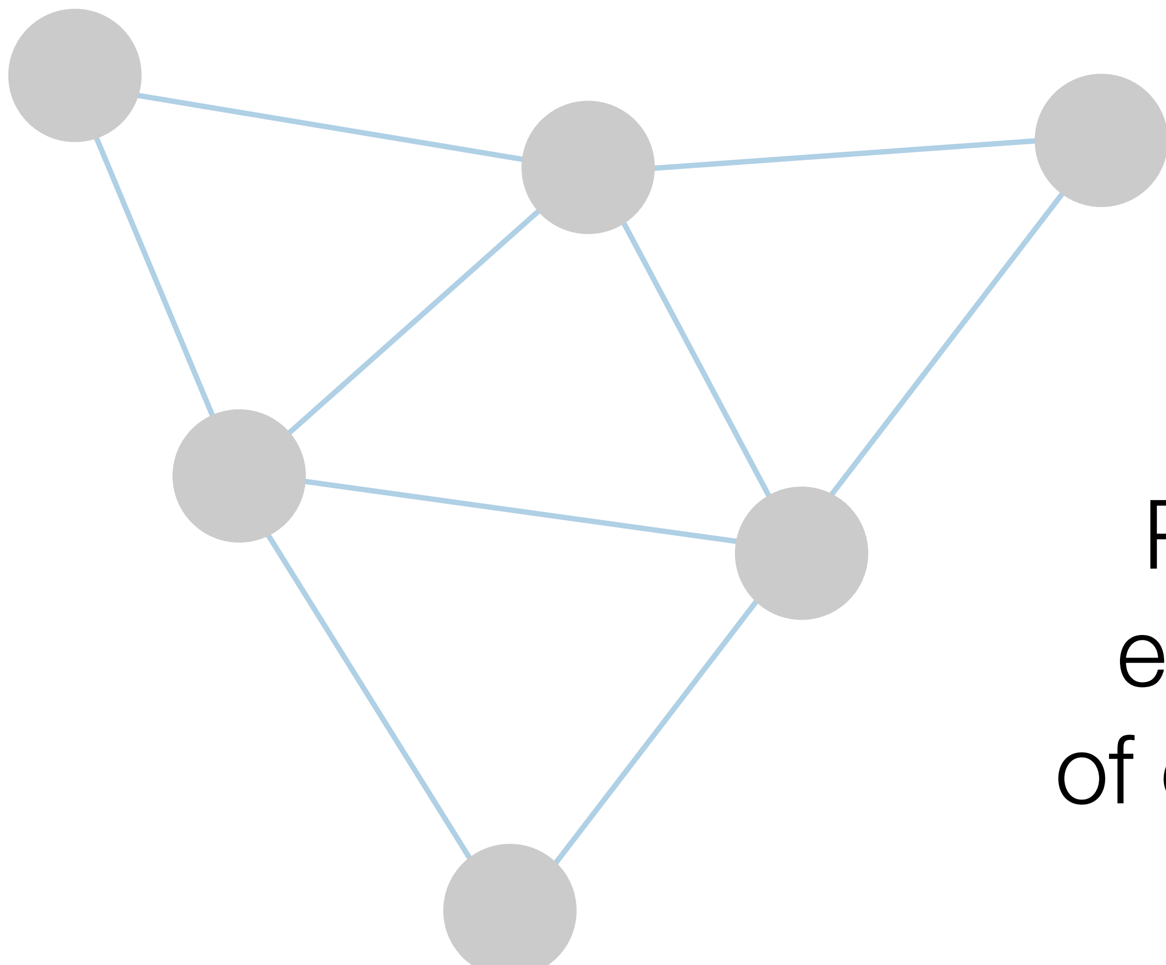
Start with graph **node features**
(hit position, amplitude, RMS, etc)

Message-passing network



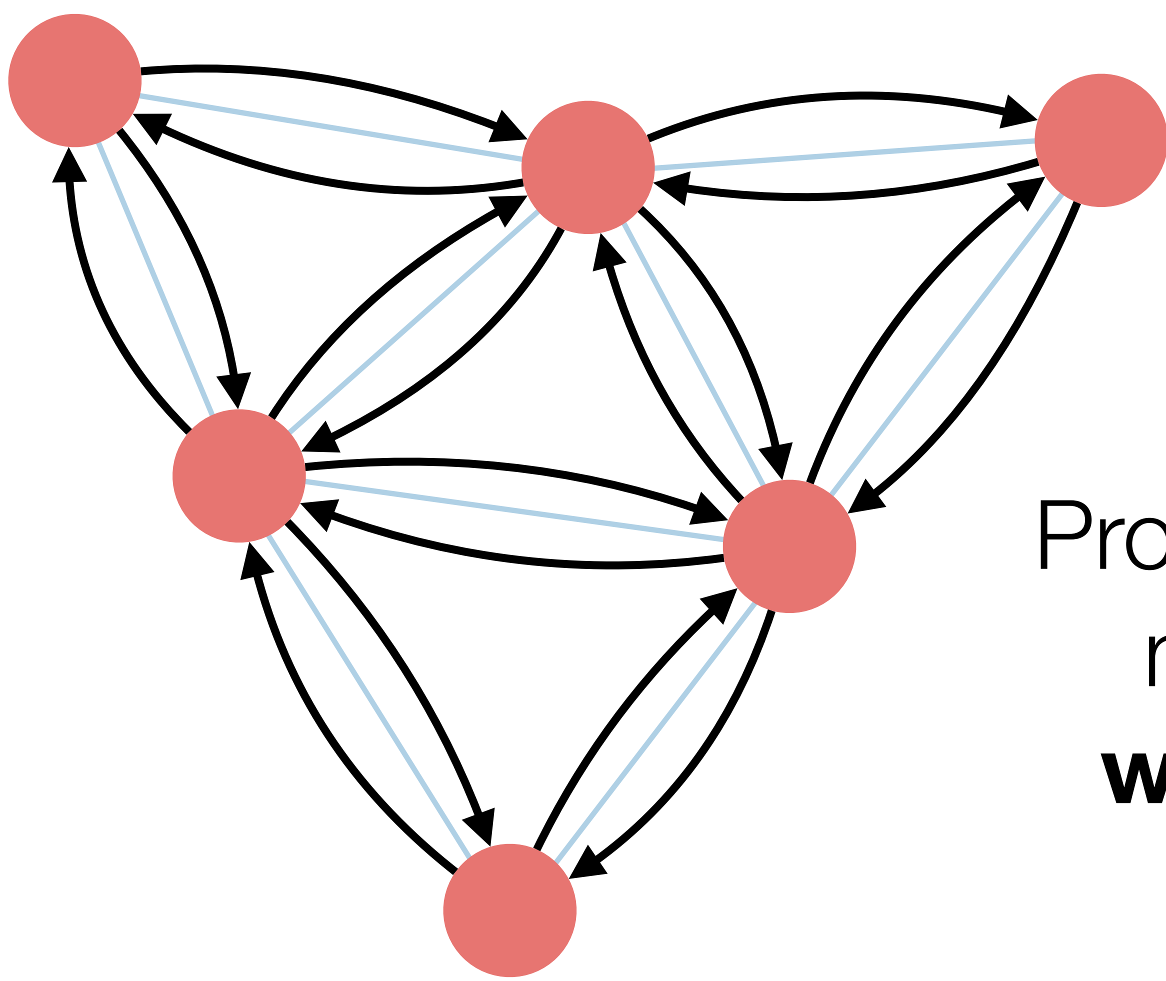
Form **edge features** by pulling in features from incoming and outgoing node

Message-passing network



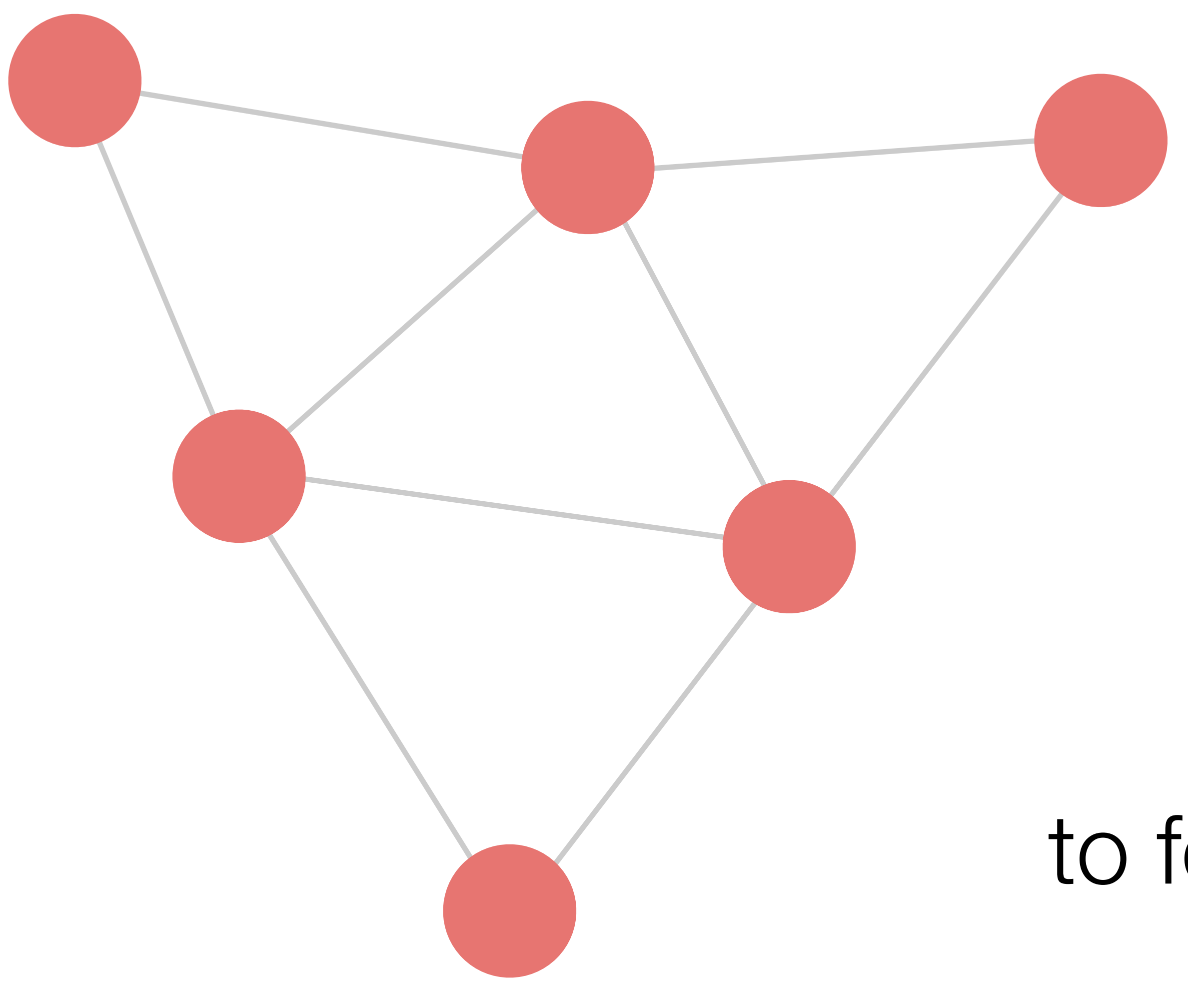
Perform convolutions on edge scores to form a set of **class-wise probabilities**

Message-passing network



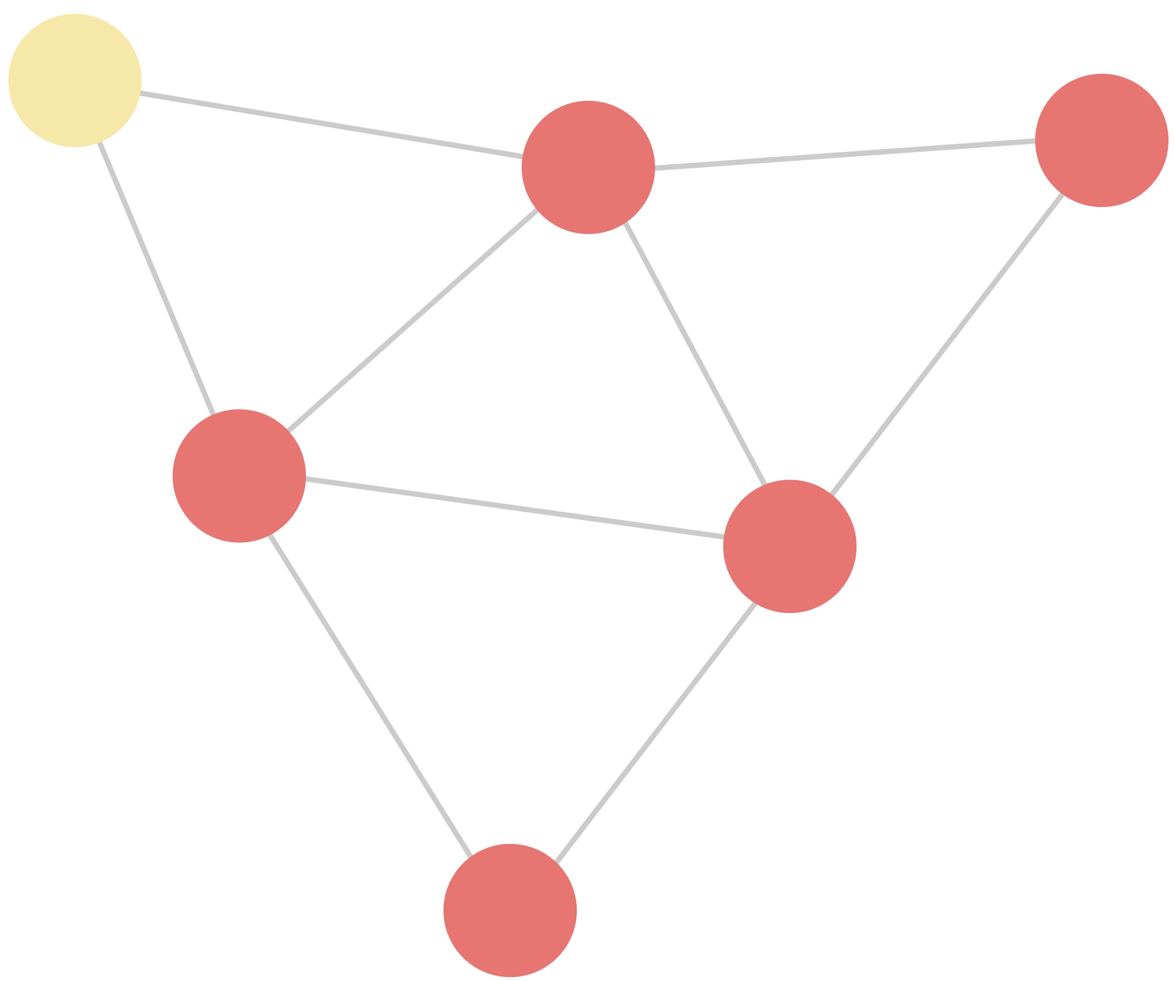
Propagate features from each node to adjacent nodes, **weighted by edge score**

Message-passing network



Perform convolutions
to form new **node features**

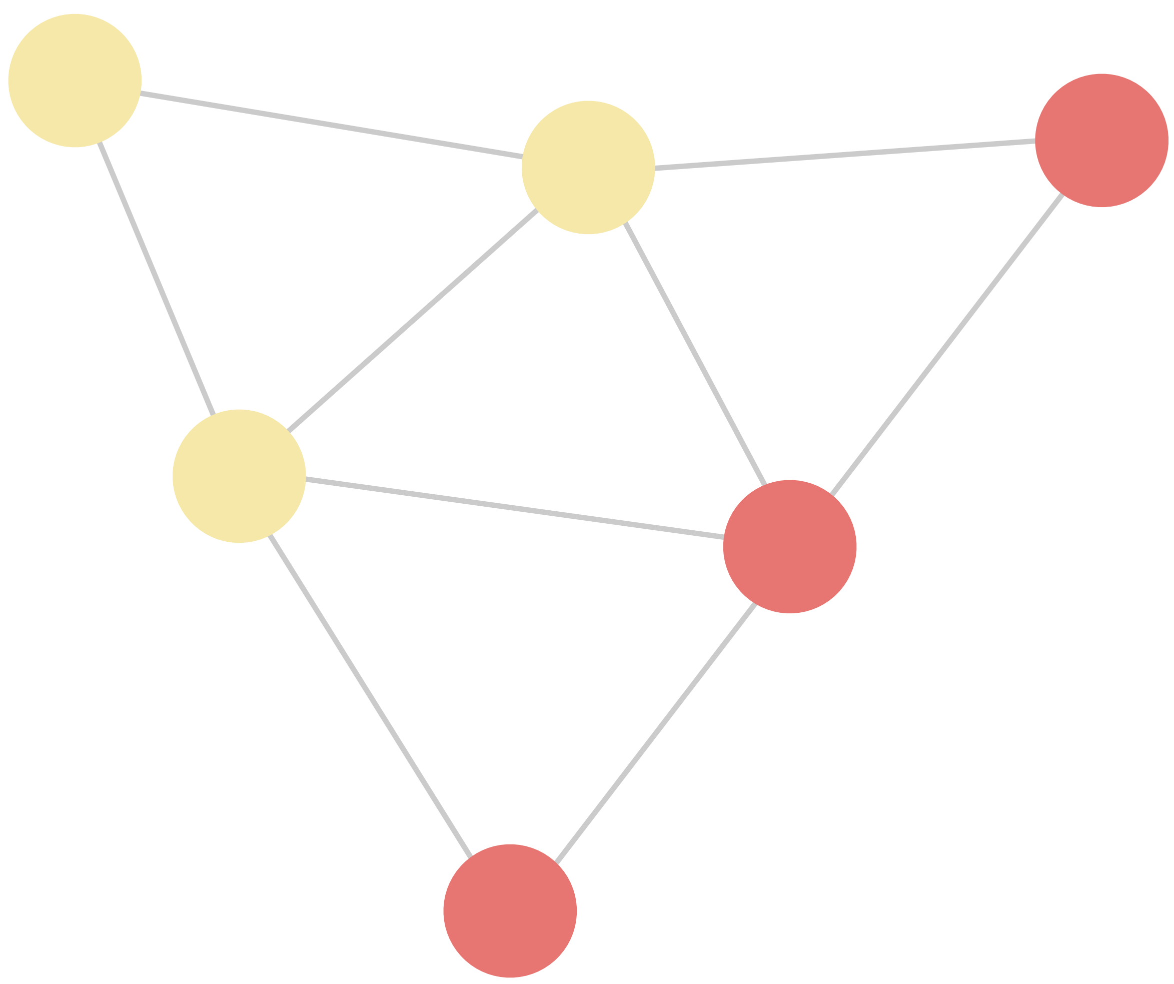
Message-passing network



Repeating this process causes information to spread across the graph

Iteration 0

Message-passing network



Repeating this process causes information to spread across the graph

Iteration 1

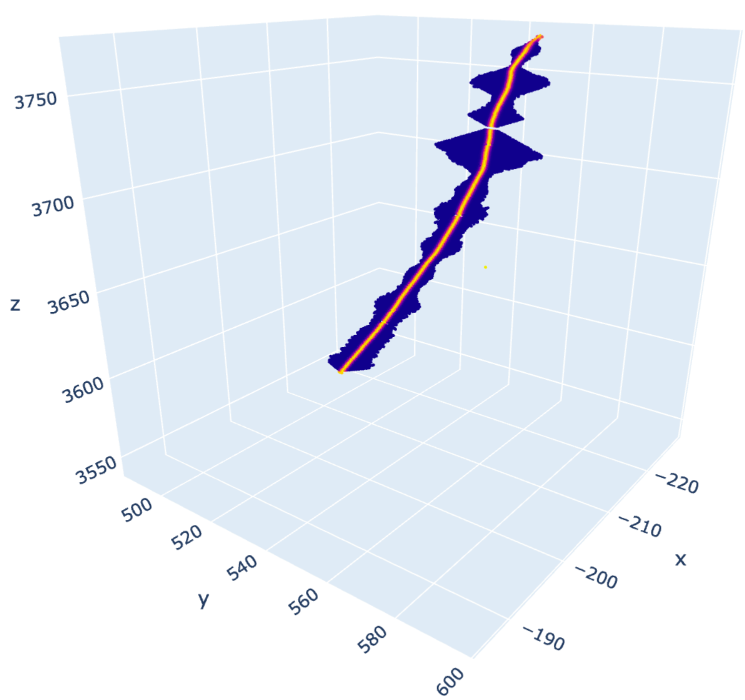
Message-passing network

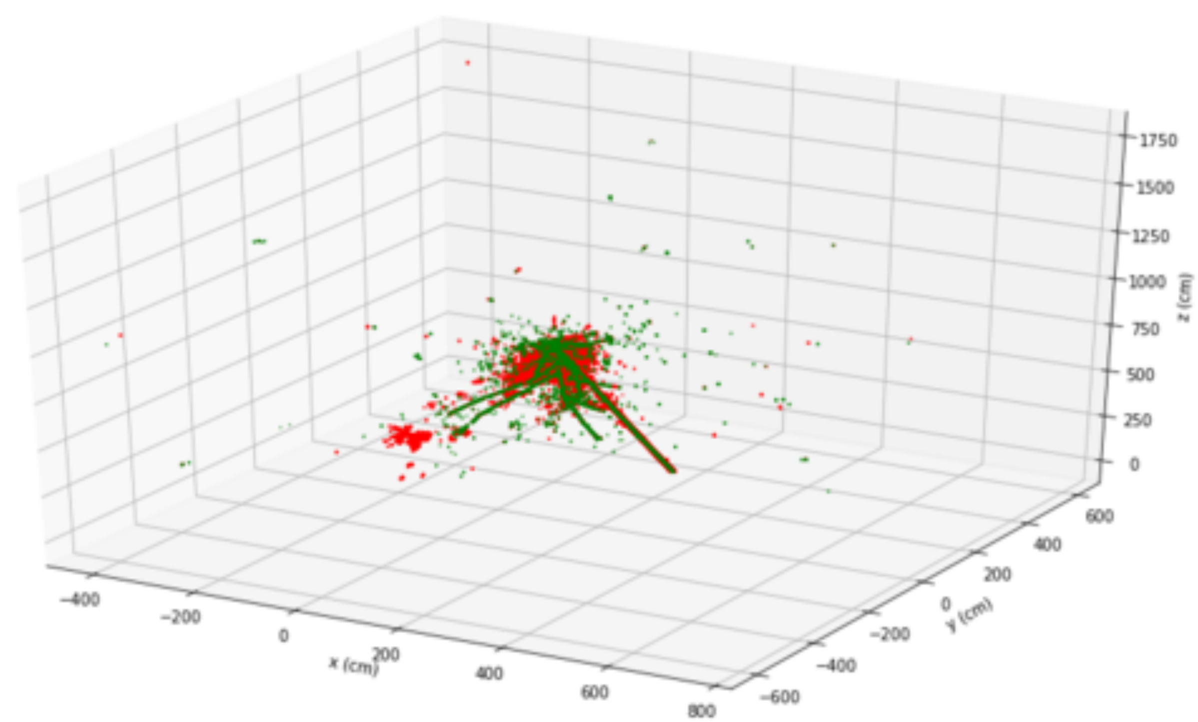
Repeating this process causes information to spread across the graph

Iteration 2

Spacepoint reconstruction

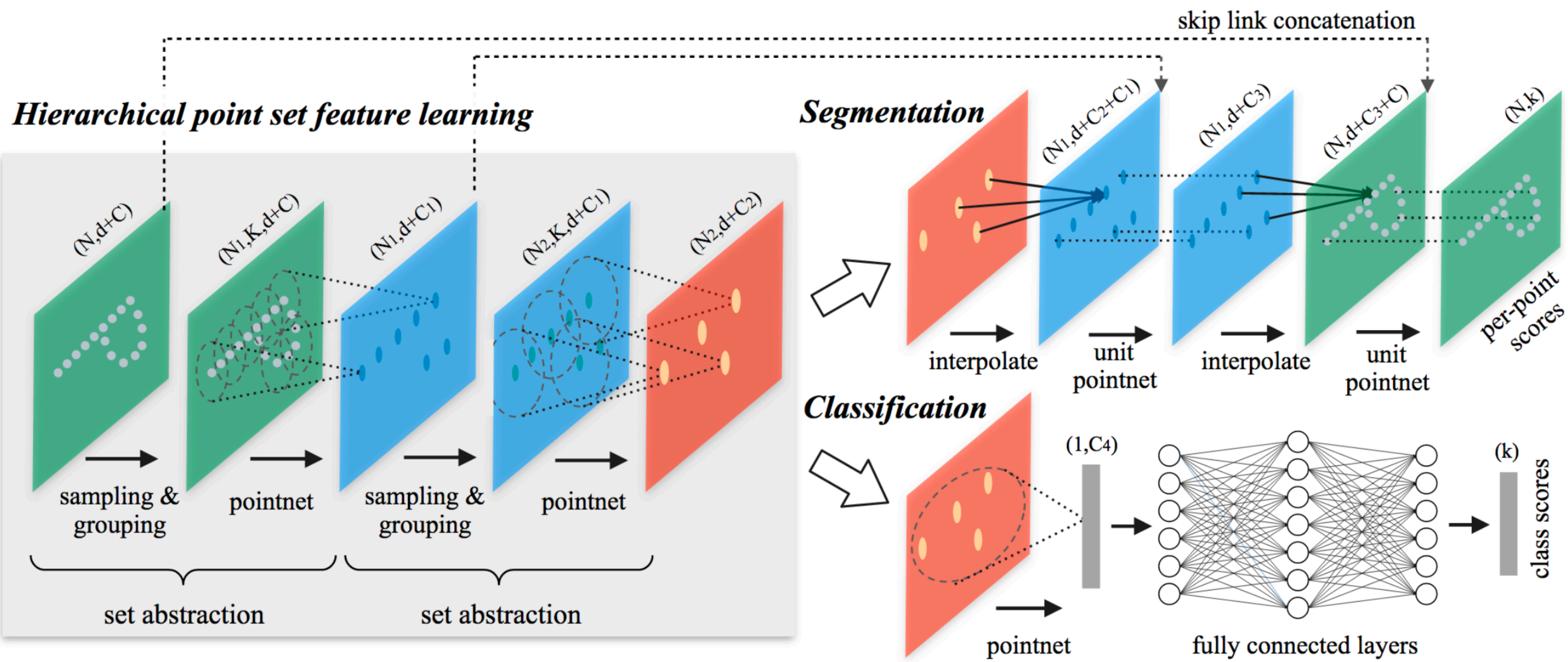
- Moving from three 2D representations of an energy deposition to one 3D representation is a noisy procedure.
- Early attempt: utilise **graph node** classification to retain good 3D representations and remove spurious ones.
- Construct graph edges using k-nearest-neighbour (kNN) technique.





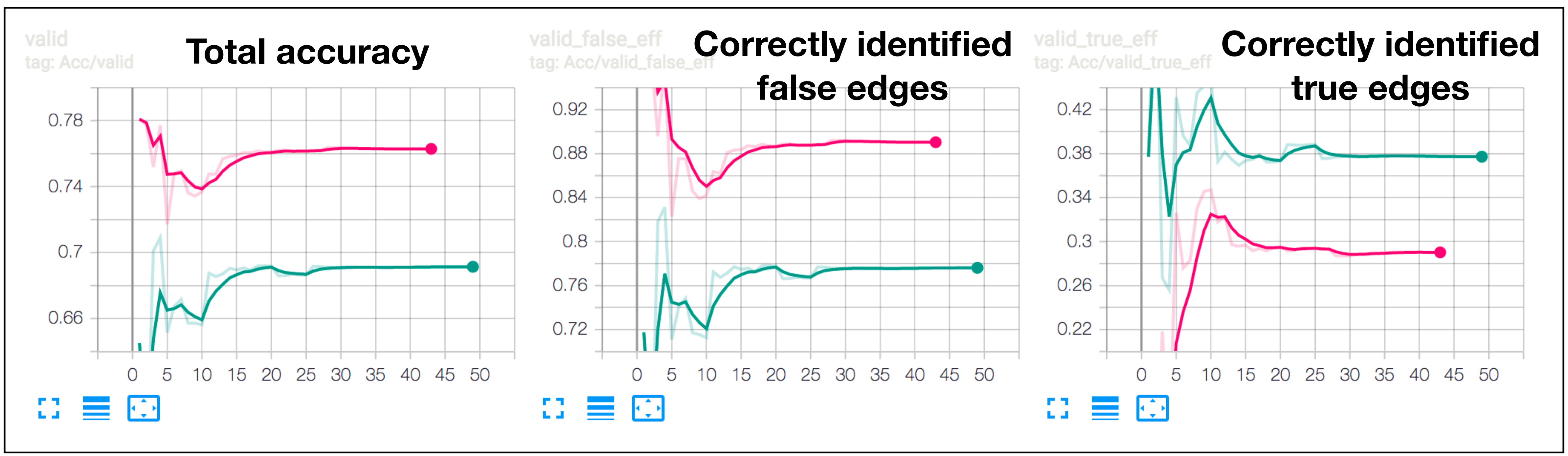
Spacepoint clustering

- Investigated use of **PointNet++** spacepoint graph network (arxiv:1706.02413).
  - This network is specifically designed to operate on point clouds.
  - Utilises **set abstraction** to aggregate local features, similar to a U-net for CNNs.
- PyTorch implementation of up & down-sampling too slow for large point clouds.



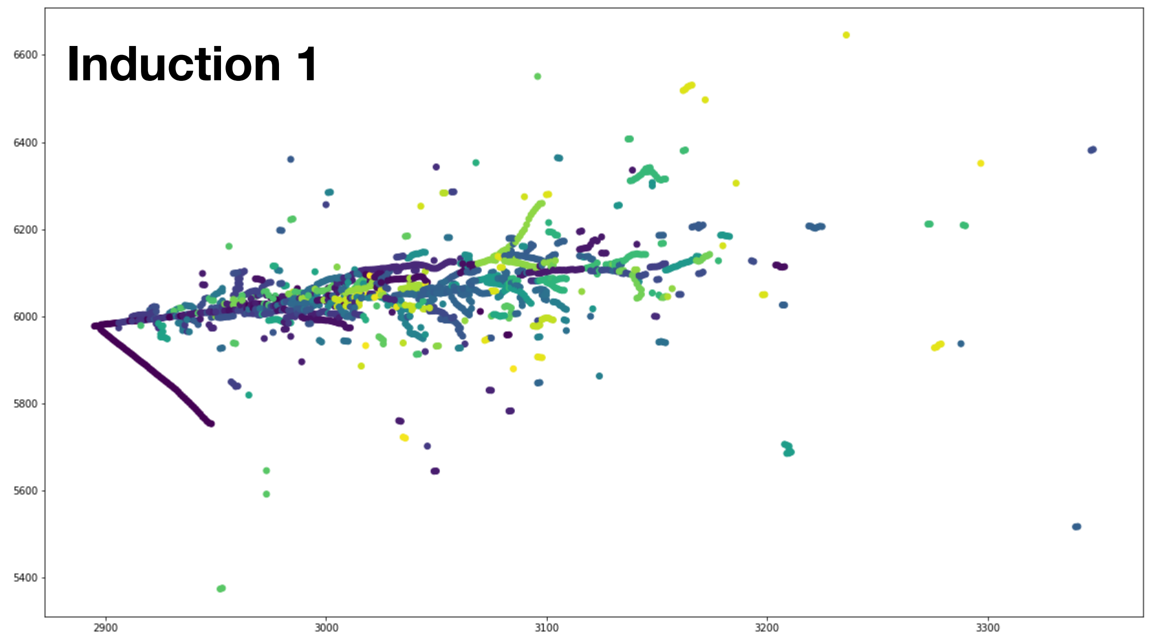
2D approaches

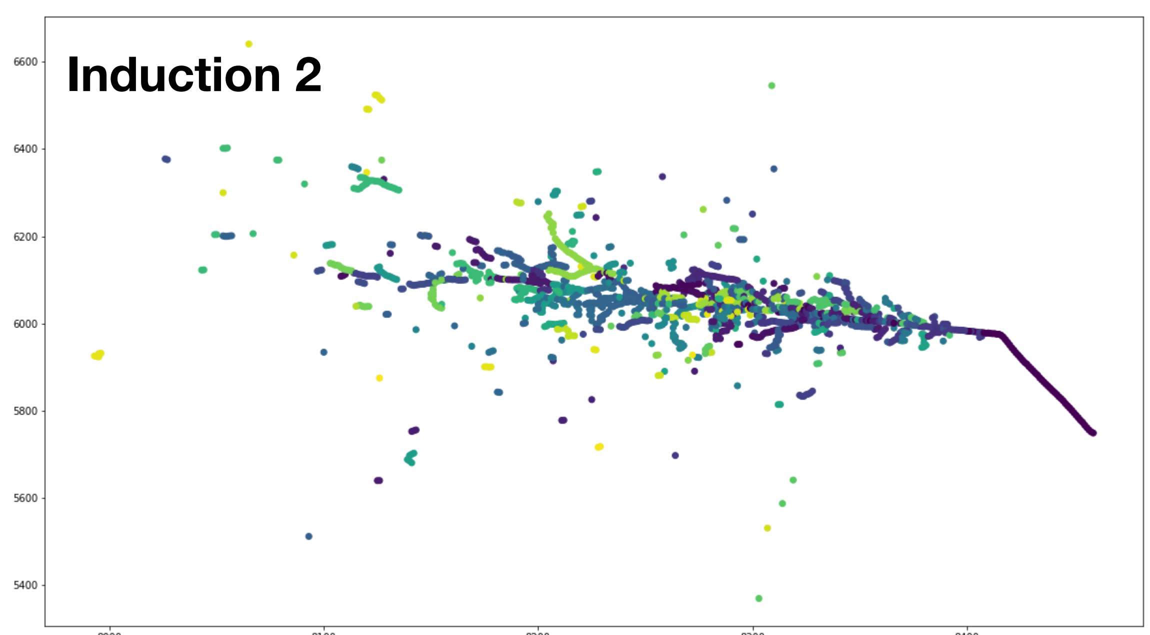
- The 3D approaches explored were not found to be effective.
  - Only learn marginally above noise level.
- Next step: investigate reconstruction of interactions in 2D representations.
  - Conceptually closer to LHC approach.
  - Can leverage structure of detector to sparsify number of edges and reduce graph size.

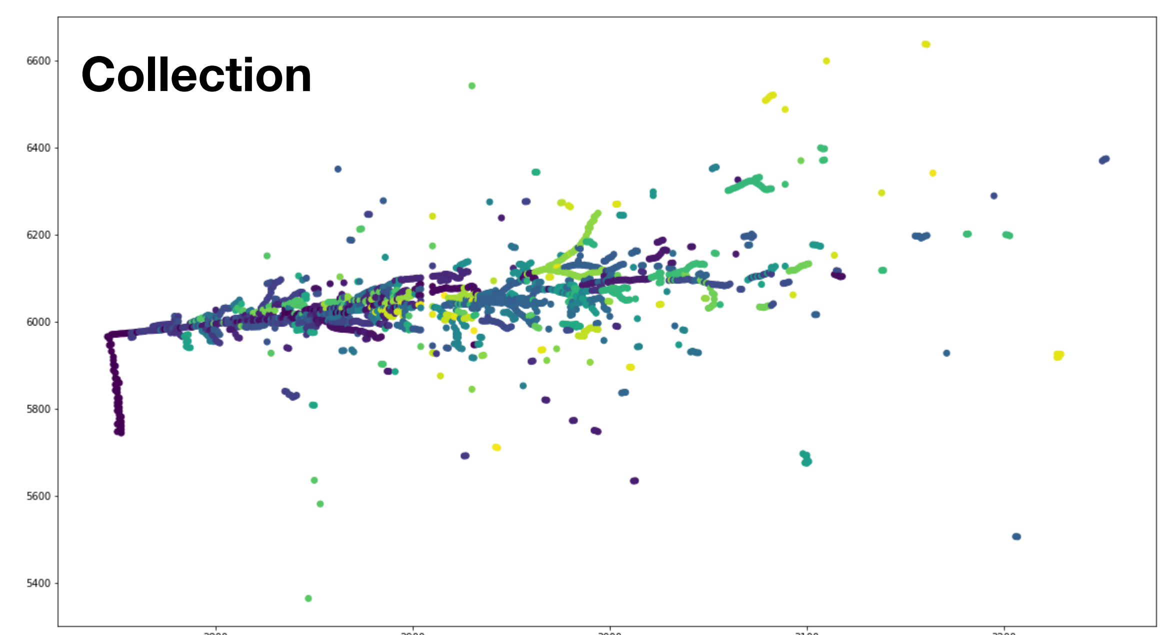


2D reconstruction

- Alternate approach: start with 2D representation and build up using graph network.
- Colour coded according to **true simulated particle**.
- Three 2D representations of the same 3D interaction.

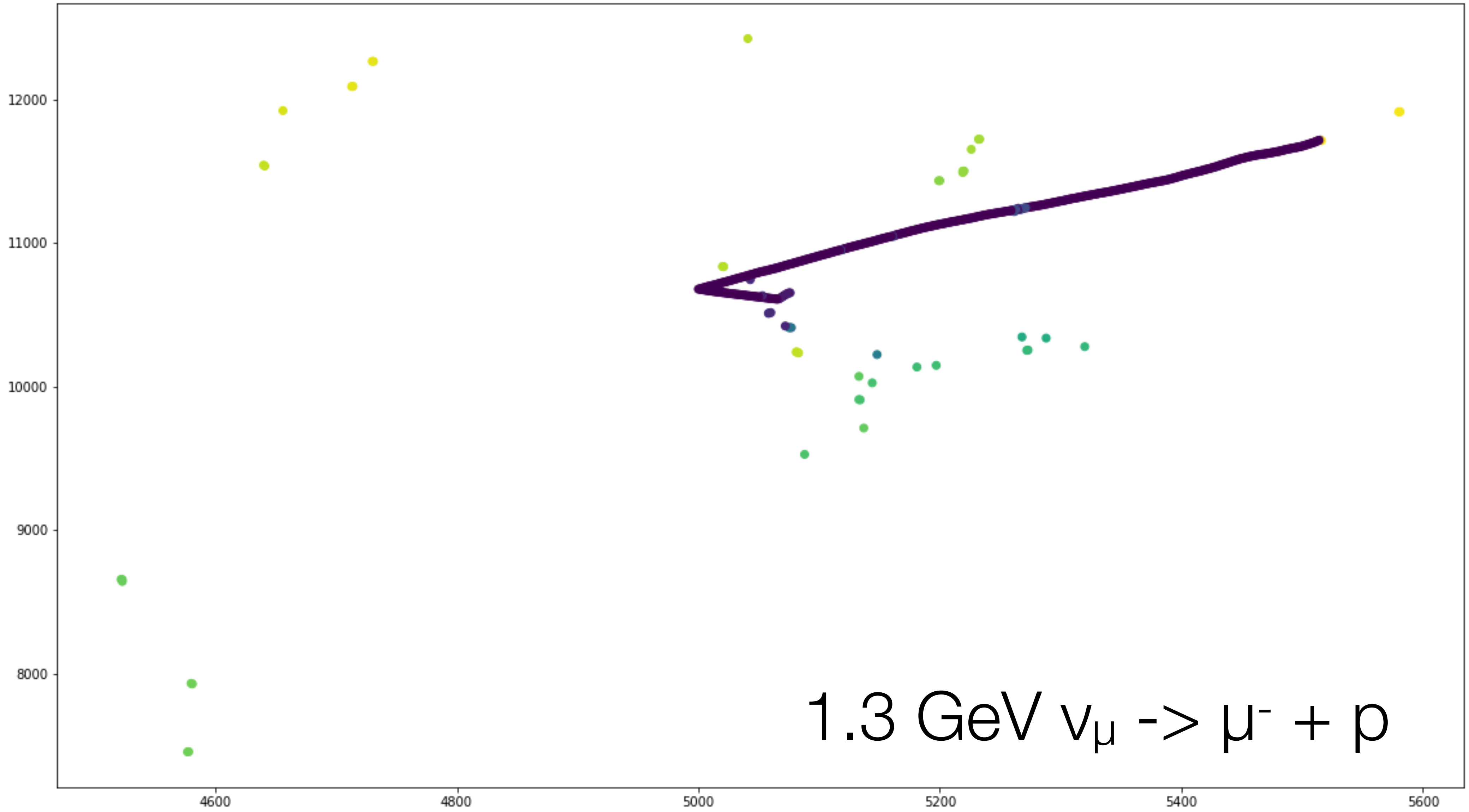






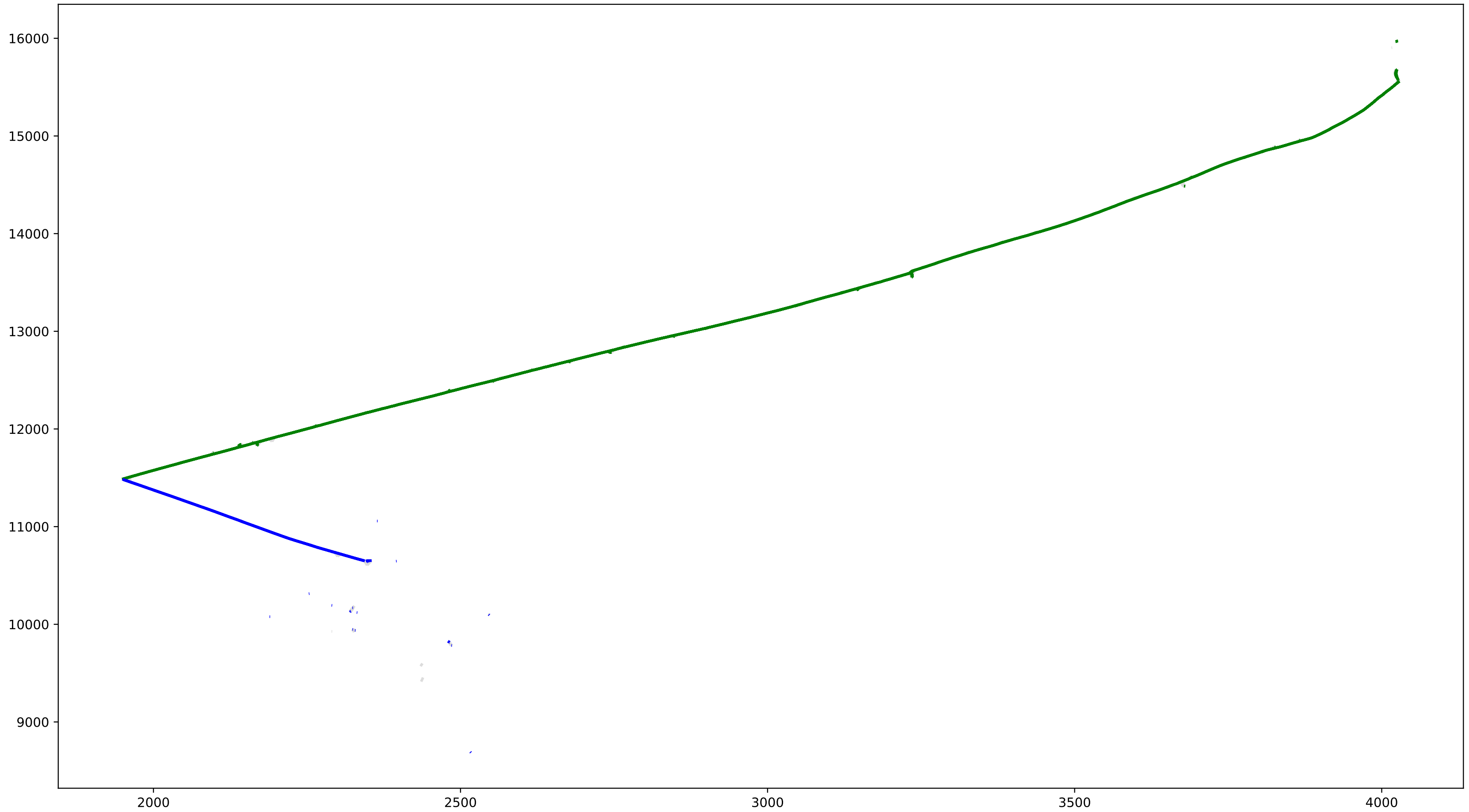
ν_μ graph construction

- Connect hits that are adjacent in wire and time with **potential edges**.
- Potential edges drawn in grey between nodes.



ν_μ graph construction

- Potential graph edges formed for **hits in close proximity** (5 wires & 50 time ticks).
- Potential edges then classified as **hadronic**, **muon**, **shower** or false as an objective for learning.



- Edges are classified as false if the two hits were not produced by the same particle in the underlying simulation.
- **Muon** edges are hits produced by the primary muon, **shower** edges by the primary electron, and **hadronic** edges are the remainder.

ν_e graph construction

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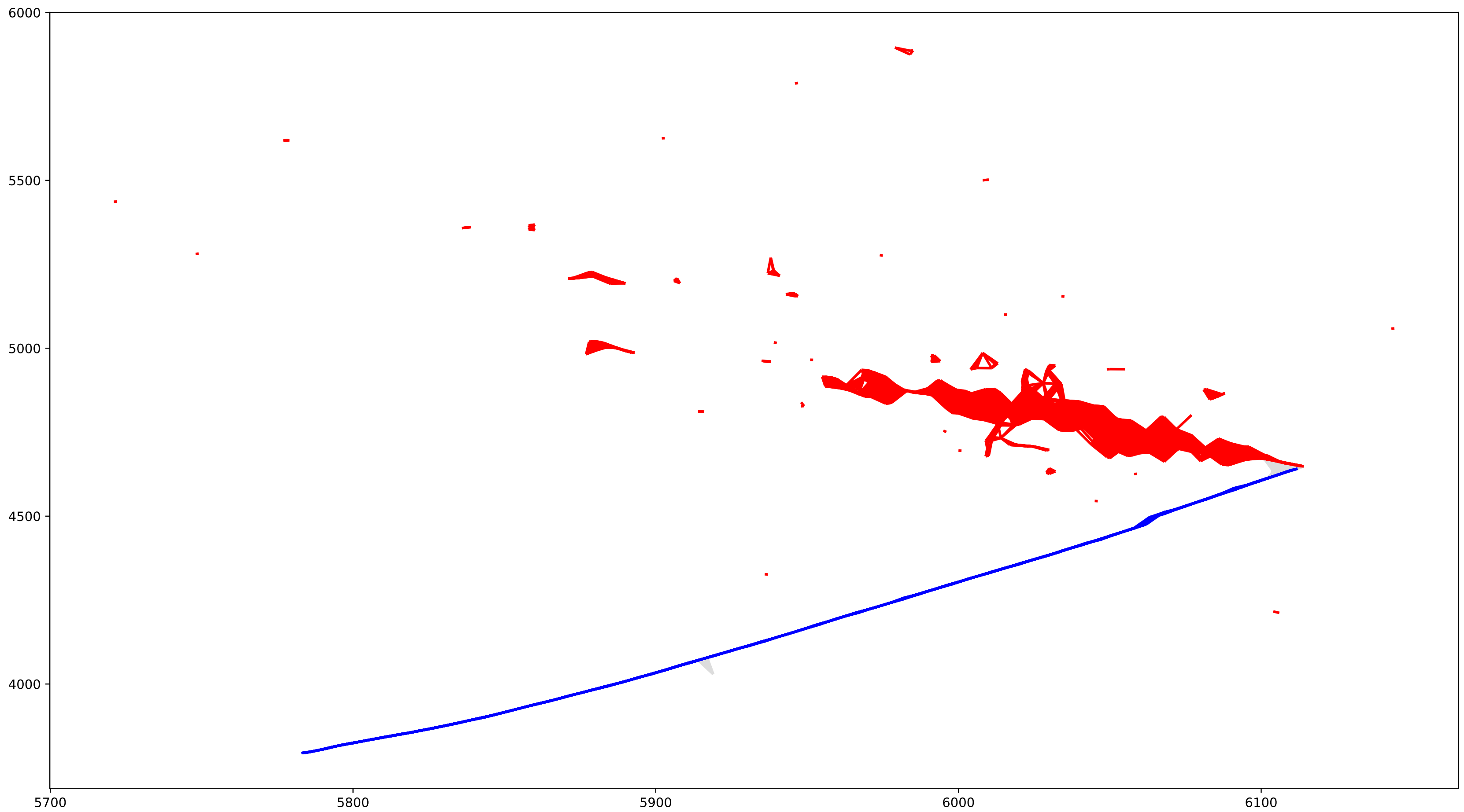

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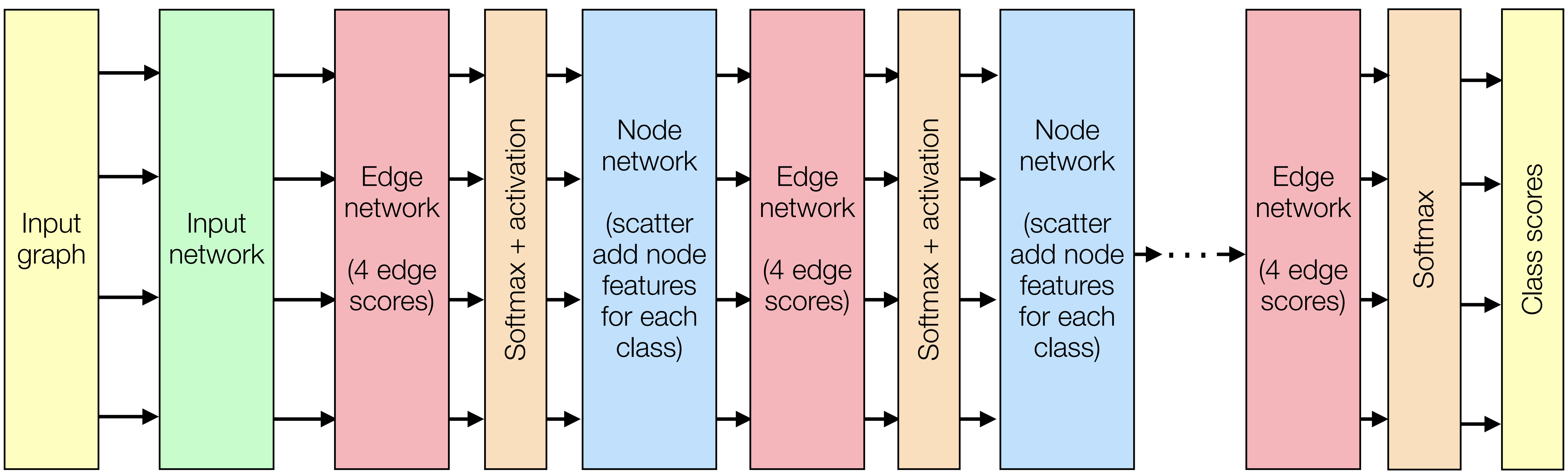
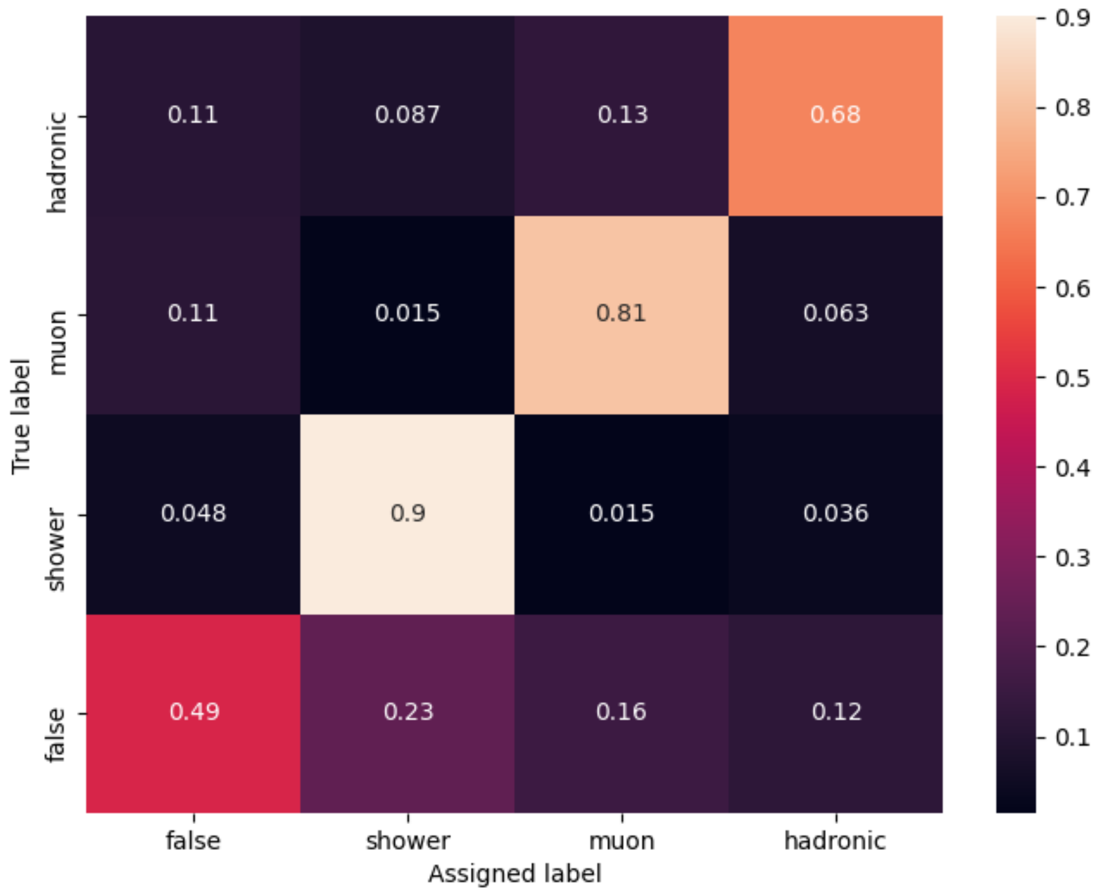
Multihead attention message-passing network

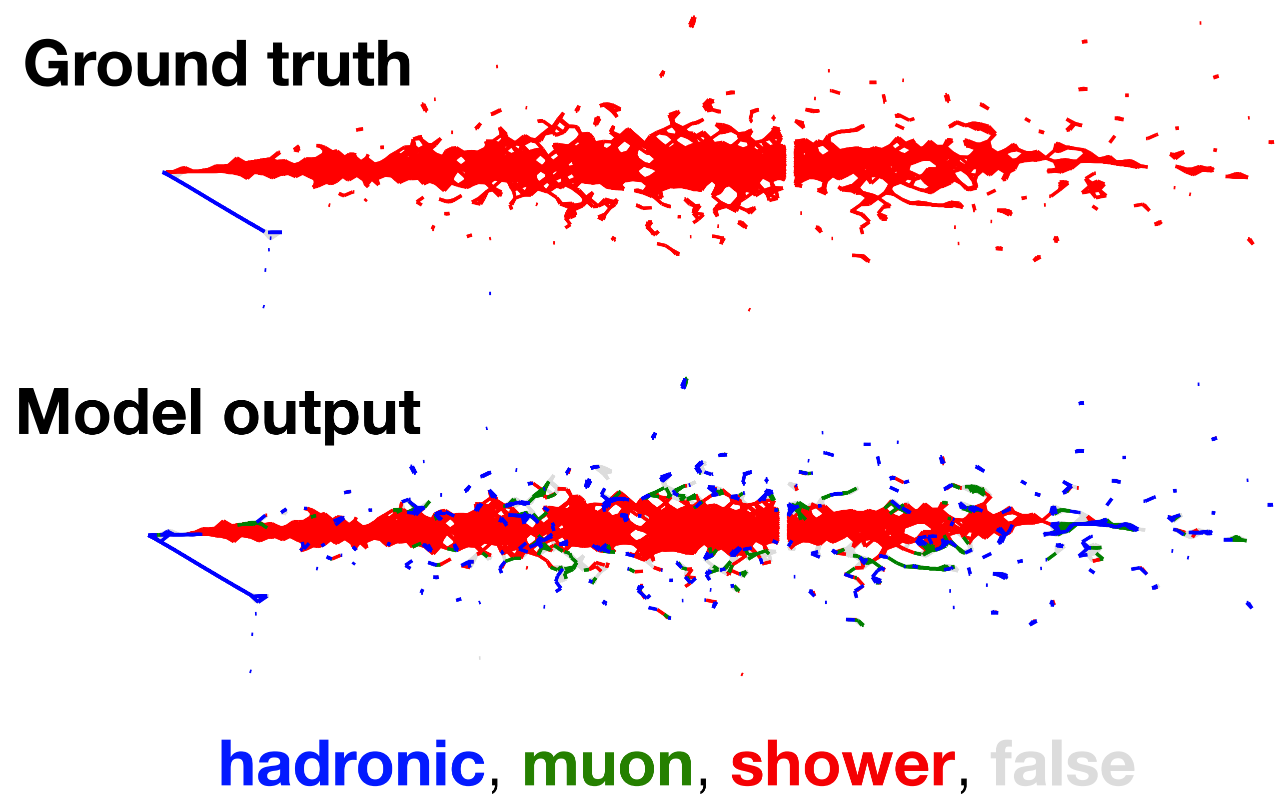
- Build on Exa.TrkX binary edge classifier.
  - Pass messages + form node features independently for each class.
  - Produce 4 edge attention scores on each edge.
  - Take the softmax of those edges **with each iteration**.
  - If an edge is strongly shower-like, the track-like classes will be weighted down accordingly.



2D edge classification network

- Current iteration achieves 84% accuracy in classifying graph edges.
- Performs well on showers, but still room for improvement in tracks.





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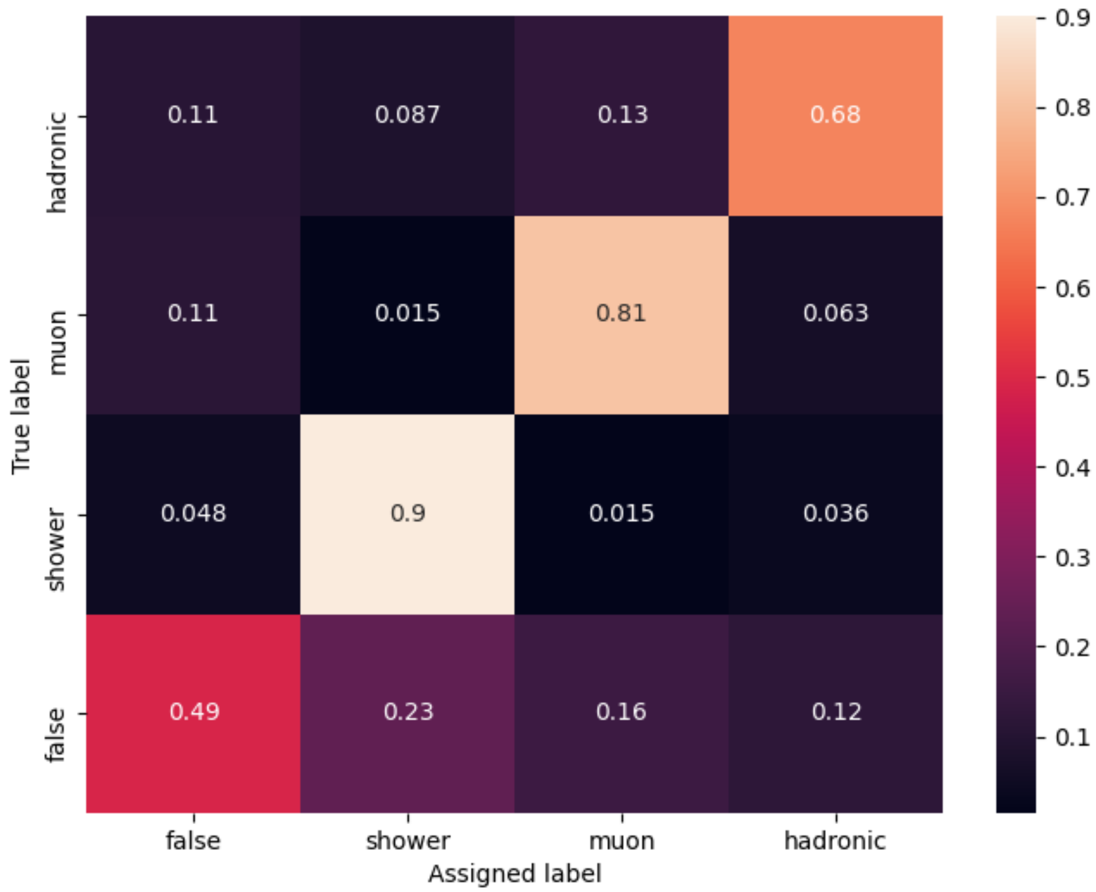
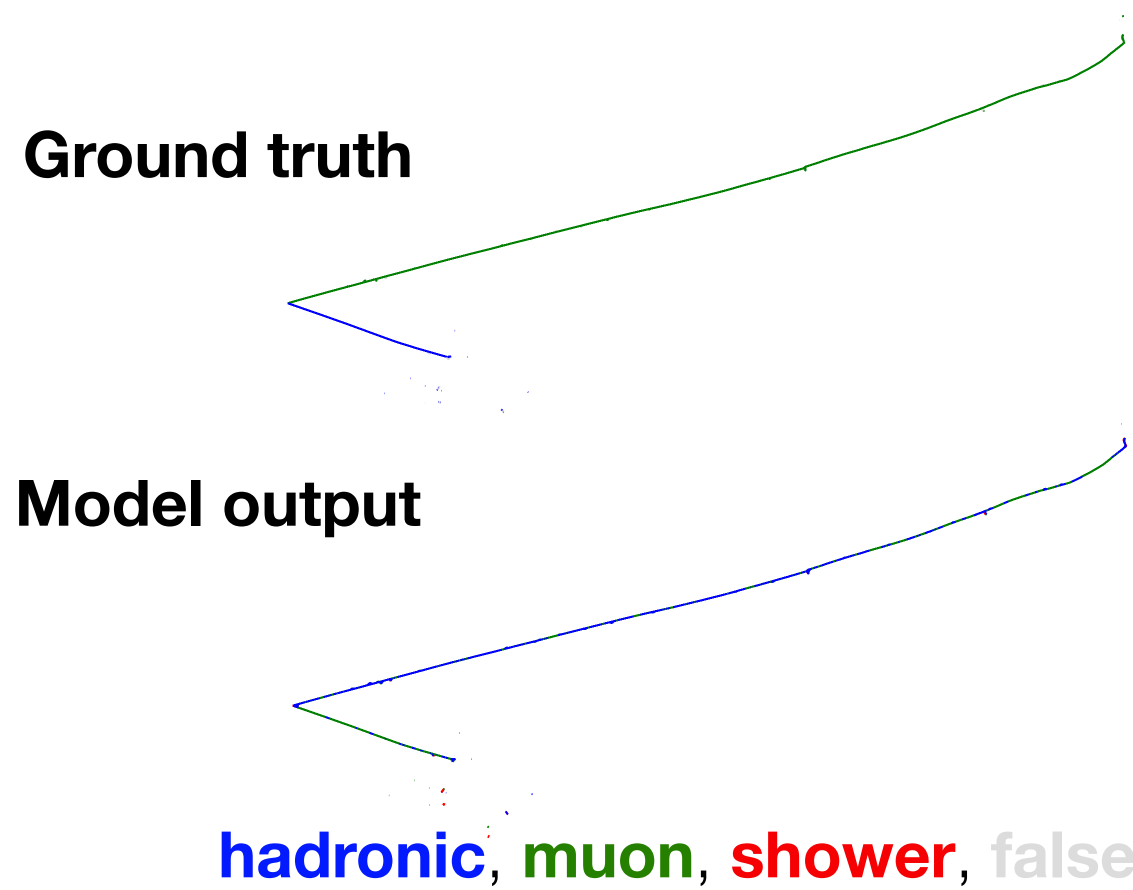
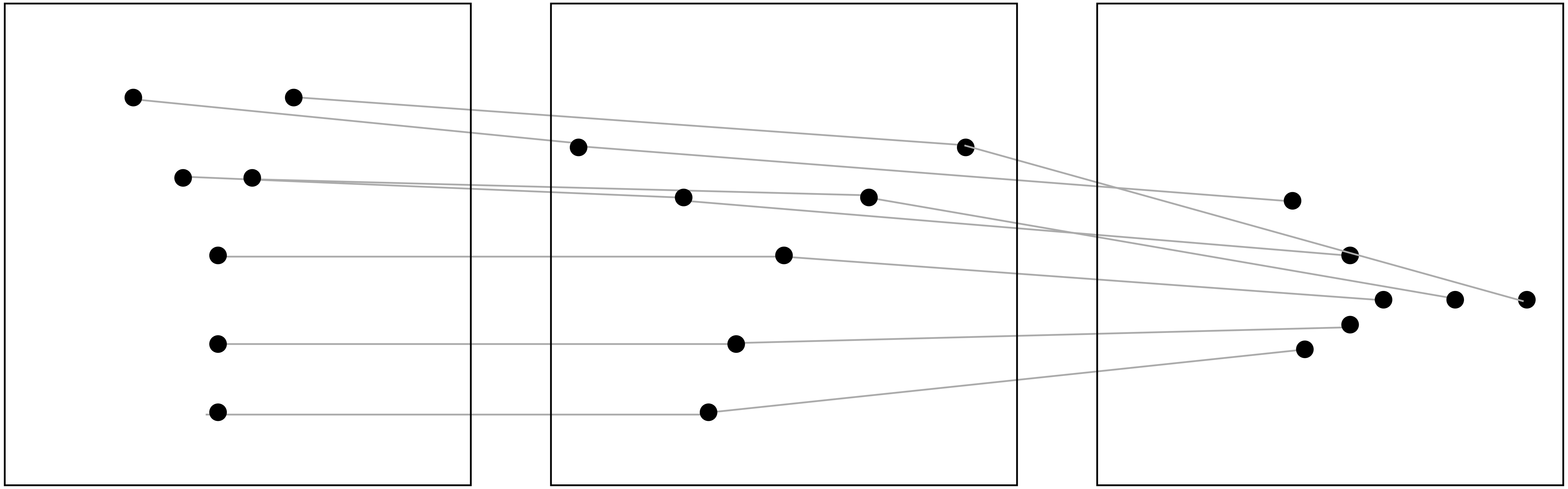




Next steps

- In current setup, the three views are categorised independently.
- Match hits produced concurrently in time to allow information flow between views.
  - Message-passing *between* planes may aid with clustering *within* each plane.
- Long-term goal: combine with heterogeneous graph nodes such as LArTPC optical detector system for time matching.



Next steps

- Edge classification was a natural fit for track-forming in HL-LHC.
- Clearly shows promise in neutrino physics too, but less well-suited to the problem of clustering hits into dense objects.
  - Need a scheme to collapse disparate classified edges into objects.
  - Objective function scores each edge independently, and doesn't have any wider context.
- Considering newer techniques such as graph pooling and instance segmentation.
- Move beyond simple CCQE interactions to more complex event topologies
  - Build more sophisticated definitions of the ground truth.
  - Scale up from 2D representations to 3D.