GRAPH NEURAL NETWORKS FOR HIGH LUMINOSITY TRACK RECONSTRUCTION

EP-IT DATA SCIENCE SEMINAR, CERN, 18 MAY 2022

DANIEL MURNANE ON BEHALF OF THE EXATRKX AND L2IT PROJECTS AND THE ATLAS COLLABORATION



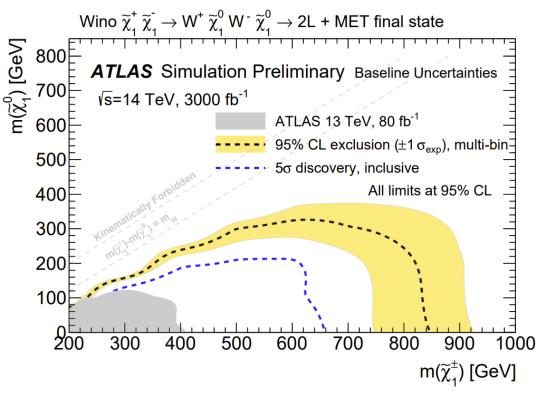
HIGH LUMINOSITY TRACK RECONSTRUCTION



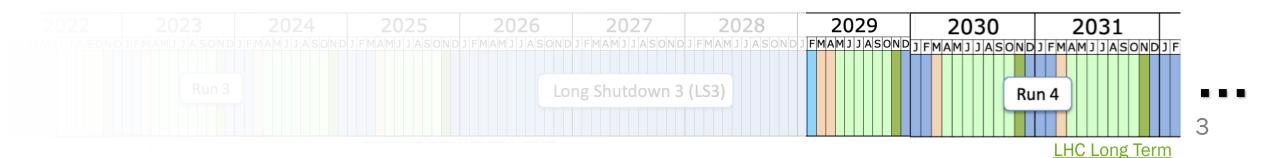
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WHY HIGH LUMINOSITY PHYSICS?

- 1. Better reach for Supersymmetry discovery:
 - a) Electroweakino particles produced by much greater range of chargino masses
 - b) Gluino exclusion from channels across 0.7-2.0TeV to channels across 2.5-3.2TeV
- 2. Sensitive to resonances (W', Z') up to 6-8TeV
- W mass precision improvement from <u>+9.4MeV</u> to <u>+6MeV</u>

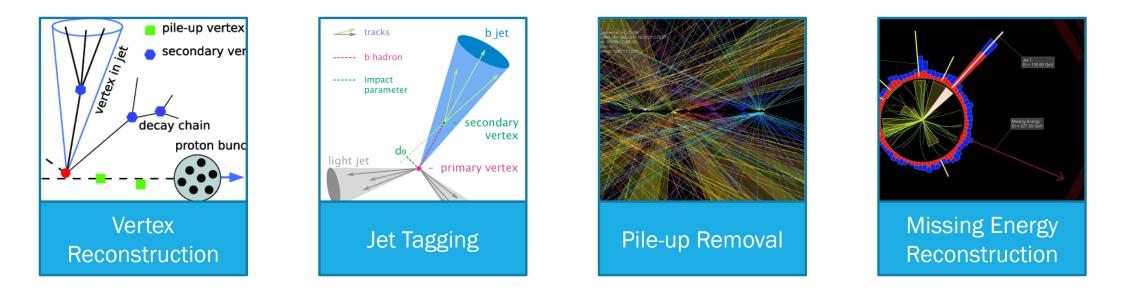


ATL-PHYS-PUB-2018-048



TASKS IN AN HL-LHC DETECTOR

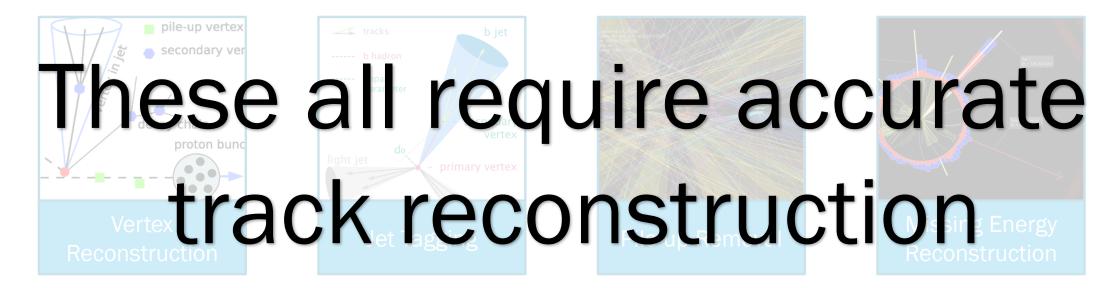
- In order to perform the analysis that leads to discovery (e.g. of dark matter, extra dimensions, SUSY, ...), need to make sense of the detector read-out
- There are many tasks required to reconstruct the physics event behind the read-out





TASKS IN AN HL-LHC DETECTOR

- In order to perform the analysis that leads to discovery (e.g. of dark matter, extra dimensions, SUSY, ...), need to make sense of the detector read-out
- There are many tasks required to reconstruct the physics event behind the read-out



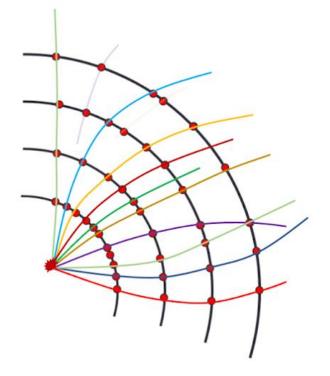


TRACK RECONSTRUCTION

- Protons collide in center of detector, "shattering" into thousands of particles
- The charged particles travel in curved tracks through detector's magnetic field (Lorentz force)
- A track is defined by the hits left as energy deposits in the detector material, when the particle interacts with material
- The goal of track reconstruction:

Given set of hits from particles in a detector, assign label(s) to each hit.

Perfect classification: All hits from a particle (*and only those hits*) share the same label



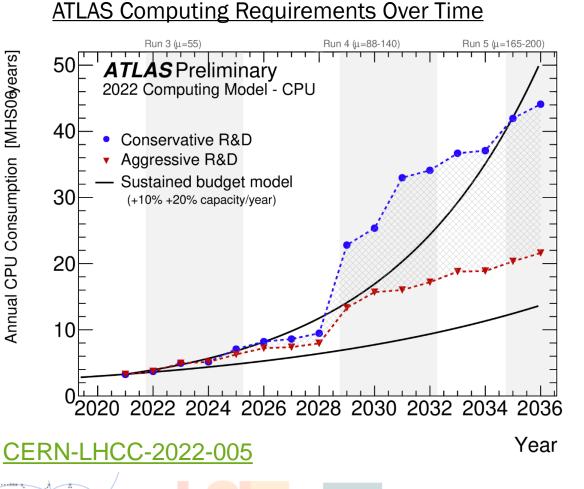
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REPRESENTATION OF COLLISIONS

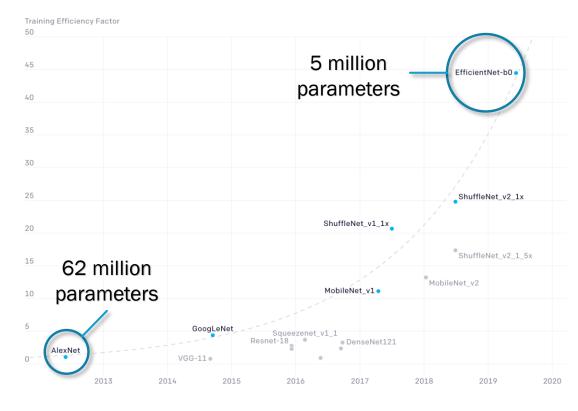


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COMPUTE SCALING FOR HIGH LUMINOSITY



ML Image Classification Efficiency Over Time



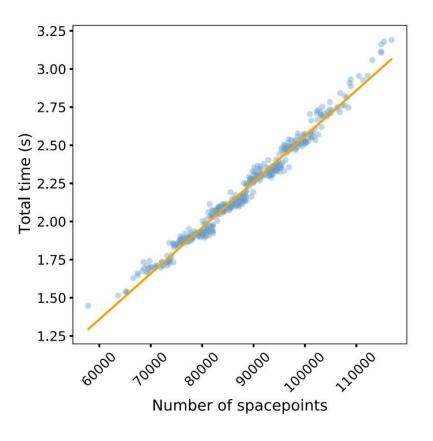
44x less compute required to get to AlexNet performance 7 years later (linear scale)

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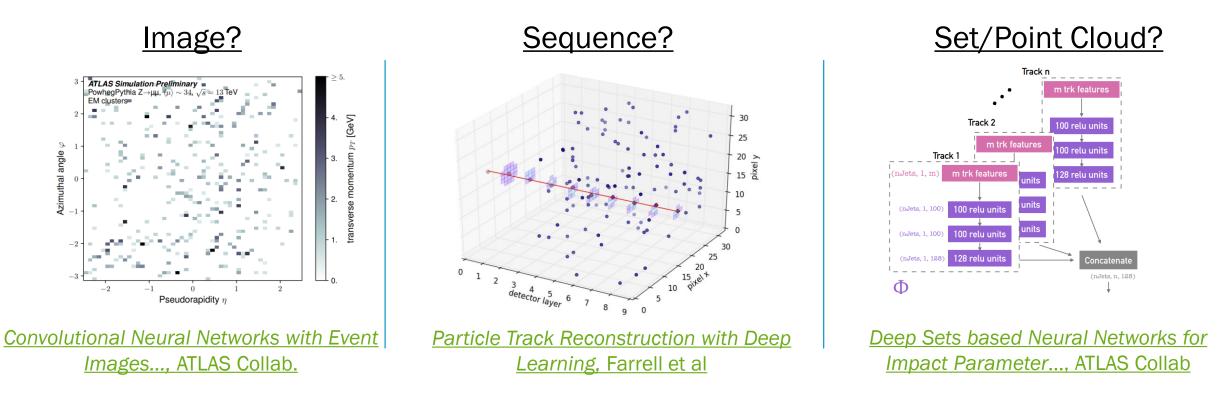
TEASER: GRAPH-BASED PIPELINE FOR TRACK RECONSTRUCTION

- Using graph-based ML, can perform track reconstruction on High Luminosity detector events
- Comparable efficiency and fake rates to traditional algorithms
- Scaling that is approximately linear in event size (on open-source TrackML dataset)

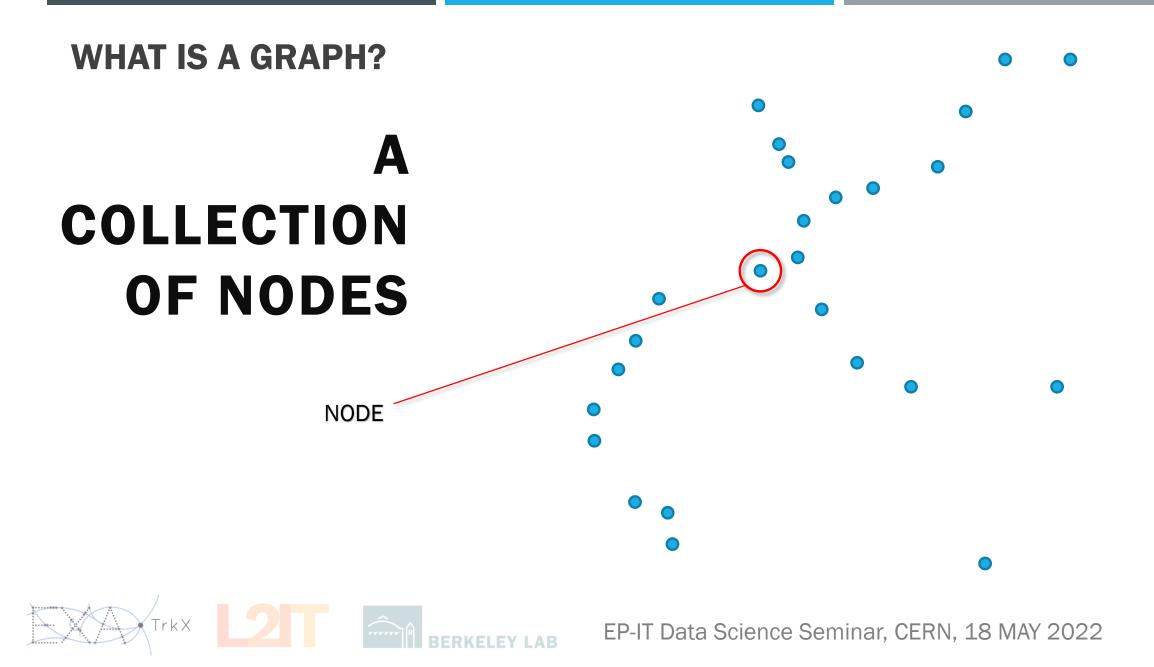


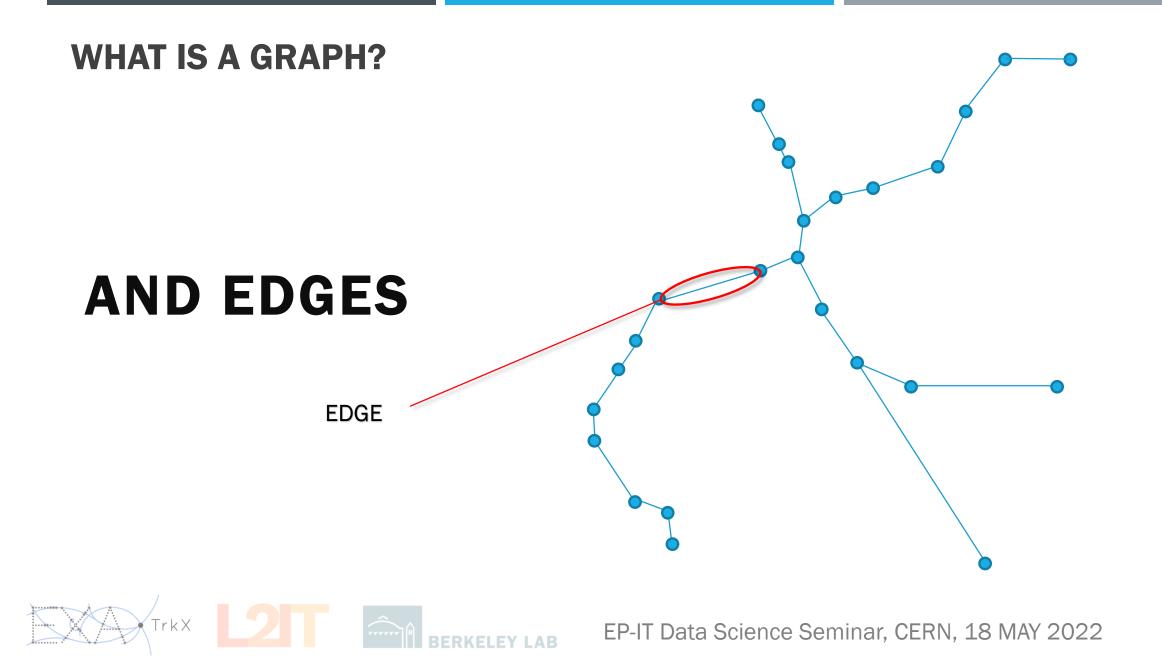
HOW SHOULD WE REPRESENT PARTICLE COLLISIONS?

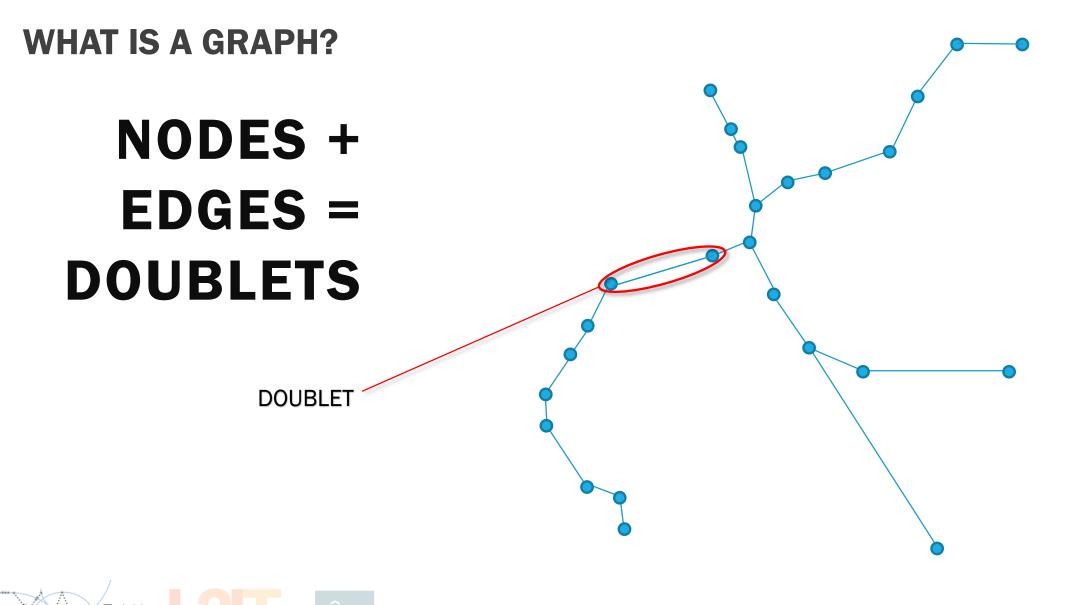
Assuming we want to use deep learning, how can we represent a particle collision?



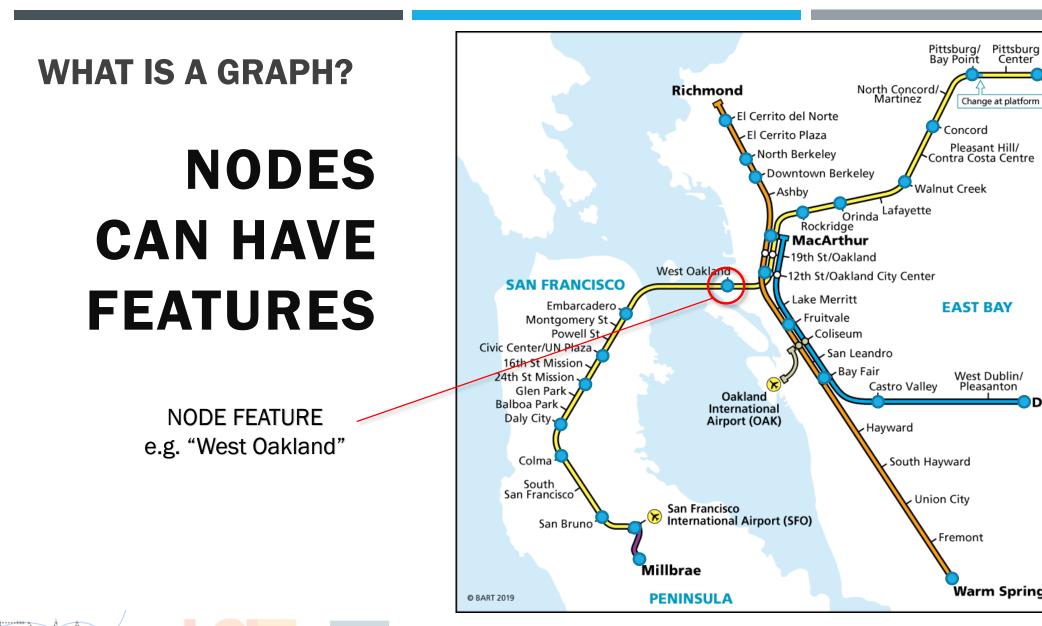
For event collision as point cloud, with relationships between points, this is a graph.







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Antioch

Dublin/Pleasanton

Warm Springs/South Fremont

Change at platform

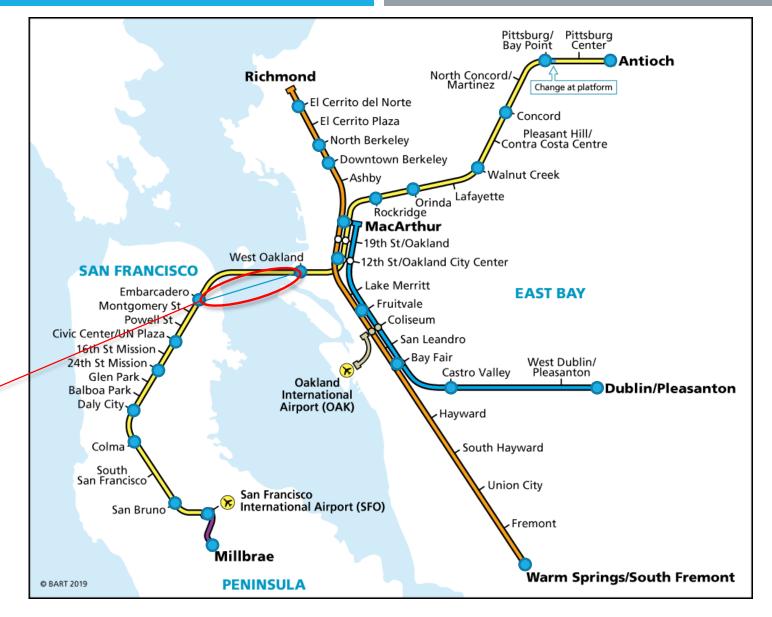
West Dublin/

Pleasanton

EDGES CAN HAVE FEATURES

WHAT IS A GRAPH?

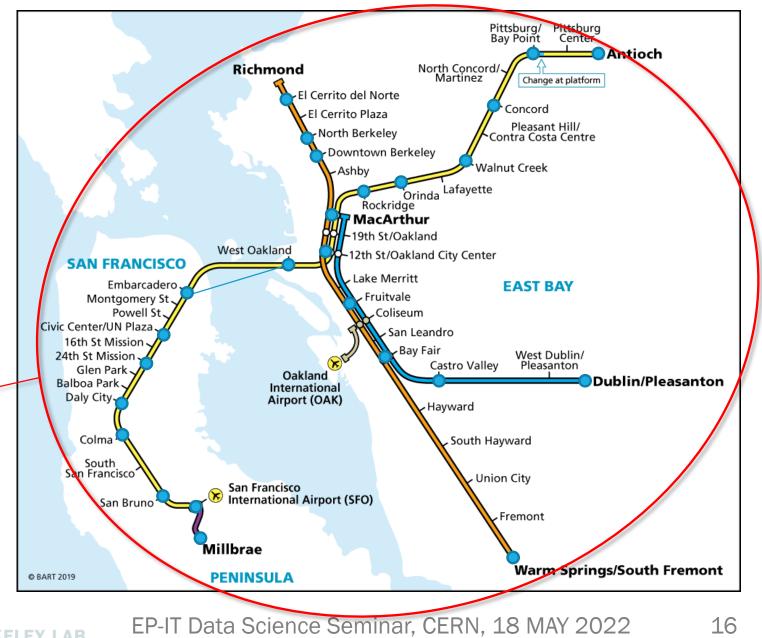
EDGE FEATURE e.g. "Under Maintenance – Single Track"



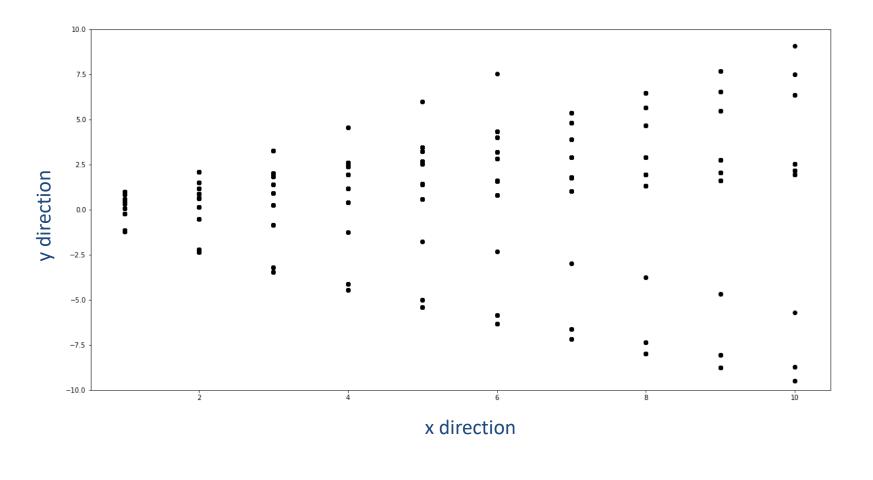
BERKELEY LAE

THE WHOLE GRAPH **CAN HAVE FEATURES**

GRAPH FEATURE e.g. "Sunday Timetable"



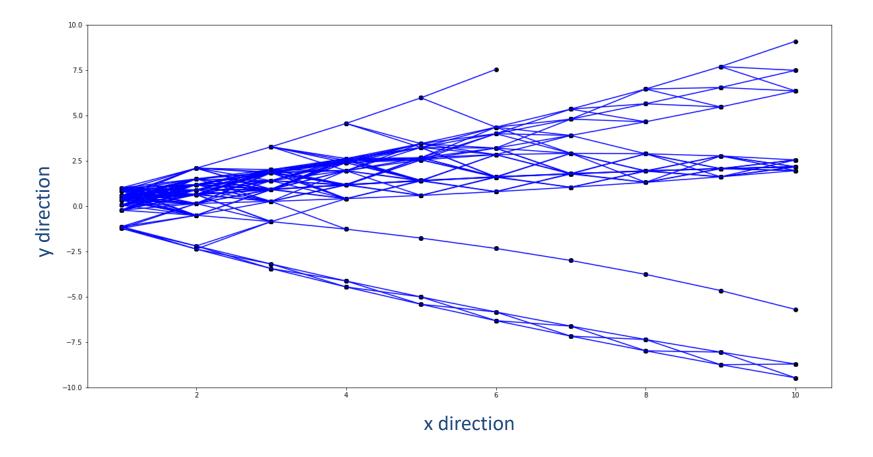
GRAPHS ARE A NATURAL WAY TO REPRESENT TRACKS



Given hits on layers of a detector

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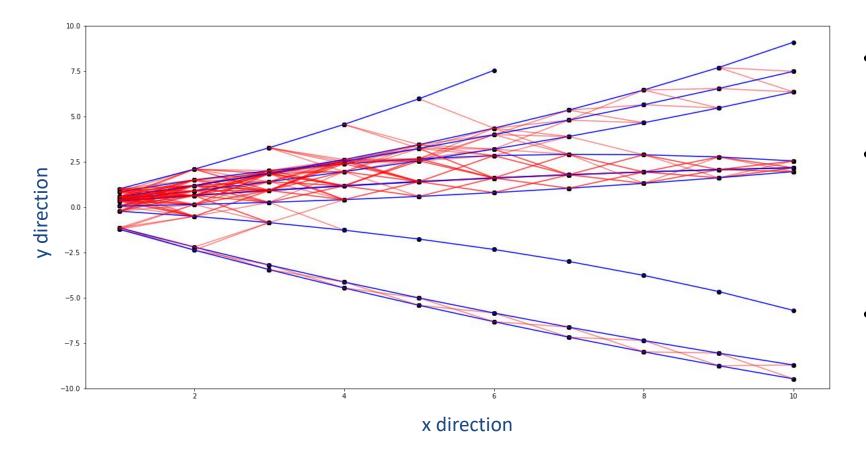
GRAPHS ARE A NATURAL WAY TO REPRESENT TRACKS



Connect the hits in some way

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GRAPHS ARE A NATURAL WAY TO REPRESENT TRACKS

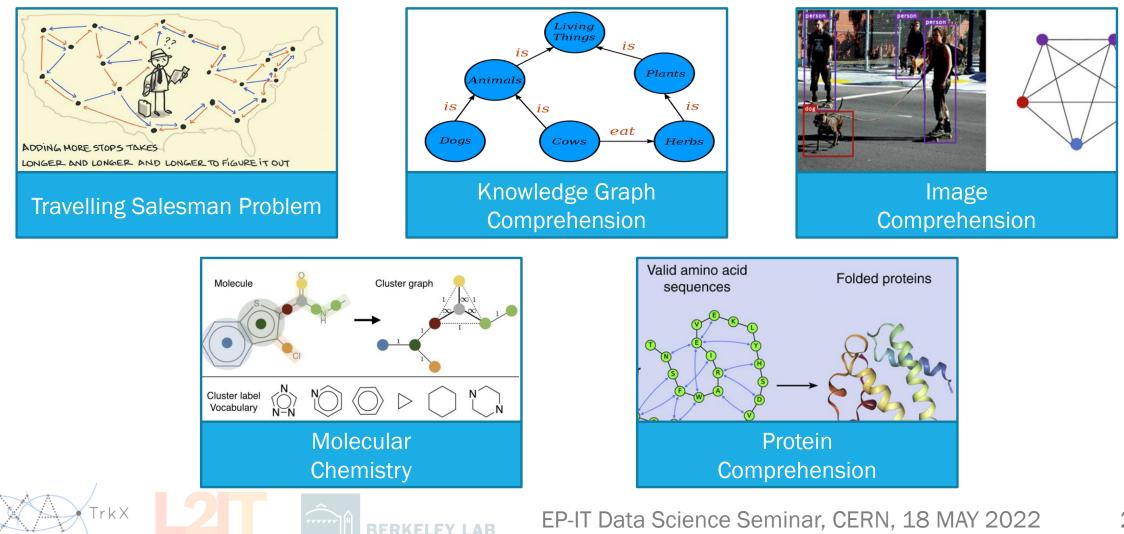


- Tracks should be found amongst the connected nodes.
- Note the trade-off: Rather than needing to classify or cluster nodes with many labels, we only need binary classification of edges
- However, introduce the extra step of building tracks from classified edges

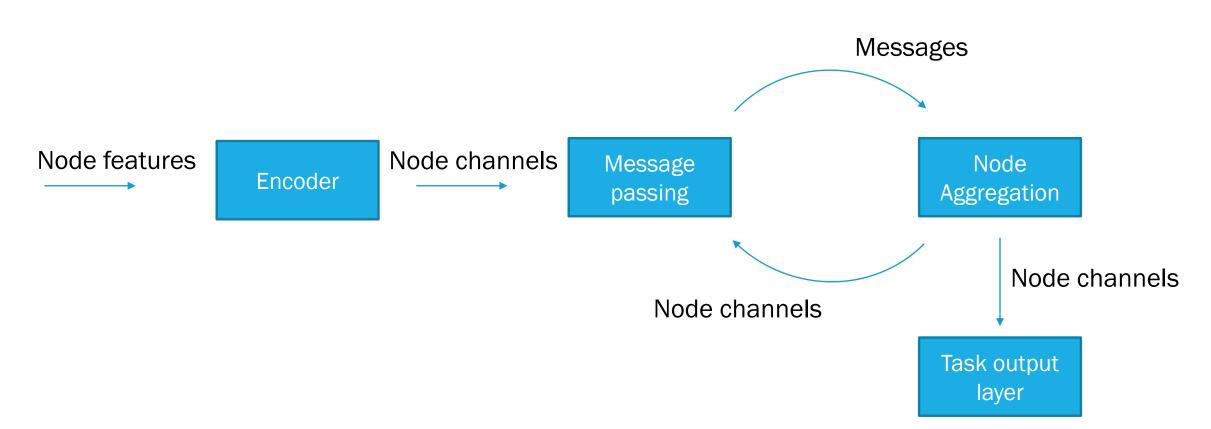
INTRO TO GRAPH NEURAL NETWORKS



GRAPH NEURAL NETWORK APPLICATIONS



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GRAPH NEURAL NETWORK PROCEDURE



STEP 1: MESSAGE PASSING MECHANISM

Input channels Encoded channels

For each node neighborhood:

- a) Pass node channels through a multi-layer perceptron (MLP) encoder
- b) Pass encoded channels along each edge to the central node of the neighborhood

Note: This is quite inexpensive since we store N_{nodes} for backpropagation

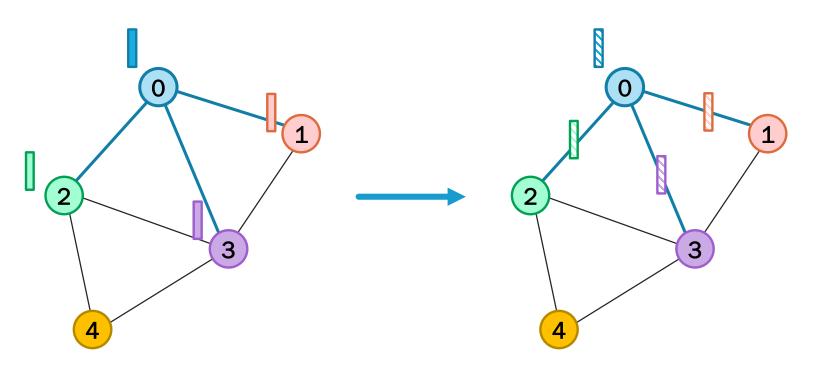
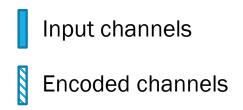


Figure inspired by Koshi et. al.

ERKELEY LAB

STEP 2: AGGREGATION



At each node:

Sum all messages

Note: Called *isotropic* message passing. Introduced as "Graph Convolution Network"

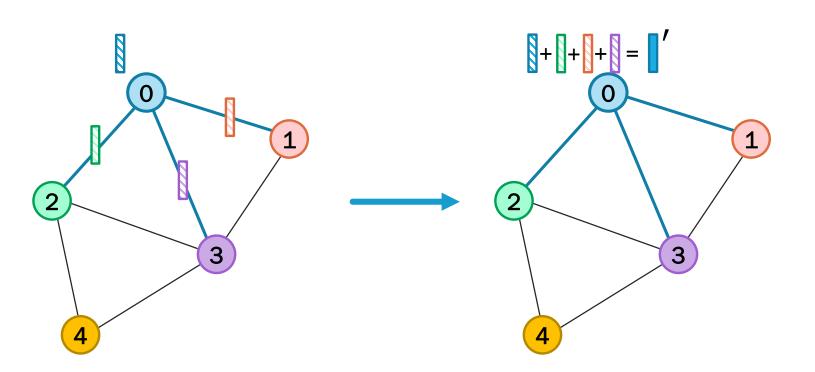


Figure inspired by Koshi et. al.

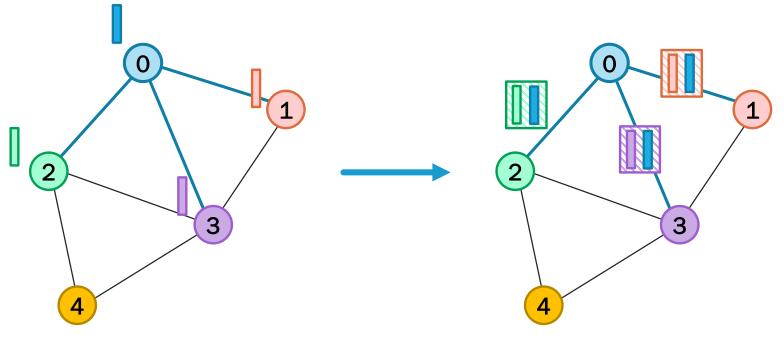


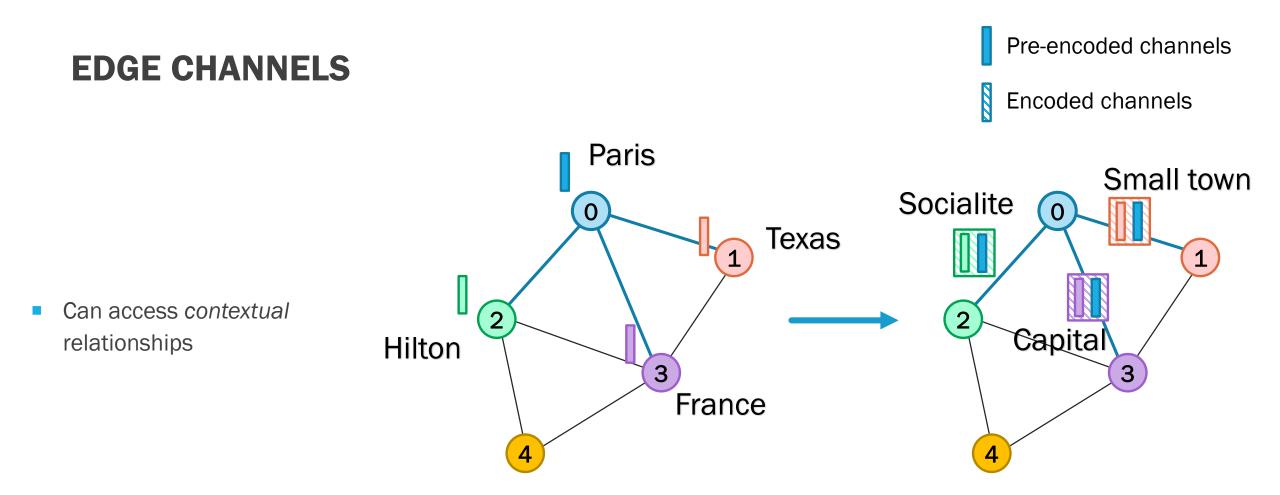
EDGE CHANNELS

- Isotropic message passing can't differentiate importance of neighbors
- Anisotropic message passing: encode a combination of node and neighbor along each edge
- Much more expensive now need to store N_{edges} for backpropagation
- But <u>much more powerful</u>

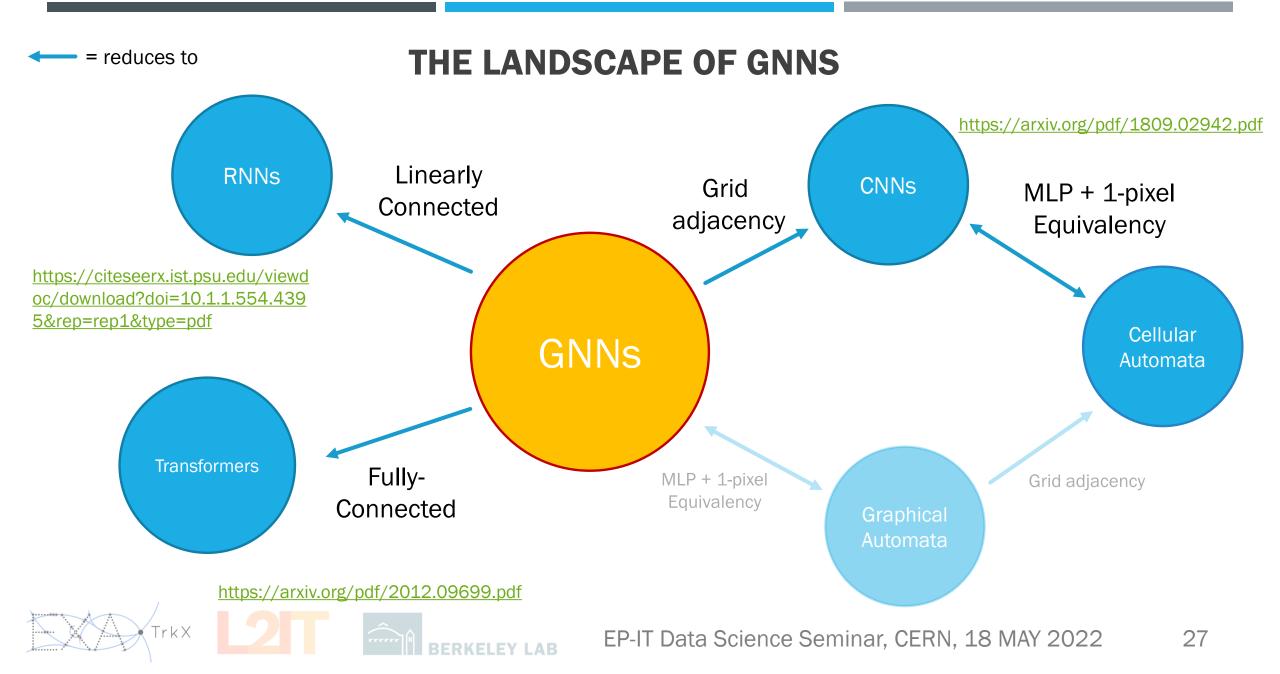
Found in "Graph Attention Network" and "Interaction Network"

Pre-encoded channelsEncoded channels

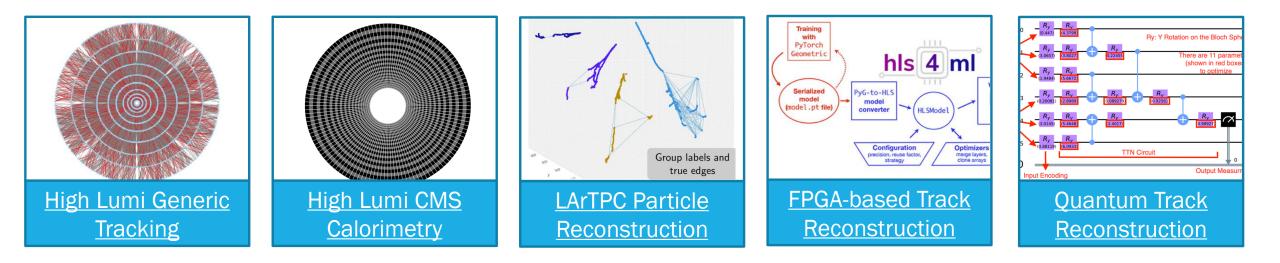








GNNS ELSEWHERE IN PARTICLE PHYSICS



- Very large and active field of study!
- Comprehensive review of GNNs for Track Reconstruction <u>- arXiv:2012.01249</u>
- White paper on progress and future of the field <u>arXiv:2203.12852</u>

GRAPH-BASED TRACK RECONSTRUCTION



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WHO IS INVOLVED?

- Two groups worked on the results in this presentation, and both first tested methods on TrackML, based on the GNN-based reconstruction introduced in arxiv:2003.11603
- L2IT: Laboratoire des deux Infinis, institute based at the University of Toulouse, within the Institute of Nuclear Physics and Particle Physics
- Exa.Trkx: A DoE Office of Science-funded collaboration of LBNL, Caltech, FNAL, SLAC and a collaboration of US institutions including Cincinnati, Princeton, Urbana-Champaign, Youngstown State, and others



GRAPH REPRESENTATION OF AN EVENT

The goal of track reconstruction:

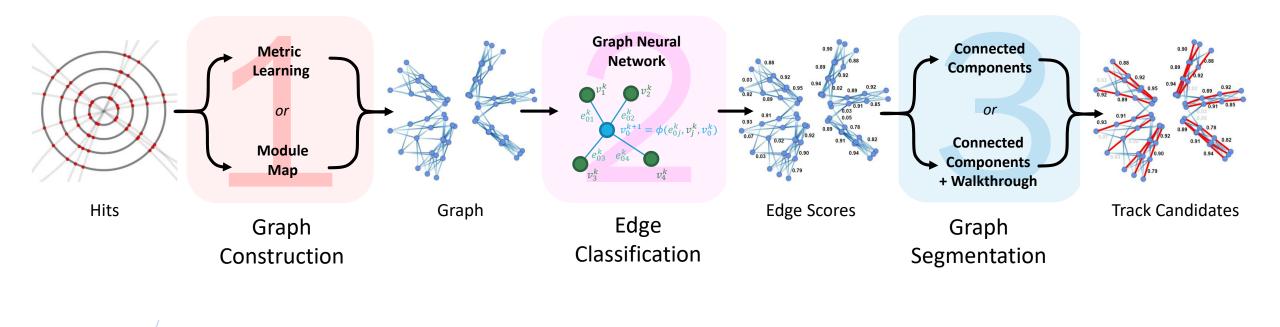
Given set of hits in a detector from particles, assign label(s) to each hit.

Perfect classification: All hits from a particle (*and only those hits*) share the same label

- What does it mean to represent an event with a graph?
 - Treat each hit as a **node**
 - A node can have features (e.g. position, energy deposit, etc.)
 - Nodes can be connected by **edges**, that represent the possibility of belonging to the same track
- Goal: Use ML and/or graph techniques to segment or cluster the nodes to match particle tracks
- Proof-of-concept: TrackML community challenge dataset with simplified simulation

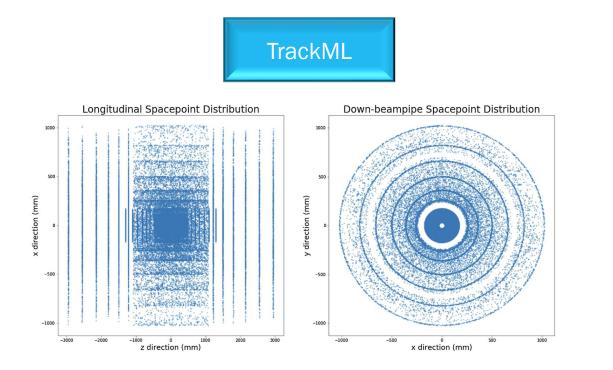
PIPELINE OVERVIEW

- Current pipeline of the L2IT-Exatrkx collaborative effort
- Each stage offers multiple independent choices, depending on hardware and time constraints

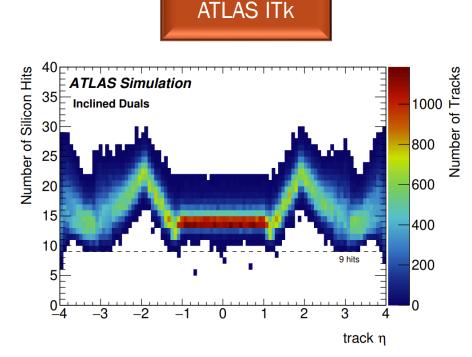


DATASETS

Two datasets used to study this pipeline. For absolute clarity, when citing a result specific to one dataset, will place the badge of TrackML or ATLAS ITk on slide:



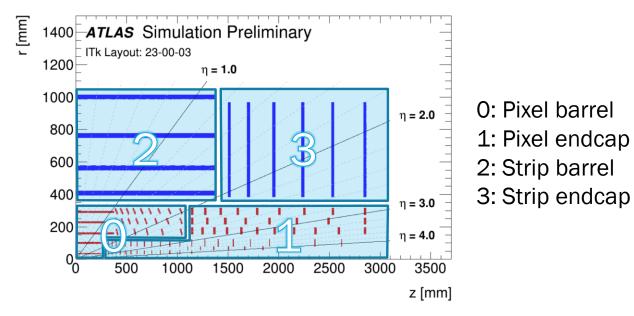
- Mean number of spacepoints: 110k
- Simplified simulation: No secondaries and optimistic charge information



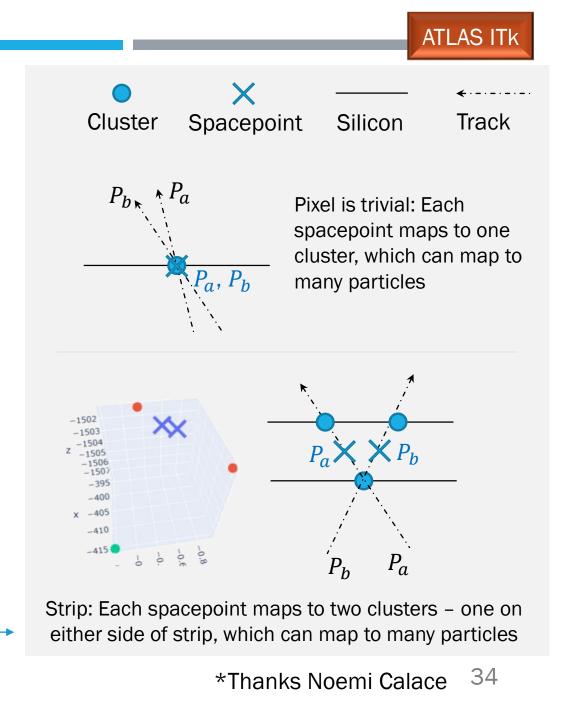
- Mean number of spacepoints: 310k
- Full simulation

ATLAS ITK GEOMETRY

- <u>Generation script</u>* using Athena, $t\bar{t}$ at $\mu = \langle 200 \rangle$: with statistics dominated by soft interactions
- ITk consists of barrel and endcap, each with pixels and strips:

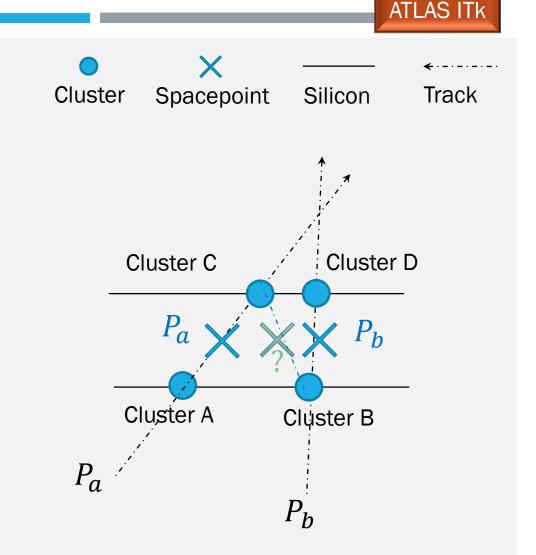


 Spacepoints (3D representations of track hits) are defined depending on strip or pixel:

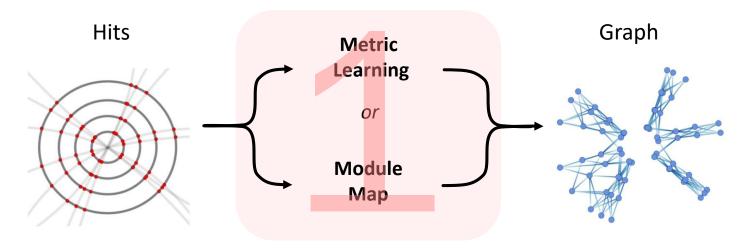


ATLAS ITK GEOMETRY

- Fiducial particles are charged, with η ∈ [-4, 4],
 and production radius < 260mm
- Each event has O(15k) fiducial particles, O(300k) spacepoints
- We define background spacepoints as including:
 - Those left by non-fiducial or intermediate particles (i.e. any particle barcodes not retained during simulation), or
 - Those mis-constructed in the strip regions as ghost ________
 spacepoints
- An event has O(170k) background spacepoints



Ghost spacepoint: Incorrectly constructed from clusters left by different particles

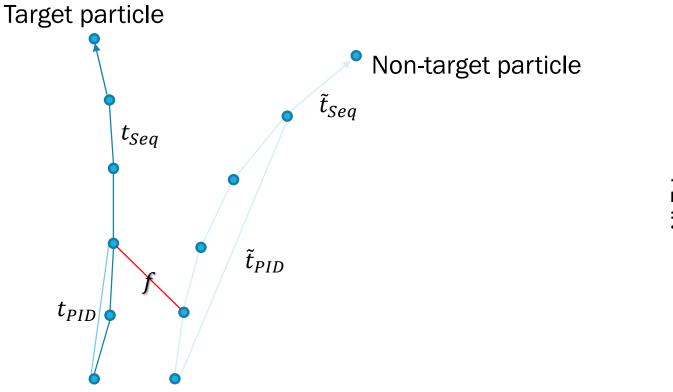


Graph Construction



LAB

EDGE TRUTH DEFINITIONS



Matching PID m_{PID} Fake fNon-target \tilde{t}_{PID} Target t_{PID} Target Seq. Truth t_{Seq}

Target particle:

- $p_T > 1$ GeV, and
- At least 3 SP on different modules, and
- Primary

Therefore, define efficiency and purity (note that we mask out sequential non-target) for a graph with edges *e*

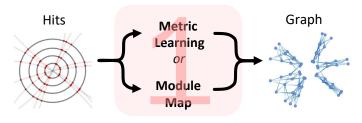
$$\text{Efficiency} = \frac{|e \cap t_{Seq}|}{|t_{Seq}|}, \text{ Purity} = \frac{|e \cap t_{Seq} - \tilde{t}_{Seq}|}{|e - \tilde{t}_{Seq}|}$$

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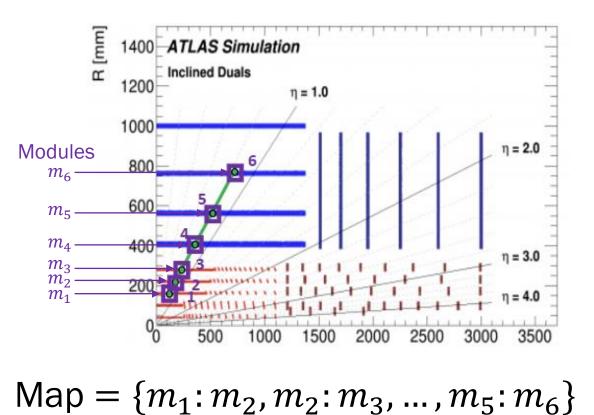


MODULE MAP - DOUBLETS

- The idea: Build a map of detector modules, where a connection *from* module A to module B means that at least one true track has passed sequentially through A to B
- Step 1: Build all combinations of sequential doublets for an event, register an A-to-B entry if a doublet passes through. O(90k) events used to build these combinations
- Step 2: For each A-to-B entry, also register/update the max and min values of a set of geometric observables. Apply these cuts when building the graph in inference

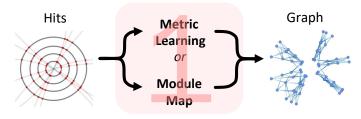


Graph Construction



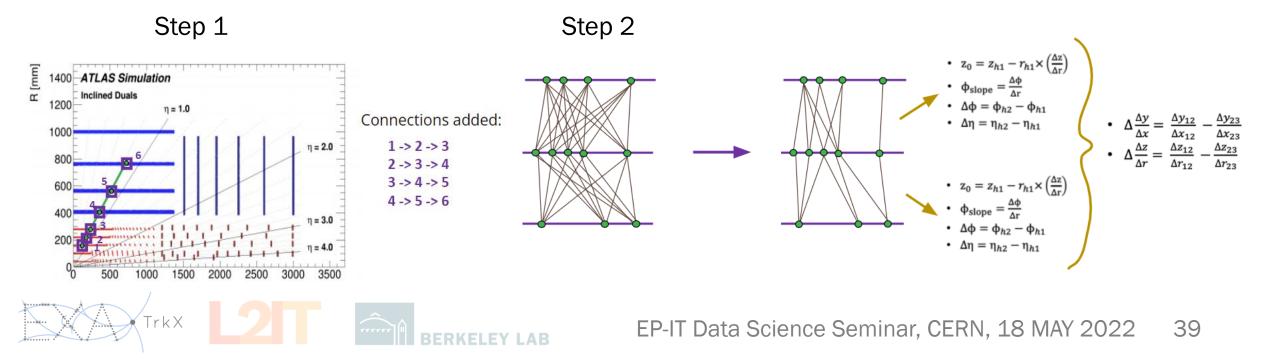
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MODULE MAP – TRIPLETS



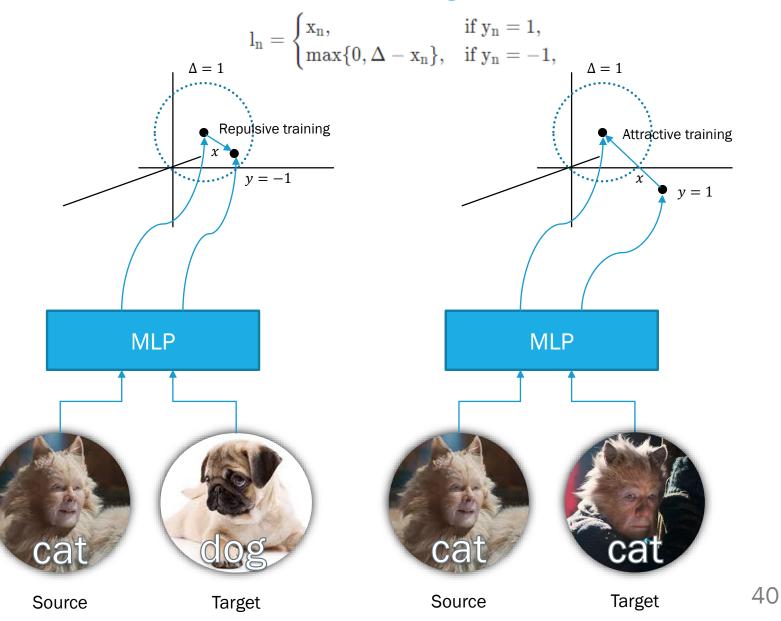
Graph Construction

- The idea: Build a map of detector modules, where a connection from module A to module B to module C means that at least one true track has passed sequentially through A to B to C
- Step 1: Build all combinations of sequential triplets for an event, register an A-to-B-to-C entry if a triplet passes through
- Step 2: For each A-to-B-to-C entry, also register/update the max and min values of a set of geometric observables. Apply these cuts when building the graph in inference



METRIC LEARNING INTUITION

- Encode / embed input into Ndimensional space
- Reward (low loss) matching pairs within unit distance
- Punish (high loss) mismatching pairs within unit distance
- Repeat for many pairs



"Contrastive" hinge loss

METRIC LEARNING



- In this embedded space, all doublets in a given particle track are trained to be near each other (Euclidean distance x), using a contrastive loss function L:
- $L = \begin{cases} x, \text{ if true pair} \\ \max(0, r x), \text{ if false pair} \end{cases}$

Metric Learning

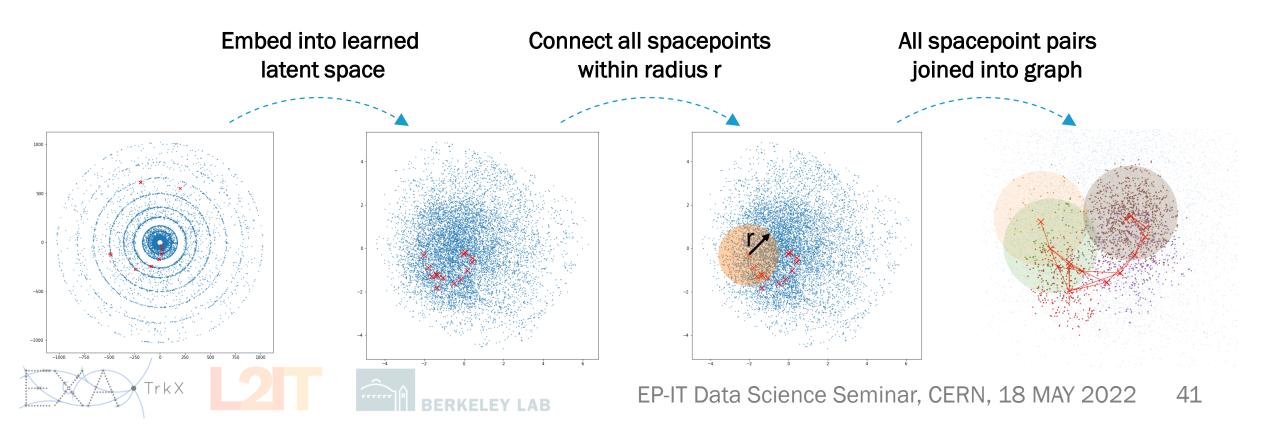
Module Map

Graph Construction

Graph

Hits

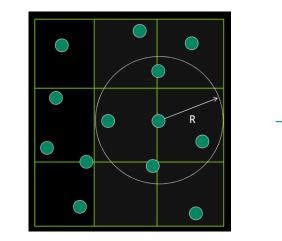
• A hit in a track is trained to be **closest** to its preceeding and succeeding track hits

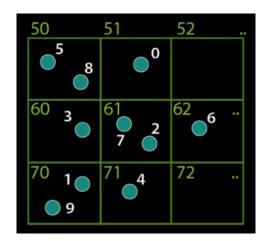


FAST GRAPH CONSTRUCTION

- Nearest neighbor search is a bottleneck of the graph construction stage
- <u>FAISS</u> finding K=500 for N=100,000 ~ 700ms
- KNN is overkill we don't need explicit list of K sorted neighbours
- Built <u>custom library</u> on Fixed Radius Nearest Neighbour (FRNN) search algorithm
- Cell-by-cell grid search is much faster: [The complexity of finding fixedradius near neighbors. Bentley, et al 1977]

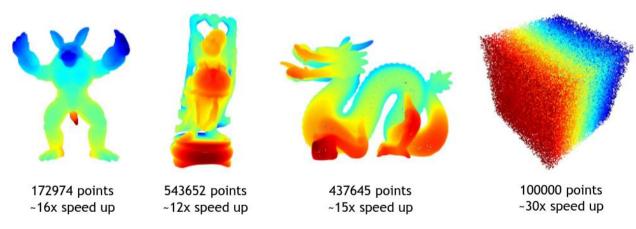
Fast fixed-radius nearest neighbors: Interactive Million-particle Fluids, Hoetzlein (NVIDIA), 2014

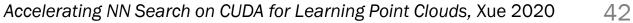




TrackML

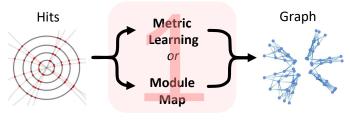
Fixed Radius NN Search vs Pytorch3D's KNN





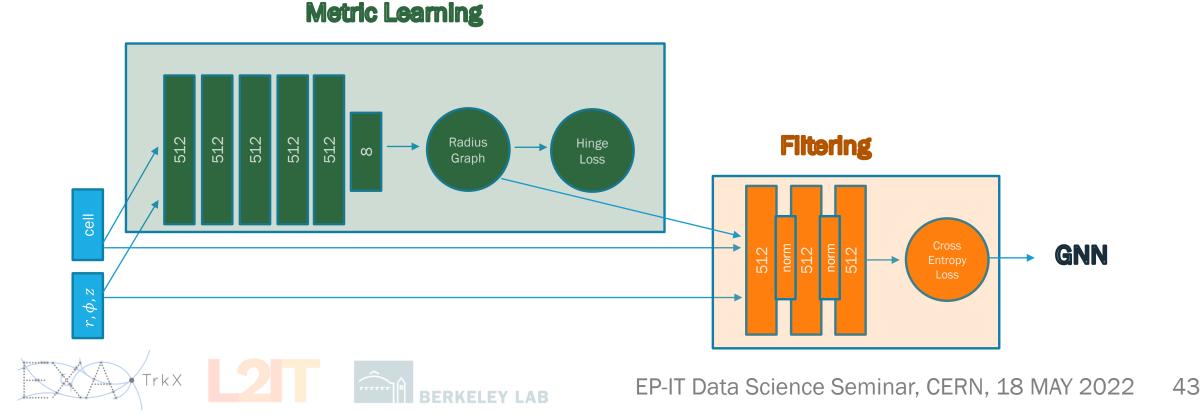
METRIC LEARNING - FILTERING

- Output graph of metric learning is impure: 0.2%
- Can pass edges through a simple MLP filter to filter out the easy fakes
- Improves purity to 2%, so graph can be trained entirely on a single GPU



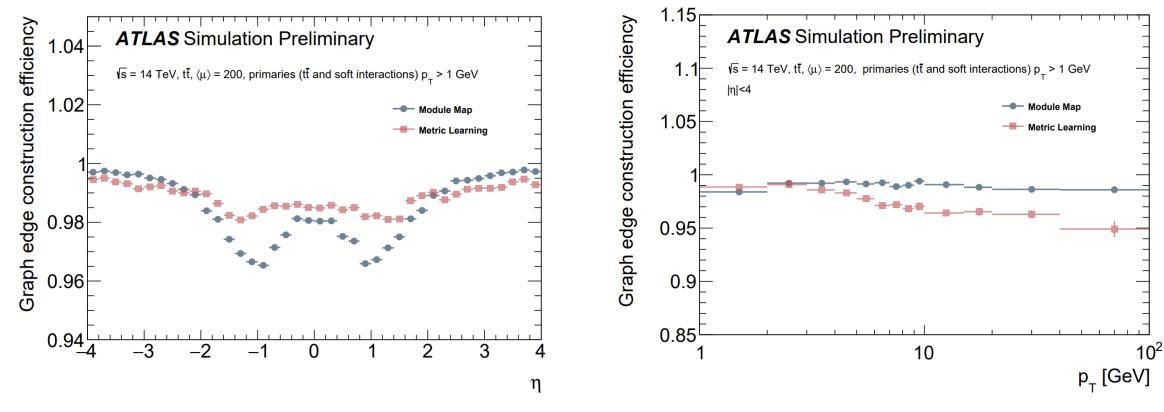
Graph Construction







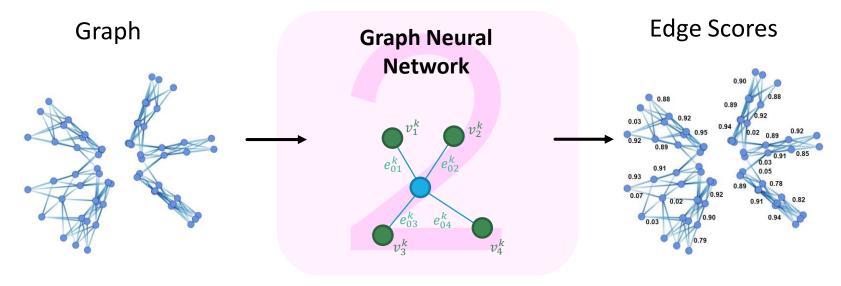
GRAPH CONSTRUCTION RESULTS



• Drop in efficiency at low η due to poor barrel strip resolution (will discuss further!)

training statistics

Drop in efficiency at high p_T due to low



Edge Labeling



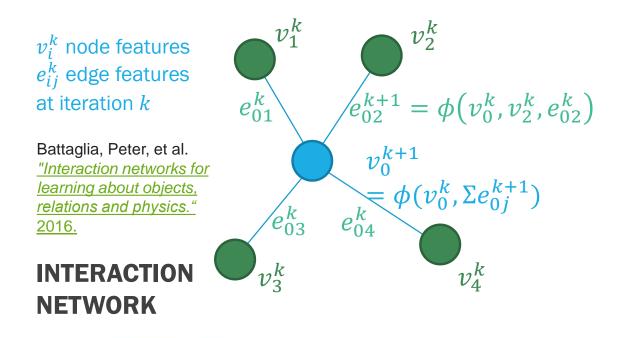
ELEY LAB

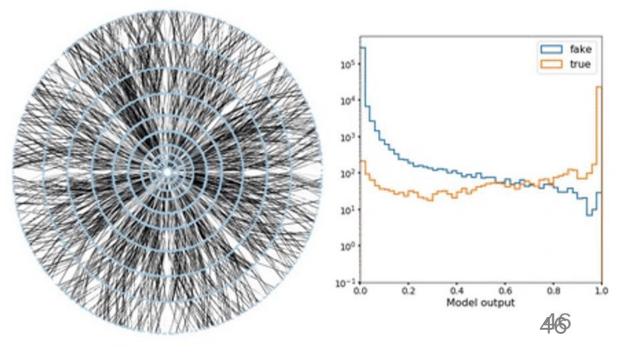
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EDGE CLASSIFICATION WITH GRAPH NEURAL NETWORK

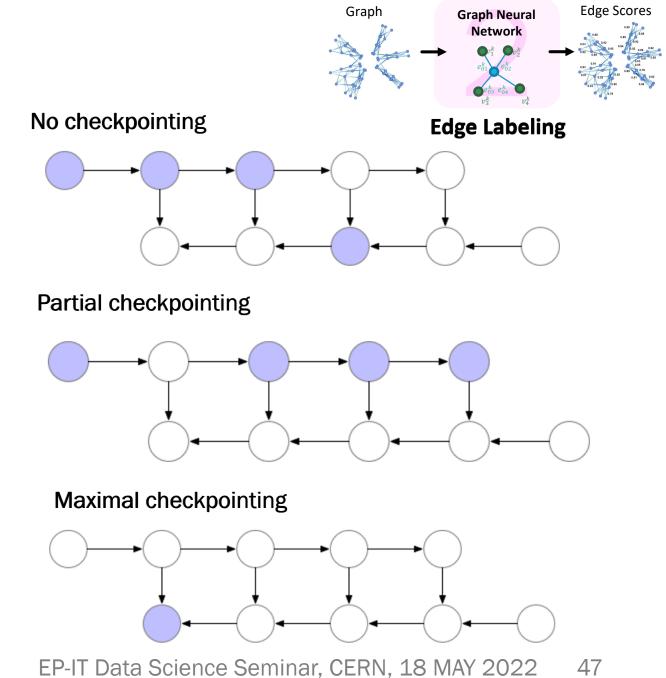
- 1. Node features (spatial position) are encoded
- 2. Encoded features are concatenated and encoded to create edge features
- Edge features are aggregated around nodes to create next round of encoded node features (i.e. message passing)
- 4. Each iteration of message passing improves discrimination power





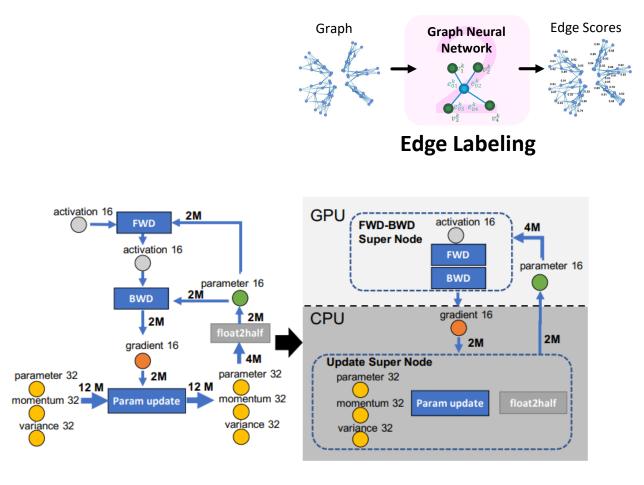
MEMORY MANAGEMENT

- Graph construction leads to very large graphs
 O(1m) edges, cannot fit training on A100 GPU
 with 32Gb memory
- Should not split the graphs up (leads to lower GNN accuracy)
- Solution A: Were previously using a compromising form of "gradient checkpointing" reduced memory by 4x
- Now using maximal checkpointing, reduce memory further by 2x – just fits on A100



TRAINING SOLUTIONS

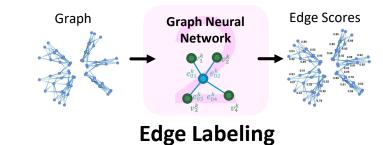
- Solution B: Model offloading
- Each layer of GNN placed on GPU for forward and backward pass, but held on CPU otherwise
- Works well with TensorFlow, enabling training of O(1m) edge graphs
- Unable to integrate with Pytorch pipeline



ZeRO-Offload: Democratizing Billion-Scale Model Training arXiv: 2101.06840

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LOSS FUNCTION DESIGN

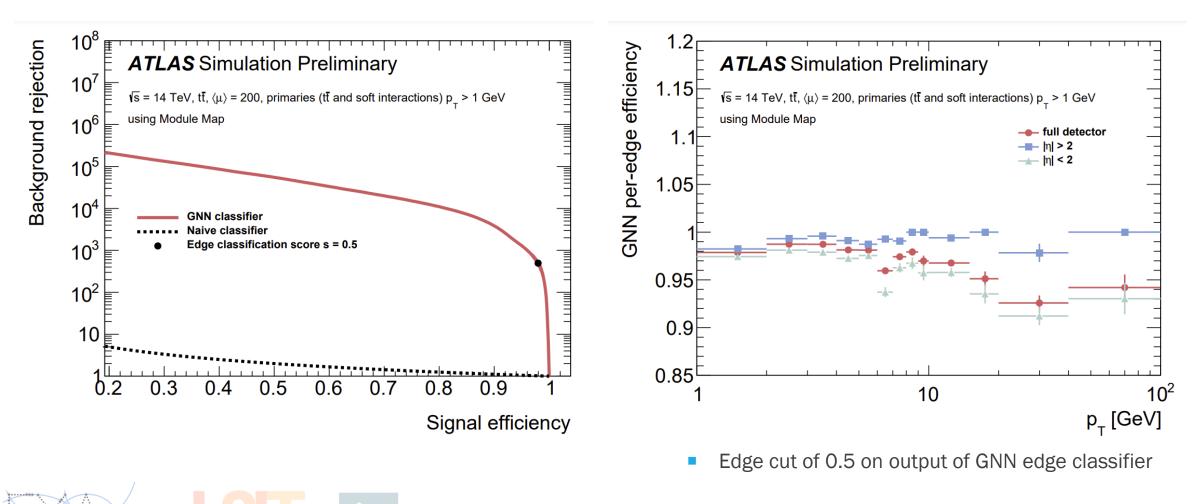


- The target of the GNN and track reconstruction is edges from primary particles with pT>1 GeV that have left at least 3 hits on different modules in the detector (see slide 12)
- Have very small set of target edges (1-2% of edges are true target t_{Seq})
- Solution: $t_{Seq} y = 1$ weighted up by $\times 10$, sequential background \tilde{t}_{Seq} masked, all others y = 0
- Weighting gives much better performance at high-efficiency
- Masking gives much better performance around the 1 GeV cutoff

ATLAS ITk

GNN EDGE CLASSIFICATION RESULTS

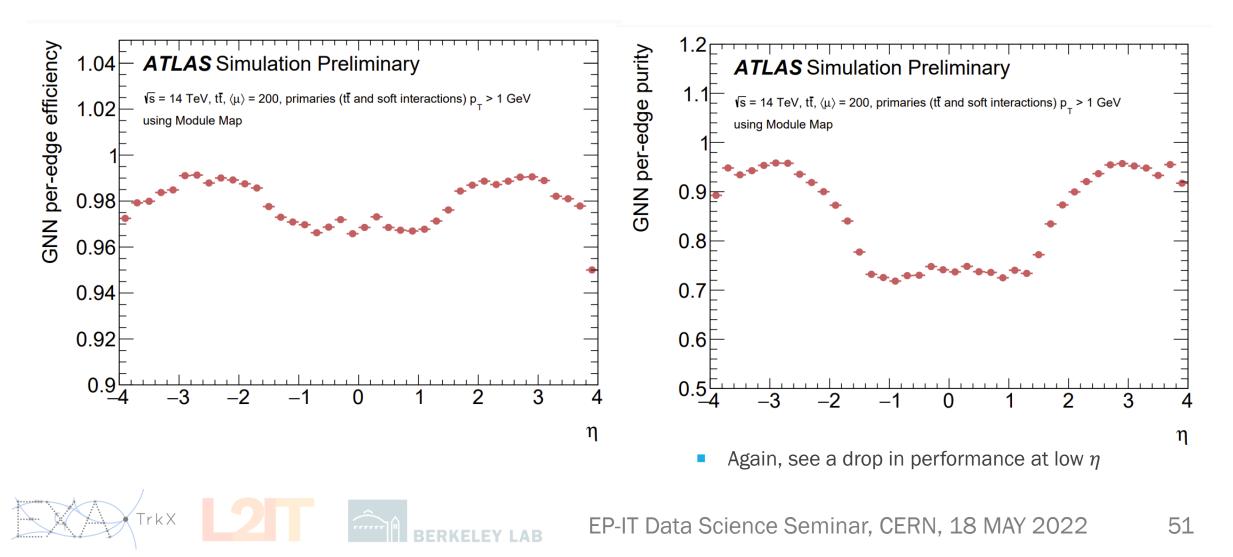
ROC CURVE & EDGEWISE PERFORMANCE VS. p_T



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GNN EDGE CLASSIFICATION RESULTS

EDGEWISE PERFORMANCE VS. η



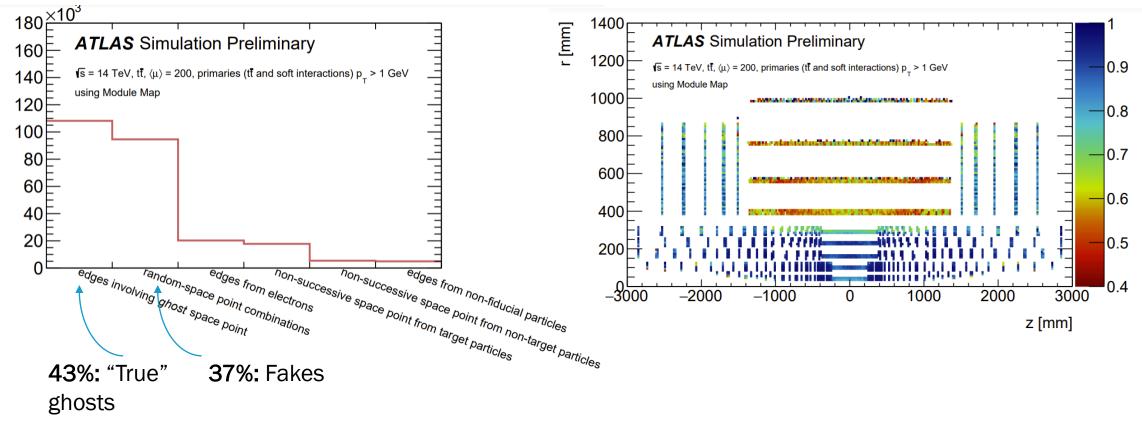
GNN per-edge purity

BARREL STRIP MISCLASSIFICATION

Nature of false positive edges

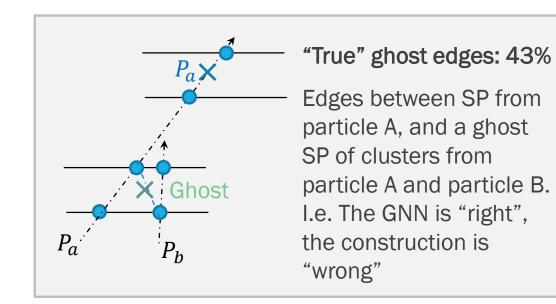
Number of edges

Location of false positive edges



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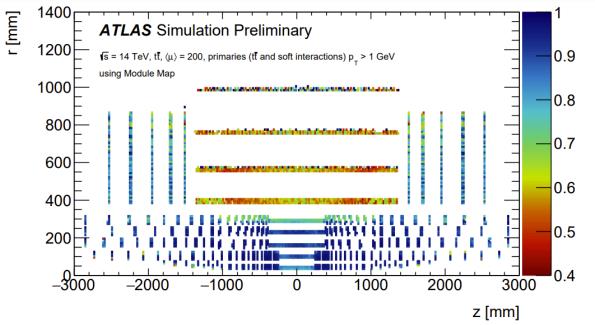
BARREL STRIP MISCLASSIFICATION



Fake edges: 37%

Edges between SP from particle A and particle B. i.e. The GNN is "wrong"

Location of false positive edges



GNN per-edge purity

ATLAS ITk

ATLAS ITk

STRIP MODULES: GHOSTS AND Z-RESOLUTION

- Since spacepoints are constructed from pairs of clusters in the strip, could mis-construct and form a ghost
- These ghosts can be cleaned up in later stages of the reconstruction chain
- However, even for correctly matched clusters, there remains low z-resolution
- Consider this example
- Easily confuses GNN!
- Could fix by including underlying cluster information somehow... (e.g. heterogeneous node features)

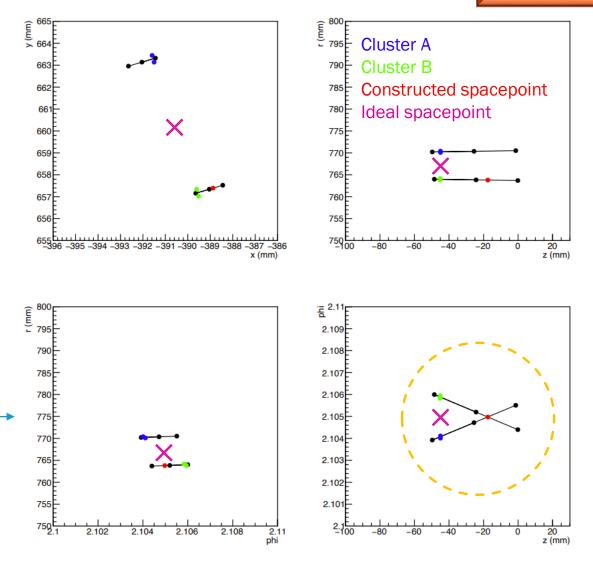
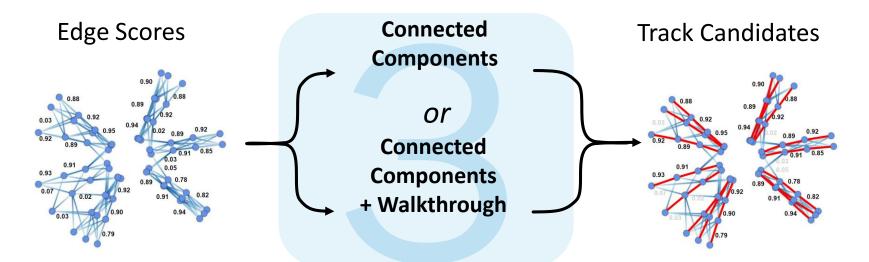


Image courtesy of Jan Stark - thanks!

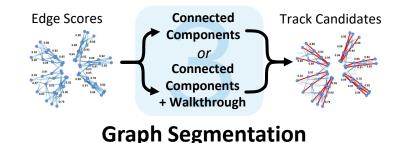


Graph Segmentation



EP-IT Data Science Seminar, CERN, 18 MAY 202255

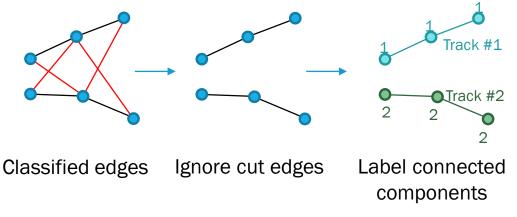
TRACK CANDIDATES CONSTRUCTION



- We now have labelled edges. Want to now label each *node* depending on connectivity.
- Two distinct approaches: **component-based** segmentation, or **path-based** segmentation.

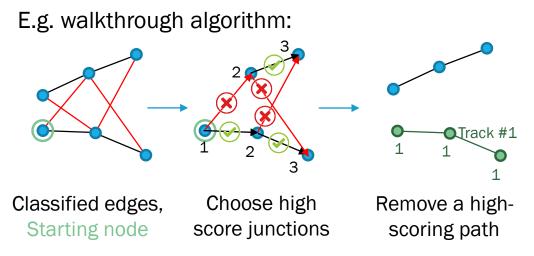
Component-based

E.g. connected components algorithm:



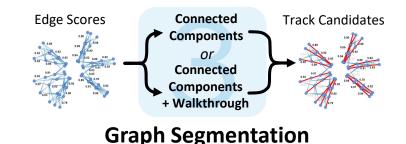
- Pros: Fast $O(N_{nodes})$
- Cons: Can merge tracks into one candidate

Path-based

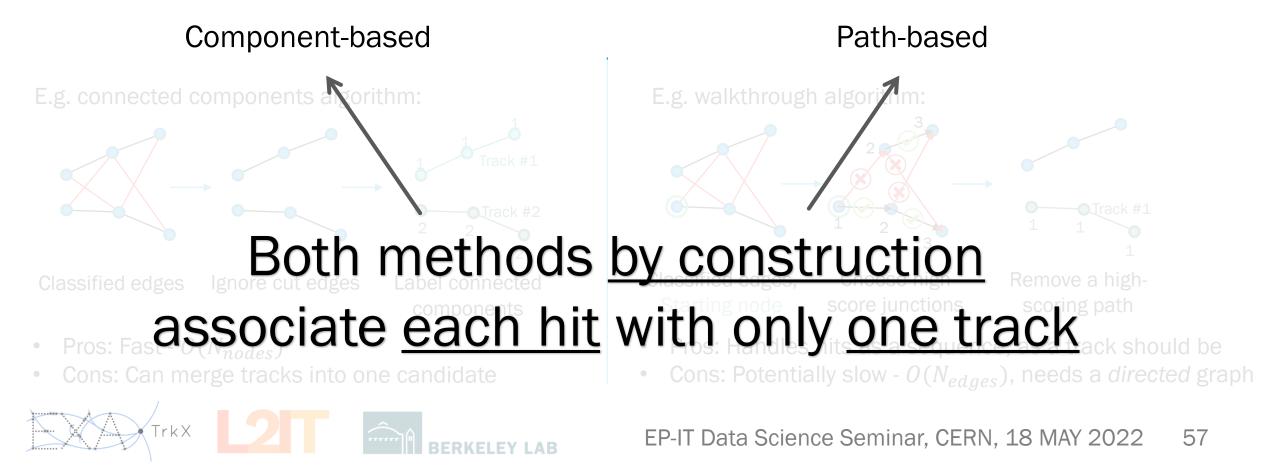


- Pros: Handles hits as a sequence, as a track should be
- Cons: Potentially slow $O(N_{edges})$, needs a directed graph

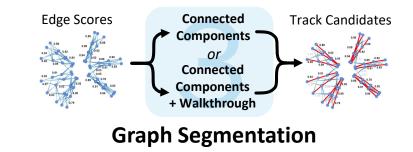
TRACK CANDIDATES CONSTRUCTION



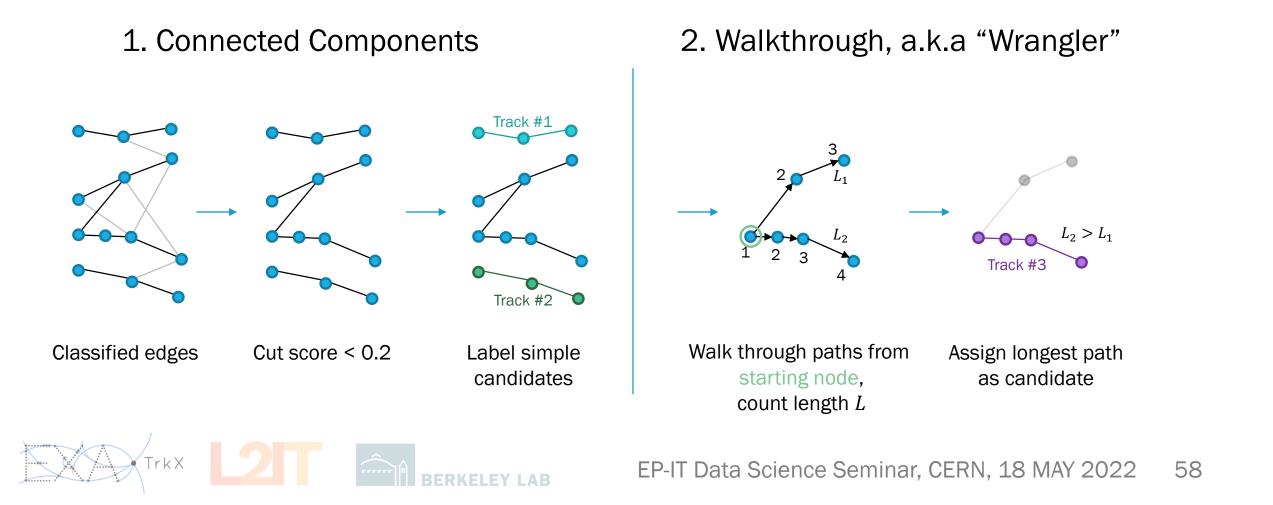
- We now have labelled edges. Want to now label each *node* depending on connectivity.
- Two distinct approaches: **component-based** segmentation, or **path-based** segmentation.



TRACK CANDIDATES CONSTRUCTION



• Our specific algorithm combines the good features of each approach:

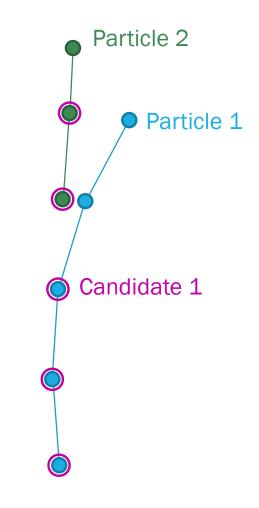


TRACK MATCHING DEFINITIONS

- $N(P_i, C_j)$ is the number of spacepoints shared by particle *i* and candidate *j*
- Particle *i* is called "matched" if, for some *j*, $\frac{N(P_i,C_j)}{N(P_i)} > f_{truth}$
- Candidate *j* is called "matched" if, for some *i*, $\frac{N(P_i,C_j)}{N(C_i)} > f_{reco}$
- Particle *i* and candidate *j* are called "double matched" if, for some *i* and *j*, $\frac{N(P_i,C_j)}{N(P_i)} > f_{truth} \text{ and } \frac{N(P_i,C_j)}{N(C_j)} > f_{reco}$

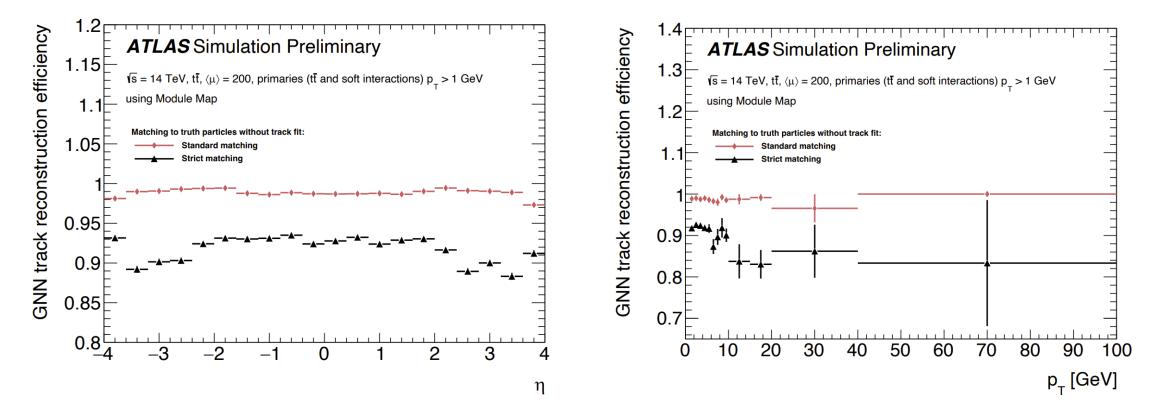
•
$$eff = \frac{\sum_{i} P_{i}(matching \ condition)}{\sum_{i} P_{i}}, \ pur = \frac{\sum_{j} C_{j}(matching \ condition)}{\sum_{j} C_{j}}$$

Standard matching: single-matched particles with $f_{truth} = 0.5$ **Strict matching:** double-matched particles with $f_{reco} = 1.0$



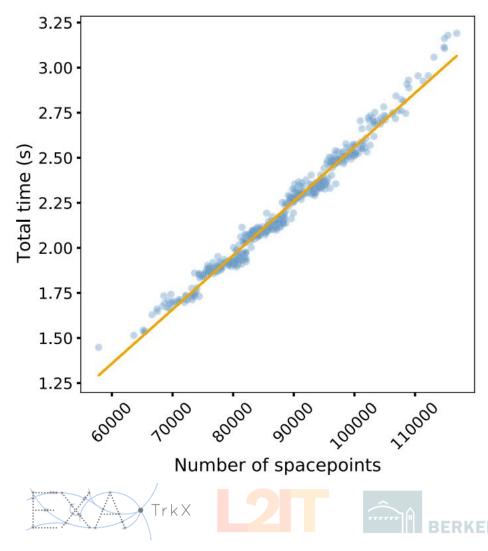


TRACK RECONSTRUCTION RESULTS



Standard matching: single-matched particles with $f_{truth} = 0.5$ **Strict matching:** double-matched particles with $f_{reco} = 1.0$ • Fake rate is $O(10^{-3})$ using standard truth matching

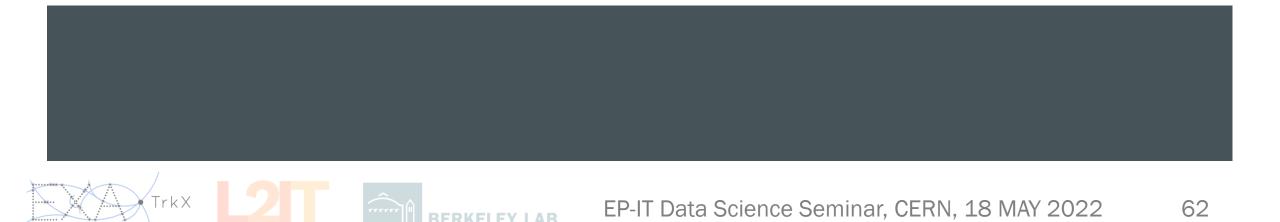
TIMING AND SCALING PERFORMANCE



	Baseline	Faiss	cuGraph	AMP	FRNN
Data Loading Embedding	$\begin{array}{c} 0.0022 \pm 0.0003 \\ 0.02 \pm 0.003 \end{array}$	$\begin{array}{c} 0.0021 \pm 0.0003 \\ 0.02 \pm 0.003 \end{array}$	$\begin{array}{c} 0.0023 \pm 0.0003 \\ 0.02 \pm 0.003 \end{array}$	$\begin{array}{c} 0.0022 \pm 0.0003 \\ 0.0067 \pm 0.0007 \end{array}$	$\begin{array}{c} 0.0022 \pm 0.0003 \\ 0.0067 \pm 0.0007 \end{array}$
Build Edges Filtering	$12 \pm 2.64 \\ 0.7 \pm 0.15$	$0.54 \pm 0.07 \\ 0.7 \pm 0.15$	$0.53 \pm 0.07 \\ 0.7 \pm 0.15$	$0.53 \pm 0.07 \\ 0.37 \pm 0.08$	$0.04 \pm 0.01 \\ 0.37 \pm 0.08$
GNN Labeling	0.17 ± 0.03 2.2 ± 0.3	0.17 ± 0.03 2.1 ± 0.3	$0.17 \pm 0.03 \\ 0.11 \pm 0.01$	$\begin{array}{c} 0.17 \pm 0.03 \\ 0.09 \pm 0.008 \end{array}$	$\begin{array}{c} 0.17 \pm 0.03 \\ 0.09 \pm 0.008 \end{array}$
Total time	$15 \pm 3.$	3.6 ± 0.6	1.6 ± 0.3	1.2 ± 0.2	0.7 ± 0.1

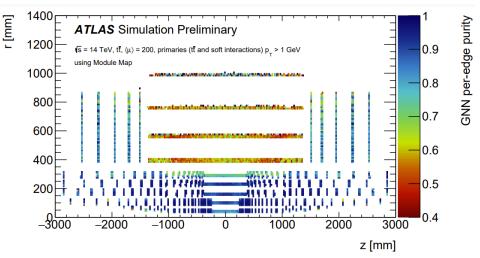
- Physics is important, but GNNs shine in scaling behavior
- When development began, graph-based pipeline started required 15 sec for TrackML
- Implemented custom Fixed Radius Nearest Neighbor (FRNN) algo., cuGraph Connected Components algo., and Mixed Precision inference
- Now have sub-second TrackML inference on 16Gb V100 GPU
- Inference time scales approximately linearly across size of event, in TrackML

ONGOING WORK



ONGOING WORK: HETEROGENEOUS NODE FEATURES

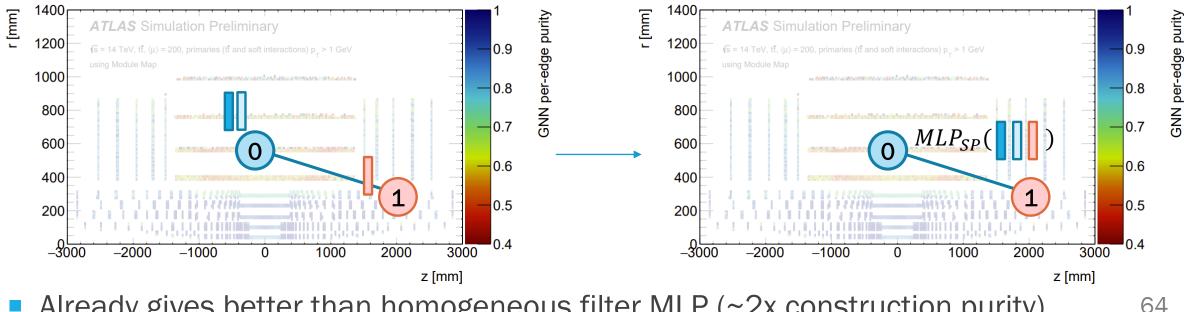
- Motivated by inconsistent performance across detector:
- Currently each node in graph uses same input feature set spacepoint $s = (r, \phi, z)$



- We could imagine using cluster-level information, e.g. position and shape of energy deposit
- But: this is not consistent across detector. Need different node and edge networks depending on detector region

ONGOING WORK: HETEROGENEOUS NODE FEATURES

- To get intuition, consider simple filter MLP applied to two pixel nodes:
- To apply a filter MLP to a pixel (single cluster) and strip (double cluster) node combination, need a *different* MLP:



0

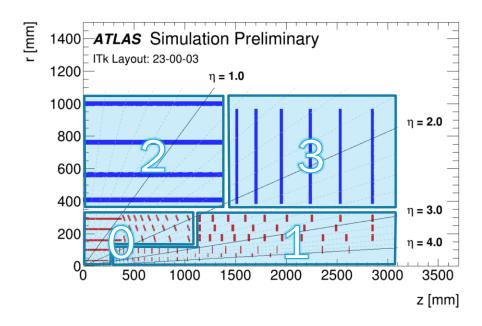
 MLP_{PP}

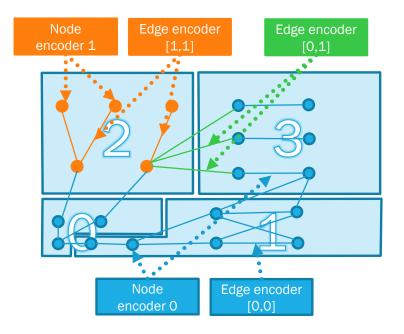
0

Already gives better than homogeneous filter MLP (~2x construction purity)

ONGOING WORK: HETEROGENEOUS GRAPH NEURAL NETWORK

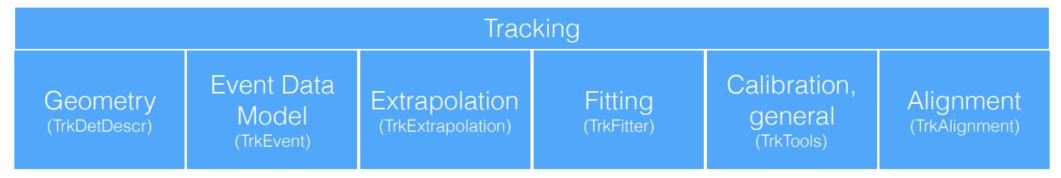
- Exact same logic applies to GNN networks
- For a four-region heterogeneous GNN, we have four node encoders/networks (N_0, N_1, N_2, N_3) and ten edge encoders/networks $(E_{00}, E_{01}, E_{02}, E_{03}, E_{11}, \dots, E_{34}, E_{44})$
- Thus, is a larger model and takes longer to train
- But reduces GNN inefficiency and fake rate by approximately half





ONGOING WORK: ACTS & ATHENA INTEGRATION

A. Salzburger, et al.



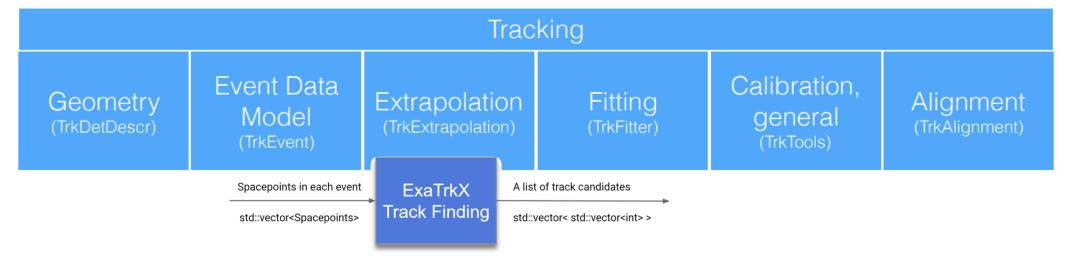
ACTS (<u>A Common Tracking Software</u>)

- A library for tracking that is independent of particular experiment or geometry
- Written in highly performant c++ and parallelized



ONGOING WORK: ACTS & ATHENA INTEGRATION





Integration of GNN pipeline with ACTS

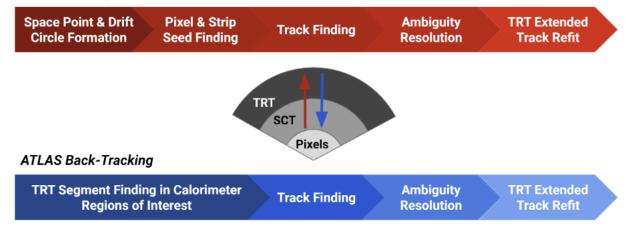
- Integration complete, with generic TrackFindingMLBased interface
- Uses TorchScript to call ML models (OnnxRuntime not yet fully compatible with GNN methods)
- Replaces seeding and track finding stages, produces protoTracks

ONGOING WORK: ACTS & ATHENA INTEGRATION

<u>Athena</u>

 Framework for ATLAS event generation, simulation, digitization, reconstruction and analysis

ATLAS Primary Tracking



Integration of GNN pipeline with Athena:

This is ongoing!

OTHER ONGOING WORK

Extending Trac



inference timing and scaling studies to



- Investigating training and inference performance on lower p_T tracks (i.e. < 1 GeV) and high p_T tracks (i.e. > 10 GeV)
- Investigating performance on large radius tracks and dense track environments
- Direct comparison with combinatorial Kalman filter (current algorithm) efficiency and track parameter resolution



CONCLUSION

- A graph-based representation of particle collisions is intuitive and rich
- GNNs and other graph techniques are well-suited even to high luminosity events
- Produced first public results on official ATLAS ITk geometry using GNN-based track reconstruction pipeline
- Promising reconstruction performance, well-positioned for comparison with traditional algorithms
- This is very early in development many more improvements are in progress within Exatrkx+L2IT
- Also new techniques being invented in GNN/ML community every day

THANKS FOR TUNING IN!

Links

<u>ExaTrkx website</u> • <u>L2IT website</u> • <u>ExaTrkx paper</u> • <u>L2IT paper</u> • <u>Codebase</u>