Charged Particle Tracking with Graph Neural Networks

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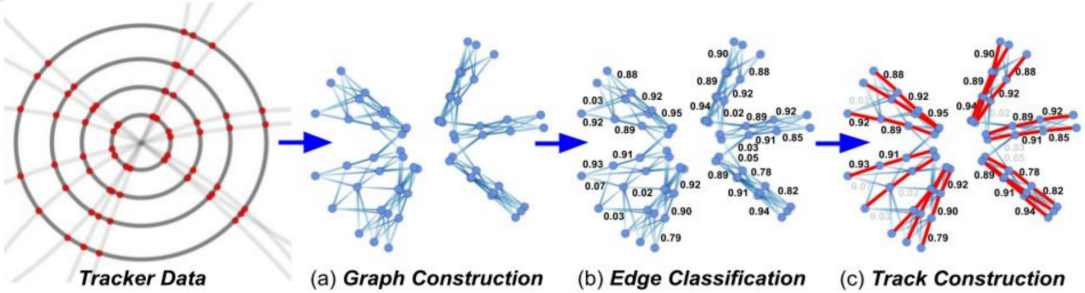
...along with many collaborators, including numerous IRIS-HEP fellows and researchers at UCSD, FNAL, Exa.TrkX, ...

Tracking with Edge Classifier GNNs

General approach



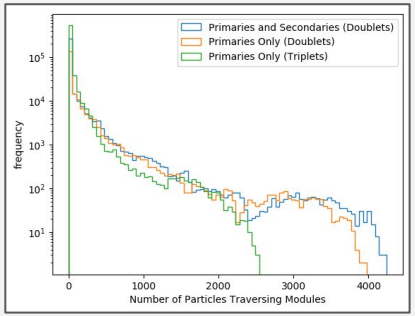
[Interaction Networks for Tracking (github)]

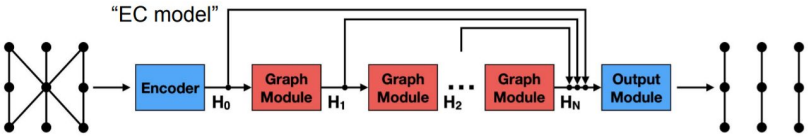
[Graph Construction and Edge Classifier (github)]

Graph Construction

Graphs constructed using **module map** (MM) approach

Both doublet and triplet MMs have been studied for TrackML & ATLAS ITk sim





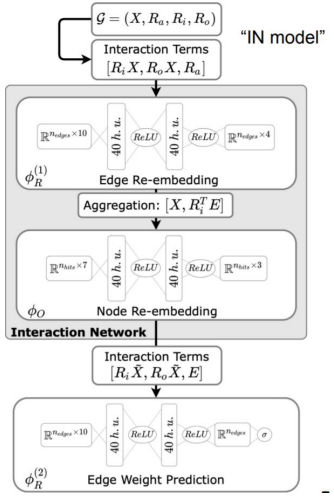
Edge Classification

Larger Model: "Edge Classifier" Network (EC)

- ~260k parameters
- Good performance observed

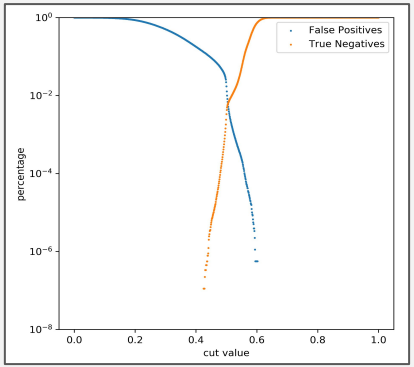
Smaller Model: "Interaction Network" (IN)

- ~6k parameters
- Comparable performance to EC, working to optimize



Track Construction

Apply **cut on edge scores**



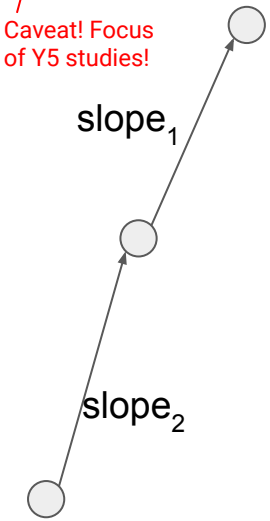
Resulting subgraphs are track candidates, created with **union find algorithm**

Tracking with Edge Classifier GNNs

Module Map Construction

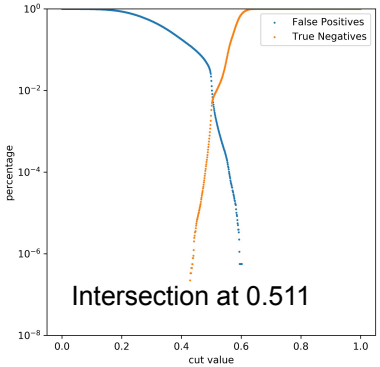
- Generated with all 8850 events
- Nodes were cut using truth level p_T cut > 1 GeV
- Noise hits removed
- All detector layers used
- Module Triplets stored

Caveat! Focus of Y5 studies!



Graph Statistics

# Nodes	**9950.4**
# Edges	**220007.1**
# True Edges	**18275.9**
Purity	**83.05%**



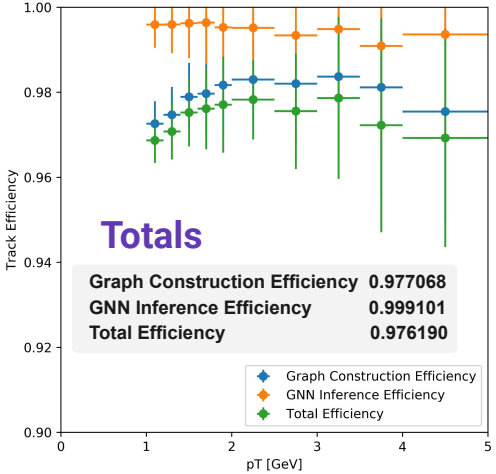
Track Building

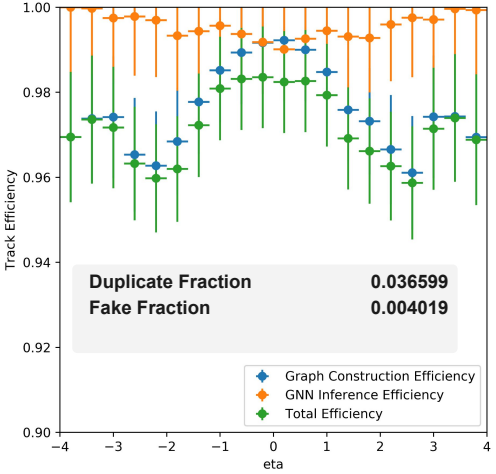
- Remove edges < 0.511
- Union Find the fragmented clusters as track candidates
- **Perfect matches**: All hits in the track candidate are from same particle

Graph Construction Cuts

- Nodes were cut using truth level p_T cut > 1 GeV
- Noise hits removed
- All Layers used
- Module Map frequency cut > 50
- Doublet Edge cuts
  - $|\phi\text{-slope}| < .0006$
  - $|z_0| < 50$
- Triplet Edge cuts
  - $|\Delta\,\phi\text{-slope}| < .00023$
  - $|\Delta\,z\text{-slope}| < .1$
- Undirected Edges

TrackML Results





We did analogous studies using ATLAS ITk simulation (not included) which shows similarly good results.

Impact: IRIS-HEP GNN work is driving forward the ATLAS Phase-II EF tracking FPGA-based demonstrator

Object Condensation Networks

new

GageDeZoort Gage DeZoort

klieret Kilian Lieret

Traditional GNN pipeline:

Hits/ point cloud → Construction of initial graphs → Edge classification & pruning → Track construction → Fit track

Track

pT, ...

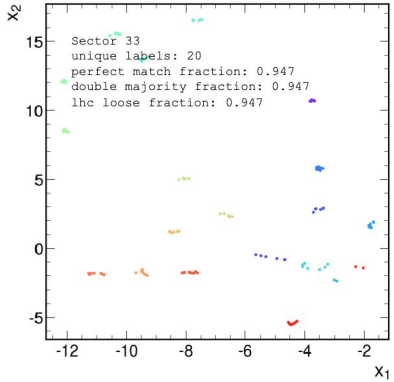
Vision:

Hits/ point cloud → **Object condensation (OC)** Learnt projection of hits to latent space → Trivial clustering

pT, ...

Track

Learnt latent space



Object condensation (OC)

- Model learns to minimize attractive and repulsive potentials that lead to **clustering in (learnt) latent space** around **condensation point** (Jan Kiesler 10.1140/epjc/s10052-020-08461-2)
- Features of condensation point correspond to pT
- OC approach has been applied successfully to calorimetry but never to tracking
- Model might involve dynamical graph-building (GravNet-style)

Status quo

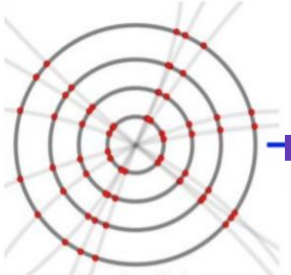
- Still using "traditional" graph construction & edge classification in front of OC
- Currently not focusing on pT prediction
- With pT > 1 GeV truth cut and w/o noise: "Easy"
- Currently training w/o these cuts: Promising

Openly developed on GitHub

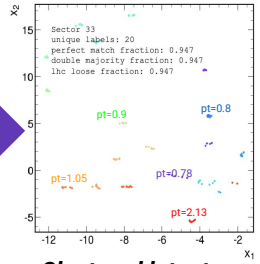
Summary / Thoughts for Y5+

- **Edge Classification Network** approach is a modular tracking approach (each stage can be studied and optimized separately) which shows **promise** to significantly speed up tracking at HL-LHC
  - IRIS-HEP work is impacting ATLAS Phase-II EF tracking developments (FPGA demonstrator)
- Further optimizing the IN model (e.g. adding additional message-passing steps, layers) to boost performance in central region without blowing up the size of model (...accelerators) is work in progress
- Plan to re-do previous studies on train/evaluation with/without truth/noise/.. cuts (generalization) and compare to more “traditional” (e.g. CKF) approaches (which themselves are in devel/optimization mode)
- Plan to perform further studies on graph/detector segmentation (likely important for EF applications)

- **Object Condensation Network** approach is new and **exploratory** approach with **potentially big payoff**
  - **Vision of one-shot model**: Feed in point cloud, get out tracks & track parameters
  - Gradually moving into this direction: First demonstrate viability with “traditional” graph building and edge classification in model, then experiment with GravNet and similar algorithms
  - Already evaluating & benchmarking on TrackML dataset **w/o truth cuts**
  - Investigate faster training by using truth cuts during training (not evaluation!)



Tracker Data



Clustered latent space

In both approaches, integration into experiment tracking software (for ATLAS→ACTS) and comparisons to more traditional (non-ML) tracking approaches planned for HL-LHC will be next IRIS-HEP phase focus

Backup

Connecting the dots…

https://indico.cern.ch/event/1103637/

Mini-workshop on Graph Neural Networks for Tracking

3 June 2022
Princeton University
US/Eastern timezone

09:00	**Welcome** — *Savannah Jennifer Thais* — Princeton University	09:00 - 09:10
	Accelerated Graph Neural Network Inference — *Javier Mauricio Duarte* — Princeton University	09:10 - 09:50
10:00	**A differentiable graph pooling method based on spatial clustering algorithms"** — *Ryan Liu* — Princeton University	09:50 - 10:10
	BESIII track finding algorithm based on edge-classifying GNN — *Xiaoqian Jia* — Princeton University	10:10 - 10:30
	Coffee — Princeton University	10:30 - 10:50
11:00	**Heterogeneous GNN for tracking** — *Daniel Thomas Murnane* — Princeton University	10:50 - 11:10

Selected Recent Papers

Abdelrahman Elabd, et al. "**Graph Neural Networks for Charged Particle Tracking on FPGAs**". *Frontiers in Big Data* 5. (2022). **Citations: 15**

Abstract:
The determination of charged particle trajectories in collisions at the CERN Large Hadron Collider (LHC) is an important but challenging problem, especially in the high interaction density conditions expected during the future high-luminosity phase of the LHC (HL-LHC). Graph neural networks (GNNs) are a type of geometric deep learning algorithm that has successfully been applied to this task by embedding tracker data as a graph -- nodes represent hits, while edges represent possible track segments -- and classifying the edges as true or fake track segments. However, their study in hardware- or software-based trigger applications has been limited due to their large computational cost. In this paper, we introduce an automated translation workflow, integrated into a broader tool called `hls4ml`, for converting GNNs into firmware for field-programmable gate arrays (FPGAs). We use this translation tool to implement GNNs for charged particle tracking, trained using the TrackML challenge dataset, on FPGAs with designs targeting different graph sizes, task complexites, and latency/throughput requirements. This work could enable the inclusion of charged particle tracking GNNs at the trigger level for HL-LHC experiments.

DeZoort, *et al.* "**Charged Particle Tracking via Edge-Classifying Interaction Networks.**" *Computer Software Big Science* **5**, 26 (2021). https://doi.org/10.1007/s41781-021-00073-z **Citations: 6**

Abstract:
Recent work has demonstrated that geometric deep learning methods such as graph neural networks (GNNs) are well suited to address a variety of reconstruction problems in high-energy particle physics. In particular, particle tracking data are naturally represented as a graph by identifying silicon tracker hits as nodes and particle trajectories as edges, given a set of hypothesized edges, edge-classifying GNNs identify those corresponding to real particle trajectories. In this work, we adapt the physics-motivated interaction network (IN) GNN toward the problem of particle tracking in pileup conditions similar to those expected at the high-luminosity Large Hadron Collider. Assuming idealized hit filtering at various particle momenta thresholds, we demonstrate the IN's excellent edge-classification accuracy and tracking efficiency through a suite of measurements at each stage of GNN-based tracking: graph construction, edge classification, and track building. The proposed IN architecture is substantially smaller than previously studied GNN tracking architectures; this is particularly promising as a reduction in size is critical for enabling GNN-based tracking in constrained computing environments. Furthermore, the IN may be represented as either a set of explicit matrix operations or a message passing GNN. Efforts are underway to accelerate each representation via heterogeneous computing resources towards both high-level and low-latency triggering applications.

Heintz, A., et al. (2020). **Accelerated charged particle tracking with graph neural networks on FPGAs**, in *3rd Machine Learning and the Physical Sciences Workshop at the 34th Conference on Neural Information Processing Systems* (Vancouver, BC). https://arxiv.org/abs/2012.01563 **Citations: 15**

Abstract:
We develop and study FPGA implementations of algorithms for charged particle tracking based on graph neural networks. The two complementary FPGA designs are based on OpenCL, a framework for writing programs that execute across heterogeneous platforms, and hls4ml, a high-level-synthesis-based compiler for neural network to firmware conversion. We evaluate and compare the resource usage, latency, and tracking performance of our implementations based on a benchmark dataset. We find a considerable speedup over CPU-based execution is possible, potentially enabling such algorithms to be used effectively in future computing workflows and the FPGA-based Level-1 trigger at the CERN Large Hadron Collider.

IRIS-HEP Fellow

Conference Papers

Savannah Thais, Gage deZoort **"Instance Segmentation GNNs for One-Shot Conformal Tracking at the LHC"**. *https://arxiv.org/abs/2103.06509*.
Citations: 2
Presented at NeurIPS Machine Learning and the Physical Sciences Workshop 2020

Abstract:
3D instance segmentation remains a challenging problem in computer vision. Particle tracking at colliders like the LHC can be conceptualized as an instance segmentation task: beginning from a point cloud of hits in a particle detector, an algorithm must identify which hits belong to individual particle trajectories and extract track properties. Graph Neural Networks (GNNs) have shown promising performance on standard instance segmentation tasks. In this work we demonstrate the applicability of instance segmentation GNN architectures to particle tracking; moreover, we re-imagine the traditional Cartesian space approach to track-finding and instead work in a conformal geometry that allows the GNN to identify tracks and extract parameters in a single shot.

Rajat Sahay, Savannah Thais **"Graph Segmentation in Scientific Datasets"**. *https://arxiv.org/abs/2103.06509*.
Presented at NeurIPS Machine Learning and the Physical Sciences Workshop 2021

Abstract:
Deep learning tools are being used extensively in a range of scientific domains; in particular, there has been a steady increase in the number of geometric deep learning solutions proposed to a variety of problems involving structured or relational scientific data. In this work, we report on the performance of graph segmentation methods for two scientific datasets from different fields. Based on observations, we were able to characterize the individual impact each type of graph segmentation methods has on the dataset and how they can be used as a precursors to deep learning pipelines.

Other Materials

Hackathons:

CMS Summer 2022

- In collaboration with the Tracking POG

Presentations:

- 8 Apr 2022 - "Representation Workshop Summary", Savannah Thais, Learning to Discover
- 22 Mar 2022 - "GNNs for Charged Particle Reconstruction at the Large Hadron Collider", Savannah Thais, US CMS HL-LHC R&D Meeting (CMS Internal)
- 8 Mar 2022 - "GNNs for Charged Particle Reconstruction at the Large Hadron Collider", Savannah Thais, Imperial College Data Learning Working Group
- 8 Mar 2022 - "Intro to GNN Approach", Markus Atkinson, EF Tracking weekly
- 22 Oct 2021 - "GNN Tracking Update", Markus Atkinson, HLS4ML Co-Processor Meeting
- 7 Sep 2021 - "Machine Learning for Tracking", Savannah Thais, HL-LHC R&D Initiative Meeting (USCMS internal)
- 26 Aug 2021 - "Machine Learning (CMS)", Savannah Thais, 10th International Conference on New Frontiers in Physics (ICNFP 2021)
- 30 Jul 2021 - "Generative Adversarial Network (GAN)", Savannah Thais, Machine Learning HATS@LPC
- 14 Jul 2021 - "AI in HEP: Current Methods and Applications", Savannah Thais, 2021 Meeting of the Division of Particles and Fields (DPF21)
- 12 Jul 2021 - "Graph Neural Networks", Savannah Thais, Machine Learning HATS@LPC
- 27 May 2021 - "Tracking with Graph Neural Networks", Markus Atkinson, ATLAS Machine Learning Forum
- 9 Apr 2021 - "GNNs for Charged Particle Reconstruction at the Large Hadron Collider", Savannah Thais, MLSys Workshop of Graph Neural Networks and Systems
- 2 Nov 2020 - "Tracking with GNN", Savannah Thais, CMS Tracking POG meeting (CMS internal)
- 23 Oct 2020 - "Graph Neural Networks Architectures", Markus Atkinson, FastML Co-processors Meeting
- 21 Oct 2020 - "Accelerated Pixel Detector Tracklet Finding with GNNs on FPGAS", Savannah Thais, 4th Annual Inter-Experiment Machine Learning Workshop
- 21 Oct 2020 - "Graph Neural Networks Architectures", Markus Atkinson, IRIS-HEP Topical Meeting
- 30 Sep 2020 - "GNNs for Tracking", Savannah Thais, CMS Machine Learning Forum
- 18 May 2020 - "Graph Neural Network Tracking using the Endcaps", Markus Atkinson, Exa.Trkx Weekly Meeting
- 4 May 2020 - "Pixel Detector Tracklet Finding", Markus Atkinson, Exa.Trkx Weekly Meeting
- 27 Feb 2020 - "New Algorithms and Computing Architectures for Tracking", Savannah Thais, IRIS-HEP 18 Month Review
- 27 Feb 2020 - "GNN Tracking and FPGA Acceleration (poster)", Markus Atkinson, IRIS-HEP Poster Session
- 16 Oct 2019 - "Semantic Segmentation for CMS Pixel Clustering", Savannah Thais, US LHC Users' Association Meeting
- 12 Sep 2019 - "Introduction and Plans", Savannah Thais, IRIS-HEP Institute Retreat
- 12 Sep 2019 - "Introduction and Plans", Markus Atkinson, IRIS-HEP Institute Retreat

Summer Students:

Aneesh Heintz (2020): Implemented IN on FPGA
Sophia Korte (2022): Apply IN + DBSCAN to CMS data (ongoing)
…