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

1

HIGH LUMINOSITY TRACK RECONSTRUCTION

EP-IT Data Science Seminar, CERN, 18 MAY 2022 2

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
- 3. W mass precision improvement from ±[9.4MeV t](https://www.science.org/doi/10.1126/science.abk1781)o ±[6MeV](https://indico.cern.ch/event/765096/contributions/3295995/attachments/1785339/2906404/HLLHC.pdf)

[ATL-PHYS-PUB-2018-048](http://cdsweb.cern.ch/record/2651927/files/ATL-PHYS-PUB-2018-048.pdf)

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)
- \blacksquare 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

6

REPRESENTATION OF COLLISIONS

EP-IT Data Science Seminar, CERN, 18 MAY 2022

COMPUTE SCALING FOR HIGH LUMINOSITY

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

EP-IT Data Science Seminar, CERN, 18 MAY 2022 8

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.

11

12

EP-IT Data Science Seminar, CERN, 18 MAY 2022 13

NODE FEATURE e.g. "West Oakland"

EP-IT Data Science Seminar, CERN, 18 MAY 2022

EDGES CAN HAVE FEATURES

WHAT IS A GRAPH?

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

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

EP-IT Data Science Seminar, CERN, 18 MAY 2022 17

GRAPHS ARE A NATURAL WAY TO REPRESENT TRACKS

Connect the hits in some way

EP-IT Data Science Seminar, CERN, 18 MAY 2022 18

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

21

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.**

EP-IT Data Science Seminar, CERN, 18 MAY 2022 23

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
- *An*isotropic message passing: encode a combination of node and neighbor along each edge
- Much more expensive now need to store N_{edges} for backpropagation
- But [much more powerful](https://arxiv.org/pdf/2003.00982.pdf)

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

0 2 1 3 4 0 2 1 3 4 Encoded channels

Pre-encoded channels

GNNS ELSEWHERE IN PARTICLE PHYSICS

- **Very large and active field of study!**
- Comprehensive review of GNNs for Track Reconstruction [arXiv:2012.01249](https://arxiv.org/abs/2012.01249)
- White paper on progress and future of the field arXiv: 2203.12852

GRAPH-BASED TRACK RECONSTRUCTION

EP-IT Data Science Seminar, CERN, 18 MAY 2022 29

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

- Generation script^{*} 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** $\eta \in [-4, 4]$, 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

EDGE TRUTH DEFINITIONS

Matching PID $m_{PID} \longrightarrow$ Fake f Non-target \tilde{t}_{PID} Target t_{PID} Target Seq. Truth t_{Seq}

ATLAS ITk

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

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

EP-IT Data Science Seminar, CERN, 18 MAY 2022 37

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

 $Map = \{m_1 : m_2, m_2 : m_3, ..., m_5 : m_6\}$

EP-IT Data Science Seminar, CERN, 18 MAY 2022 38

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**

METRIC LEARNING

- The idea: Teach an MLP to embed spacepoint features (spatial and cell information)
- 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 :
- $L=$ x , if true pair $max(0, r - x)$, if false pair

Metric Learning

Hits **Metric** Graph

or

Module Map

Graph Construction

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
- **[FAISS](https://github.com/facebookresearch/faiss)** finding K=500 for N=100,000 ~ 700ms
- KNN is overkill we don't need explicit list of K sorted neighbours
- Built [custom library](https://github.com/lxxue/FRNN/tree/larged) 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!)

Drop in efficiency at high p_T due to low training statistics

Edge Labeling

KELEY LAB

EP-IT Data Science Seminar, CERN, 18 MAY 2022 45

EDGE CLASSIFICATION WITH GRAPH NEURAL NETWORK

- 1. Node features (spatial position) are encoded
- 2. Encoded features are concatenated and encoded to create edge features
- 3. 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

EP-IT Data Science Seminar, CERN, 18 MAY 2022 48

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

GNN EDGE CLASSIFICATION RESULTS

ROC CURVE & EDGEWISE PERFORMANCE VS. p_T

EP-IT Data Science Seminar, CERN, 18 MAY 2022 50

ATLAS ITk

ATLAS ITk

GNN EDGE CLASSIFICATION RESULTS

EDGEWISE PERFORMANCE VS. η

BARREL STRIP MISCLASSIFICATION

Nature of false positive edges Location of false positive edges

BARREL STRIP MISCLASSIFICATION

Fake edges: 37%

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

$P_a \times$ The grost edges. 43%

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

LAB

EP-IT Data Science Seminar, CERN, 18 MAY 2022 55

TRACK CANDIDATES CONSTRUCTION

Connected Components Connected Components + Walkthrough *or* Edge Scores **Connected** Track Candidates

Graph Segmentation

- 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*, $\frac{N(P_i, C_j)}{N(P_i)}$ $\frac{\Gamma(\nu)}{N(P_i)} > f_{truth}$
- Candidate *j* is called "matched" if, for some *i*, $\frac{N(P_i, C_j)}{N(C_i)}$ $\frac{\Gamma(\text{C})}{N(C_j)}$ > freco
- Particle i and candidate j are called "double matched" if, for some i and j , $N(P_i,C_j)$ $\frac{N(P_i, C_j)}{N(P_i)}$ > f_{truth} and $\frac{N(P_i, C_j)}{N(C_j)}$ $\frac{\Gamma(\text{C})}{N(C_j)}$ > freco

•
$$
eff = \frac{\sum_i P_i(matching condition)}{\sum_i P_i}
$$
, $pur = \frac{\sum_j C_j(matching condition)}{\sum_j C_j}$

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

- 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

1

 $\boxed{0}$

 MLP_{PP}

1

Already gives better than homogeneous filter MLP $(\sim 2x)$ 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 $(E_{00}, E_{01}, E_{02}, E_{03}, E_{11}, ..., E_{34}, E_{44})$
- 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.](https://indico.cern.ch/event/699252/contributions/2881457)

ACTS ([A Common Tracking Software](https://arxiv.org/abs/1910.03128))

- 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,](https://github.com/xju2/acts/tree/xju/exatrkx-plugins) 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

[Athena](https://atlassoftwaredocs.web.cern.ch/athena/athena-intro/)

 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 TrackML inference timing and scaling studies to **ATLAS ITK**

- 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!

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

Links

ExaTrkx [website](https://exatrkx.github.io/) ● [L2IT website](https://www.l2it.in2p3.fr/) ● [ExaTrkx](https://link.springer.com/article/10.1140/epjc/s10052-021-09675-8) paper ● [L2IT paper](https://www.epj-conferences.org/articles/epjconf/pdf/2021/05/epjconf_chep2021_03047.pdf) ● [Codebase](https://hsf-reco-and-software-triggers.github.io/Tracking-ML-Exa.TrkX/)