

# Tagging Emerging Jets using Graph Neural Networks

The logo for Simon Fraser University (SFU), consisting of the letters "SFU" in white on a red rectangular background.

## MSc Defence

### Candidate

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**16 April 2024**

### Committee

**Dr. Andrei Frolov (Chair)**  
**Dr. Dugan O'Nei (Internal examiner)**  
**Dr. Matthias Danninger (Supervisor, Member)**  
**Dr. Bernd Stelzer (Member)**

# Search for new Physics?

- No strong indications of new physics at the modern collider experiments.
- Indicate two possibilities: either the new physics is **above the energy scale accessible to LHC** - the largest particle collider, or we have been looking at the "wrong places".
- Wrong places?
  - Most BSM physics searches have been performed with the assumption that the particles decay (promptly) near the primary interaction point of collider experiments

# Long Lived Particles (LLPs)

- LLPs: Particles that travel an observable distance from the primary collision point in particle detectors. Will have macroscopic proper lifetimes.
- Long-lived particle signatures : Unexplored phase space for BSM physics search, and requires a dedicated search
- As SM has LLPs (muons) no reason to exclude BSM searches with LLP signatures!

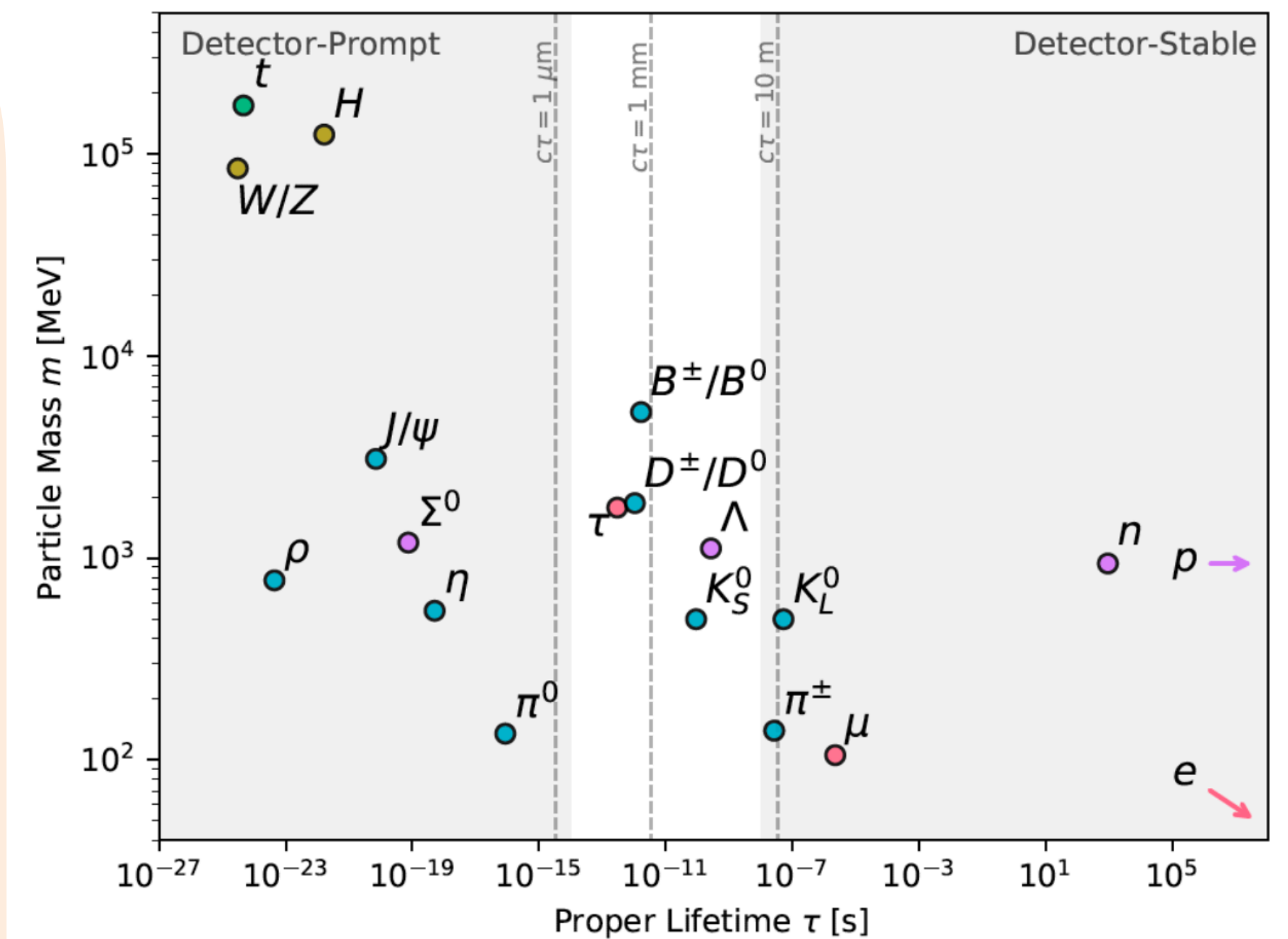
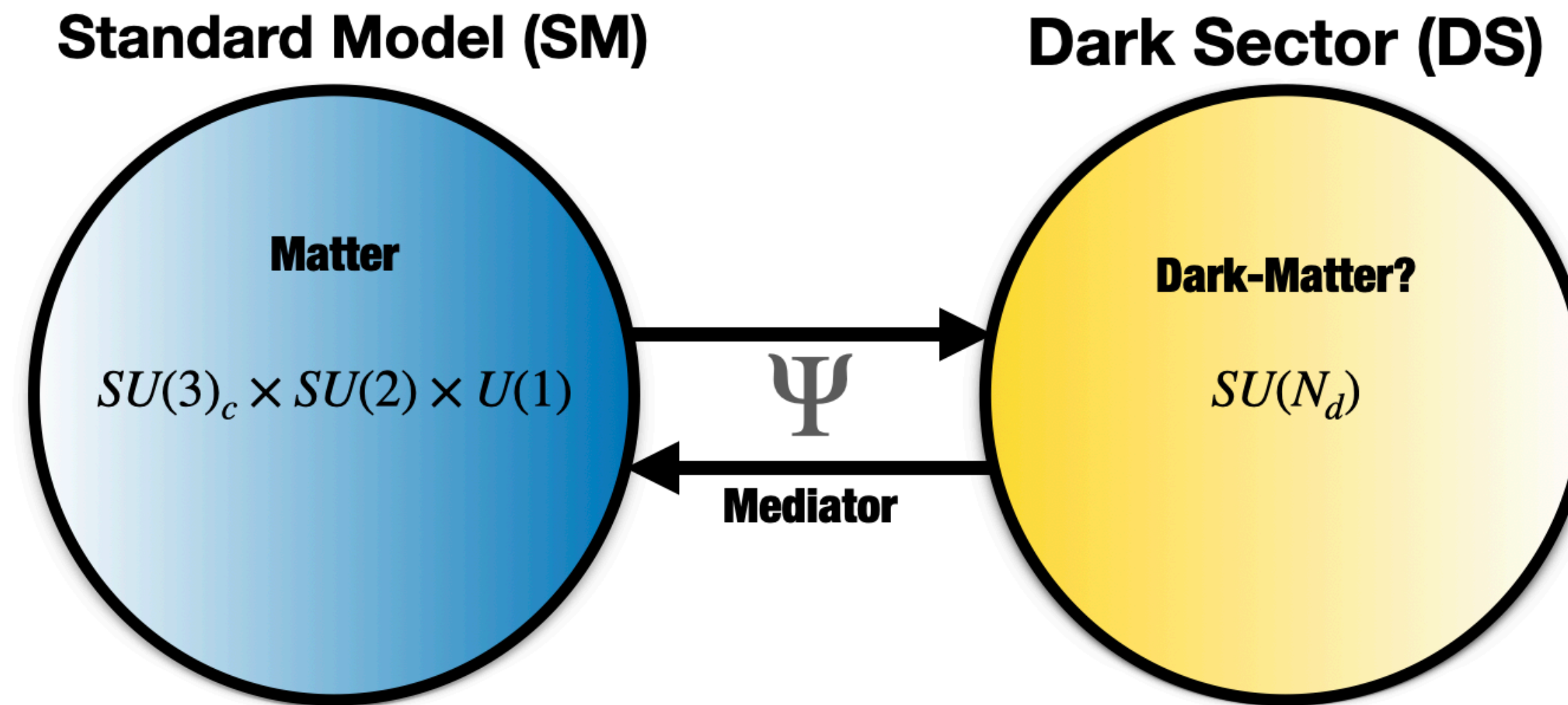


Image from Ref[1]

# Theoretical Motivation for BSM LLPs



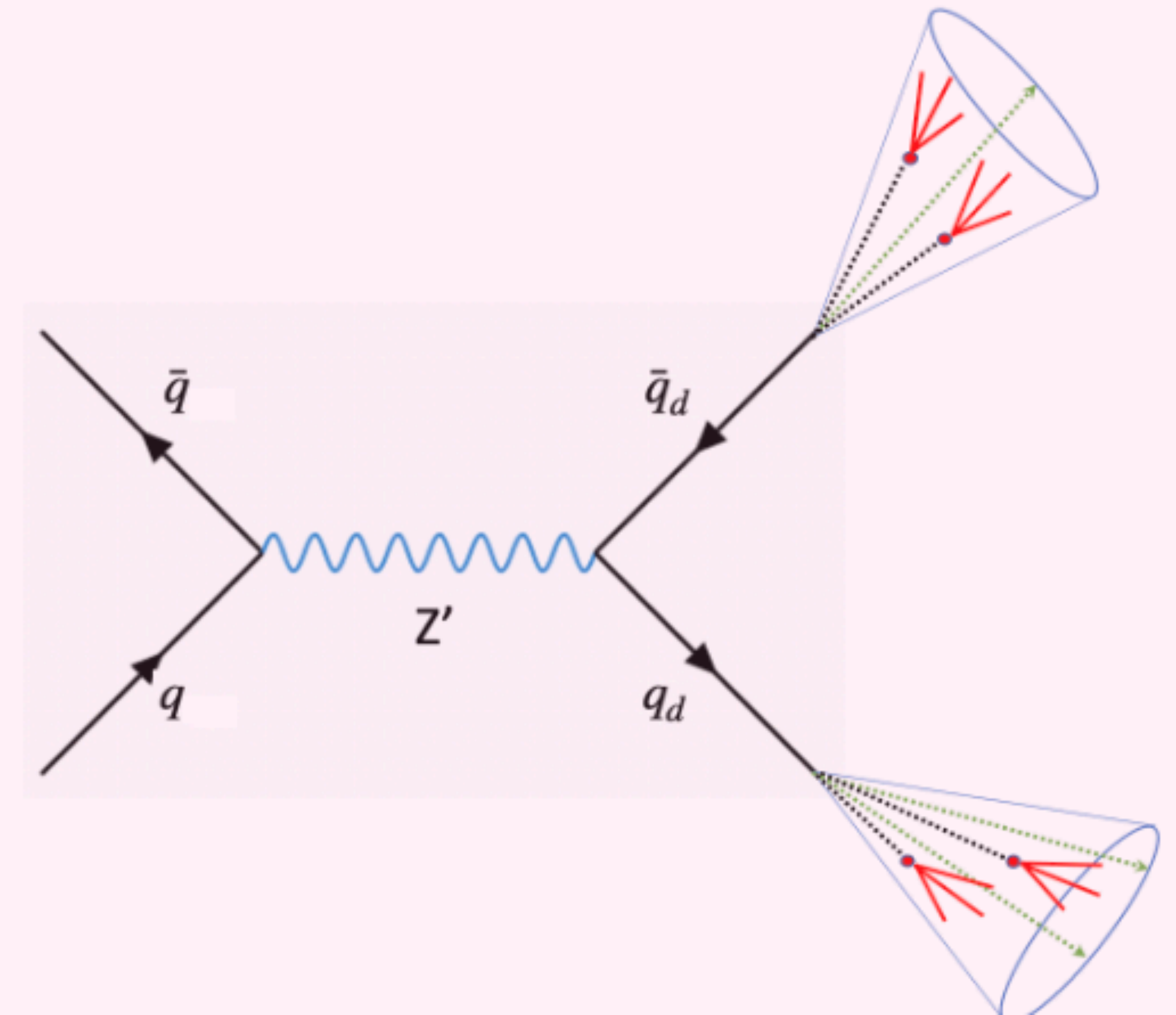
- Extended SM with additional particles and forces collectively referred as dark sector(DS).
- Weak coupling between SM and DS can give rise to LLPs

# Benchmark Model

## BSM physics processes with LLP signature

$$\mathcal{L}_{\text{med}} = -\frac{1}{4} Z'^{\mu\nu} Z'_{\mu\nu} - \frac{1}{2} M_{Z'}^2 Z'^{\mu} Z'_{\mu} + Z'_{\mu} (\bar{q}'_i \gamma^{\mu} q'_i + \bar{q}_j \gamma^{\mu} q_j)$$

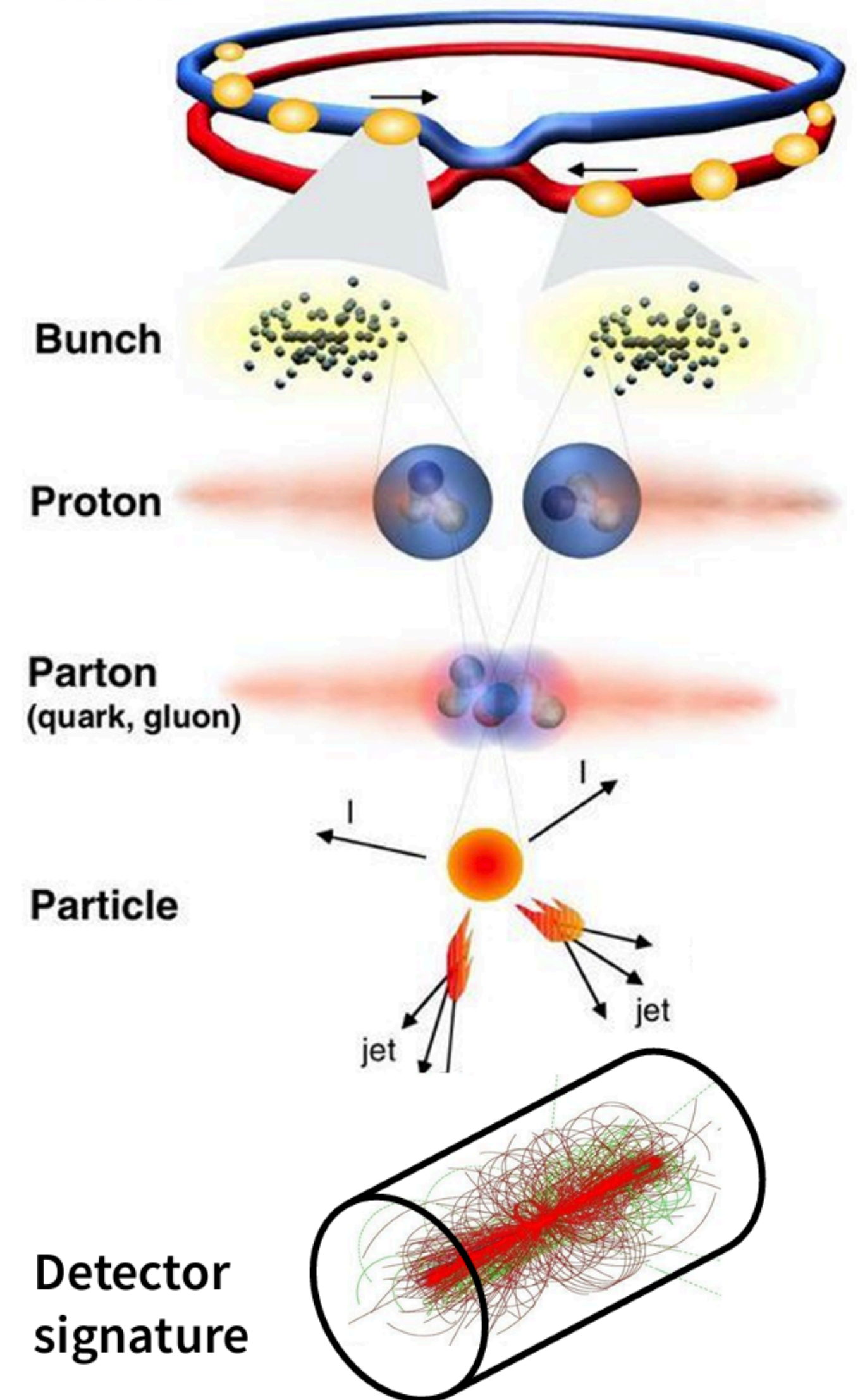
- Production of dark quarks via  $Z'$  (vector) mediator.
- Dark mesons travel sizeable distances (5mm-50mm) before decaying back to SM
- Leads to exotic LLP signature known as Emerging Jets (EJs) with with unique signature  $\rightarrow$  smoking gun for BSM physics.



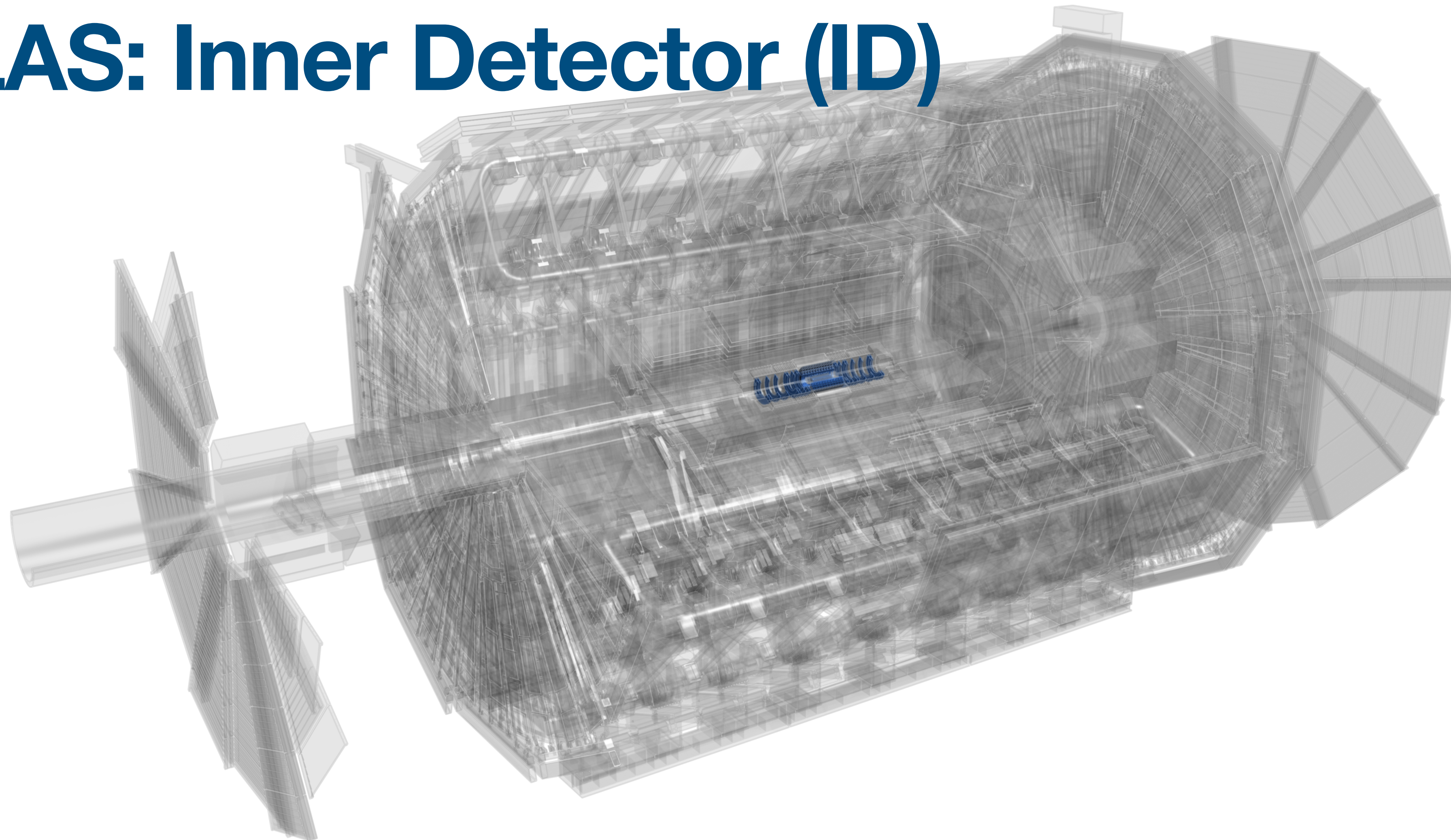
# ATLAS Detector

## Intro

- Bunches of protons are accelerated almost at the speed of light and collided at LHC, such as there are 40,000,000 interactions per second.
- A general purpose detector at LHC, ATLAS “detects” collision remnants.

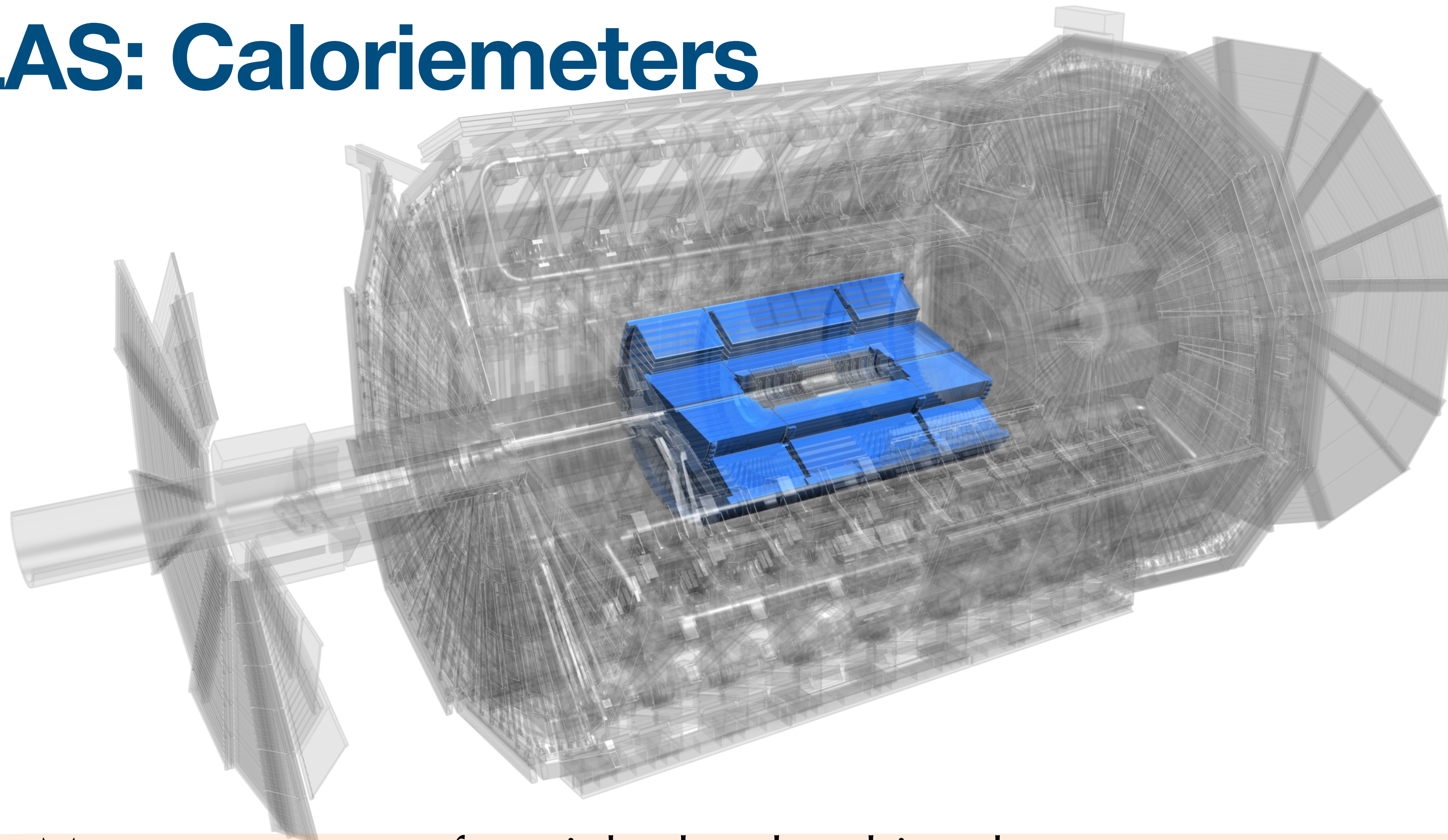


# ATLAS: Inner Detector (ID)



- Measures direction, momentum and charge of charged particles.
- Is made up of Pixel Detector, Semiconductor Tracker (SCT) and Transition Radiation Tracker (TRT)

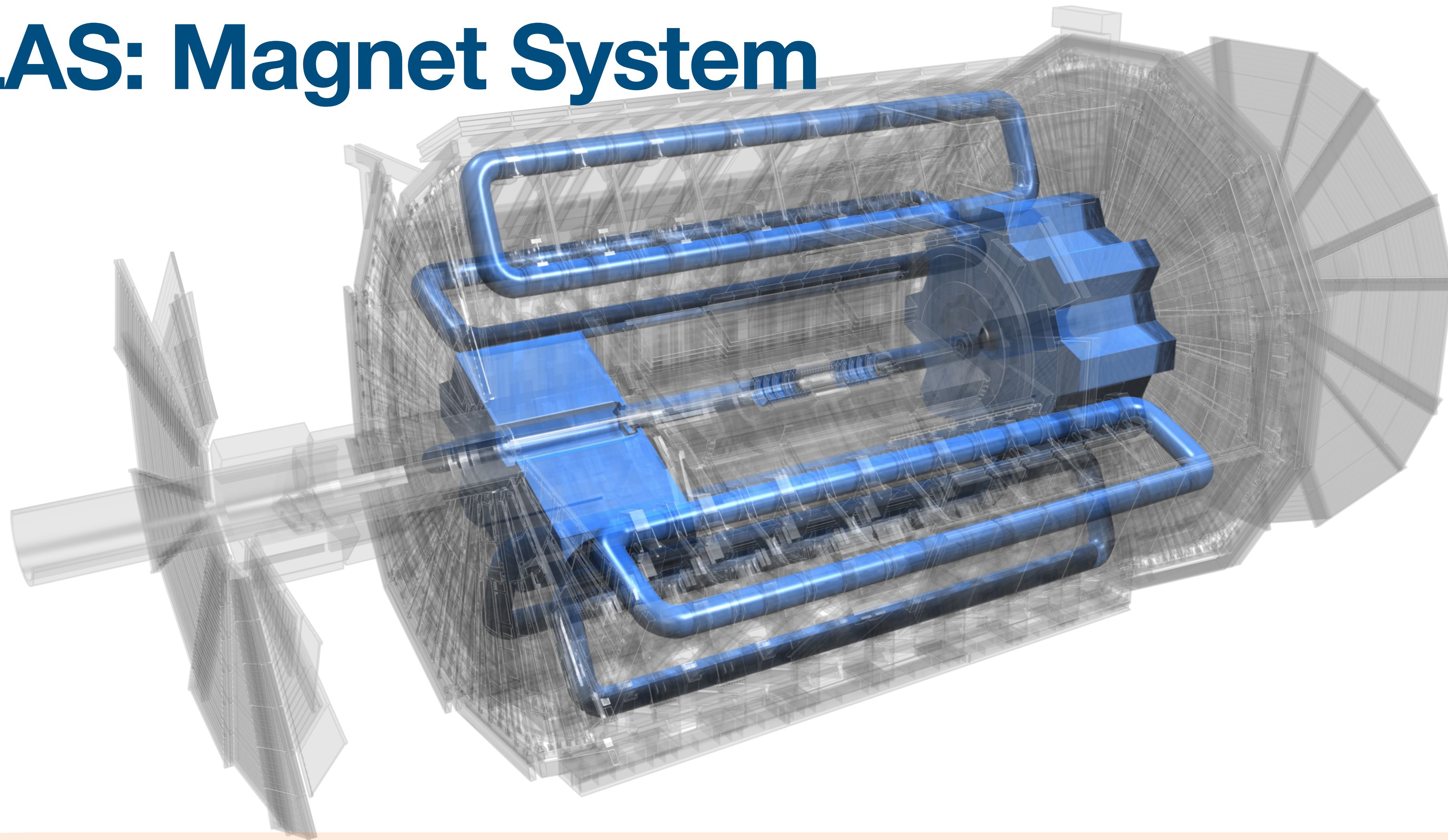
# ATLAS: Calorimeters



- Measures energy of particles by absorbing them.
- Is made up of Electronic Calorimeters (ECAL) and Hadronic Calorimeters (HCAL)

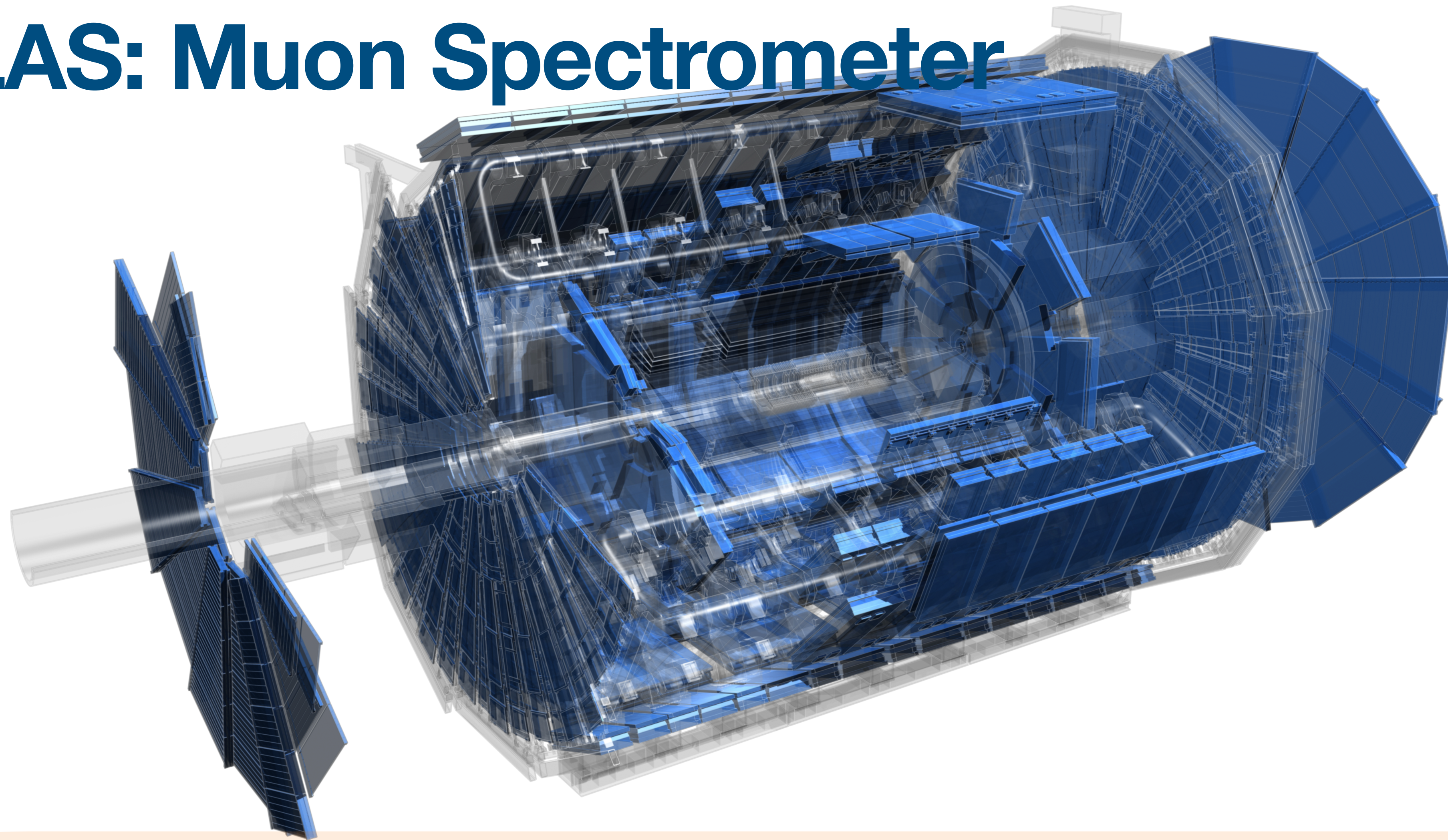


# ATLAS: Magnet System



- Magnet system bends the trajectory of charged particles to measure momentum and charge.

# ATLAS: Muon Spectrometer



- Measures momentum of muons as they escape the calorimeter without being absorbed.

# Particle Signatures in ATLAS

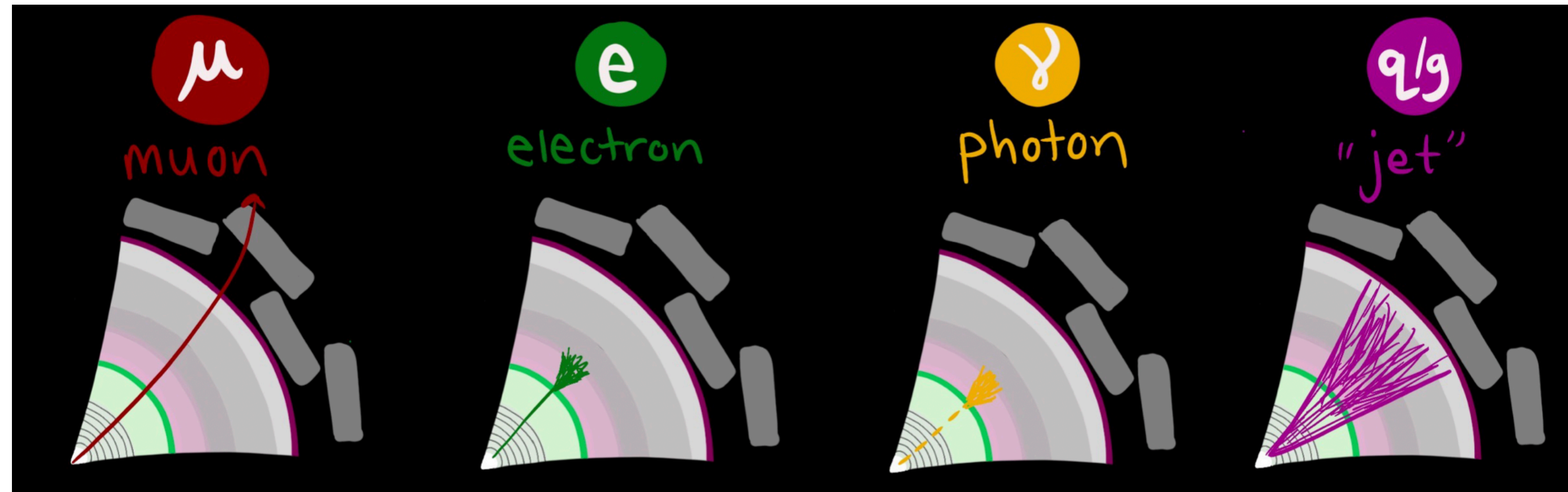


Image: Heather Russel

- Particle identification involves reconstructing the trajectory of charged particles in the ID, reconstruction of the jets from the calorimeters .. and so on.
- **Tracks** are the paths traced by charged particles as they move through the ATLAS detector.
- **Jets** are collimated sprays of particles produced when quarks and gluons (partons), ejected from the proton-proton collisions, undergo hadronization.

# Tracking: Charged particle trajectory reconstruction

- Form seeds using three hit groups (space points)

- Extend the seeds with additional space points using recursive algorithm

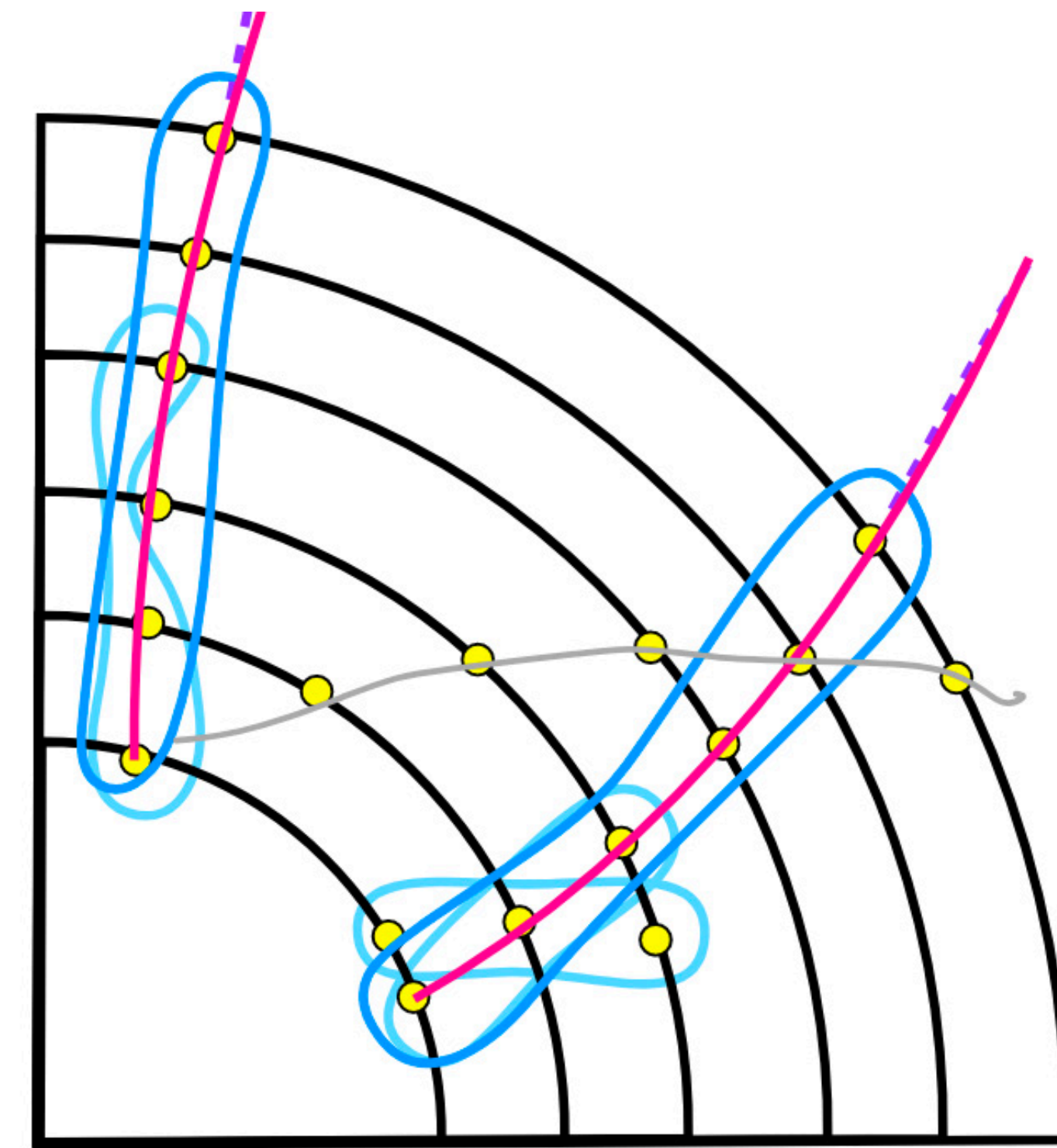
- Fit and score the track candidates using  $\chi^2$  and other metrics. Discard bad track candidates based on the score.

- Extrapolate the track candidates to TRT

- Refit with all points and score the track candidate. Also discard candidate with bad score

- Form TRT track segments are that extended back to the silicon layers

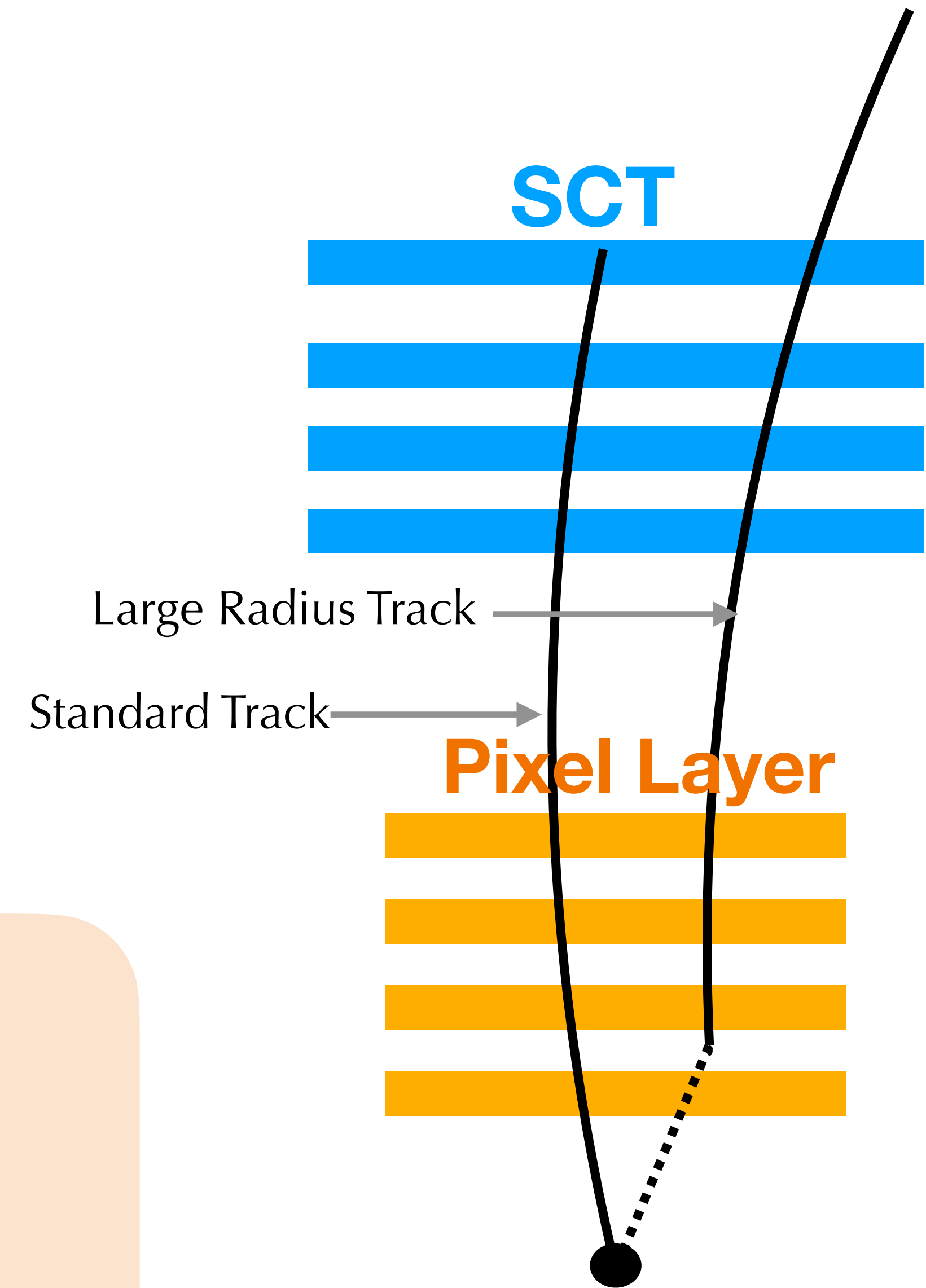
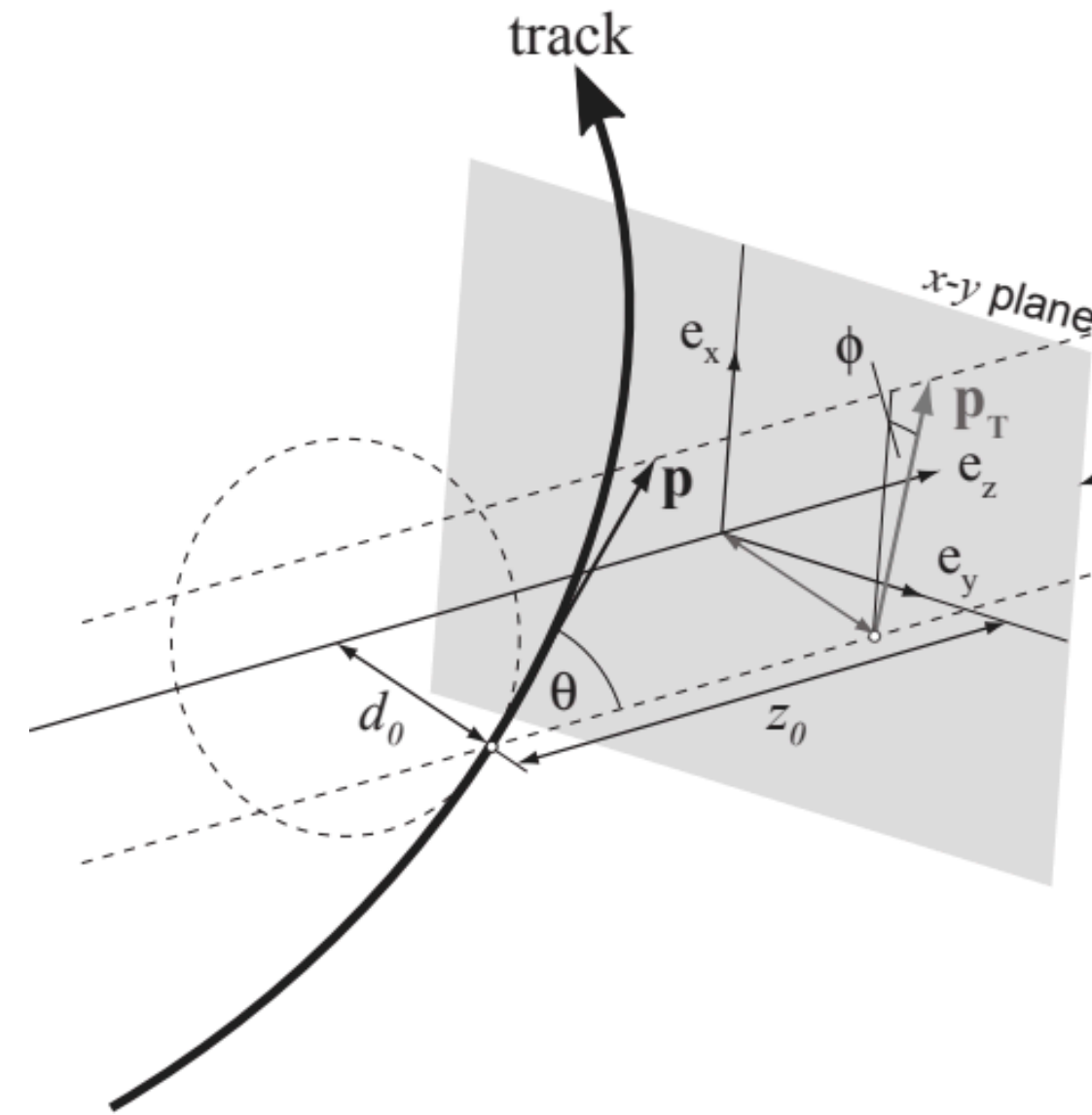
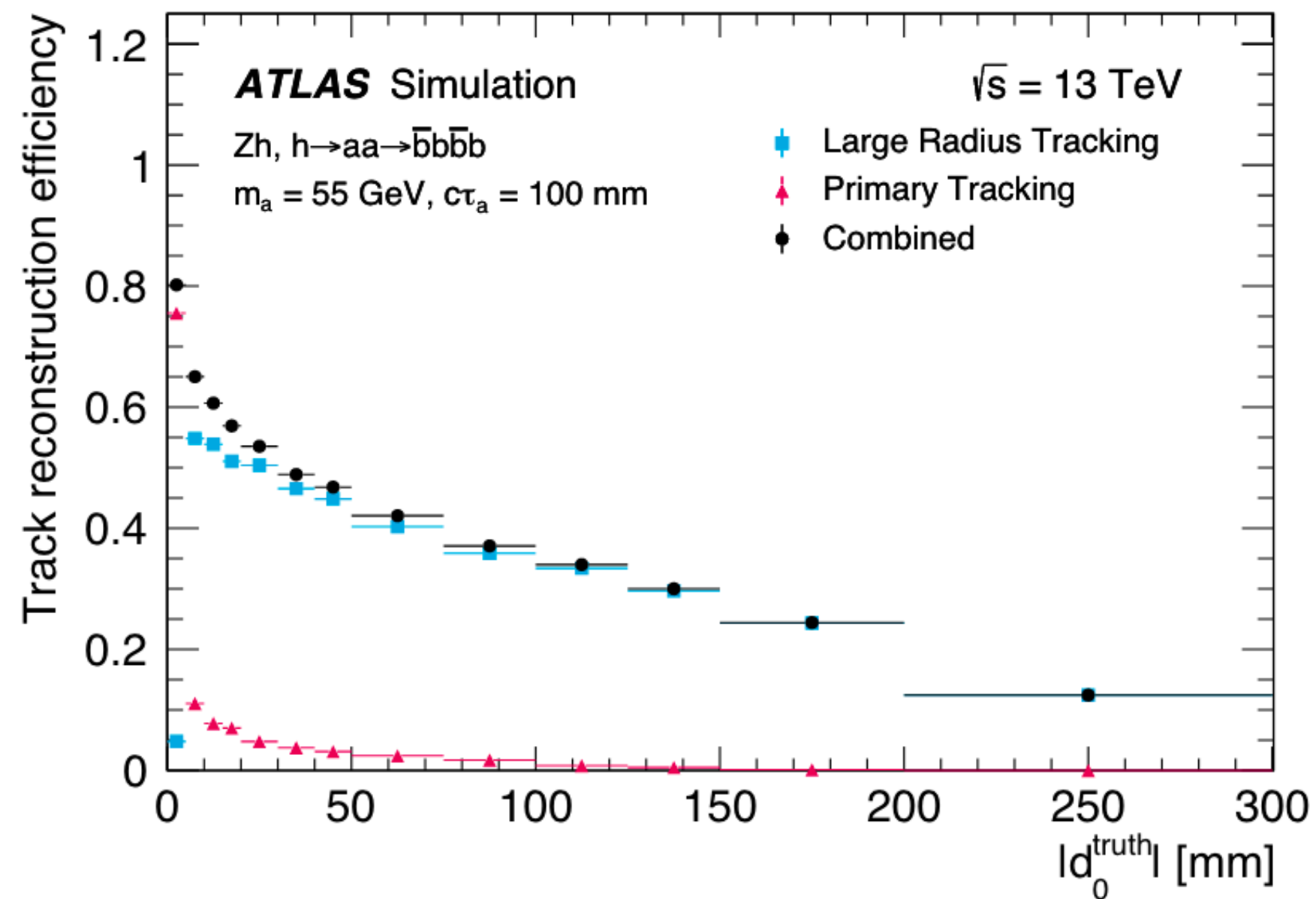
Pierfrancesco Butti



→ Inside-Out tracking

→ Outside-In tracking

# Large Radius Tracking (LRT)



- Tracks inside EJs are from LLP particle decay. Standard tracking (ST) cannot reconstruct those tracks efficiently.
- LRT run after ST and manages to retain substantial efficiency unto transverse impact parameter  $< 300 \text{ mm}$

# Jets Reconstruction

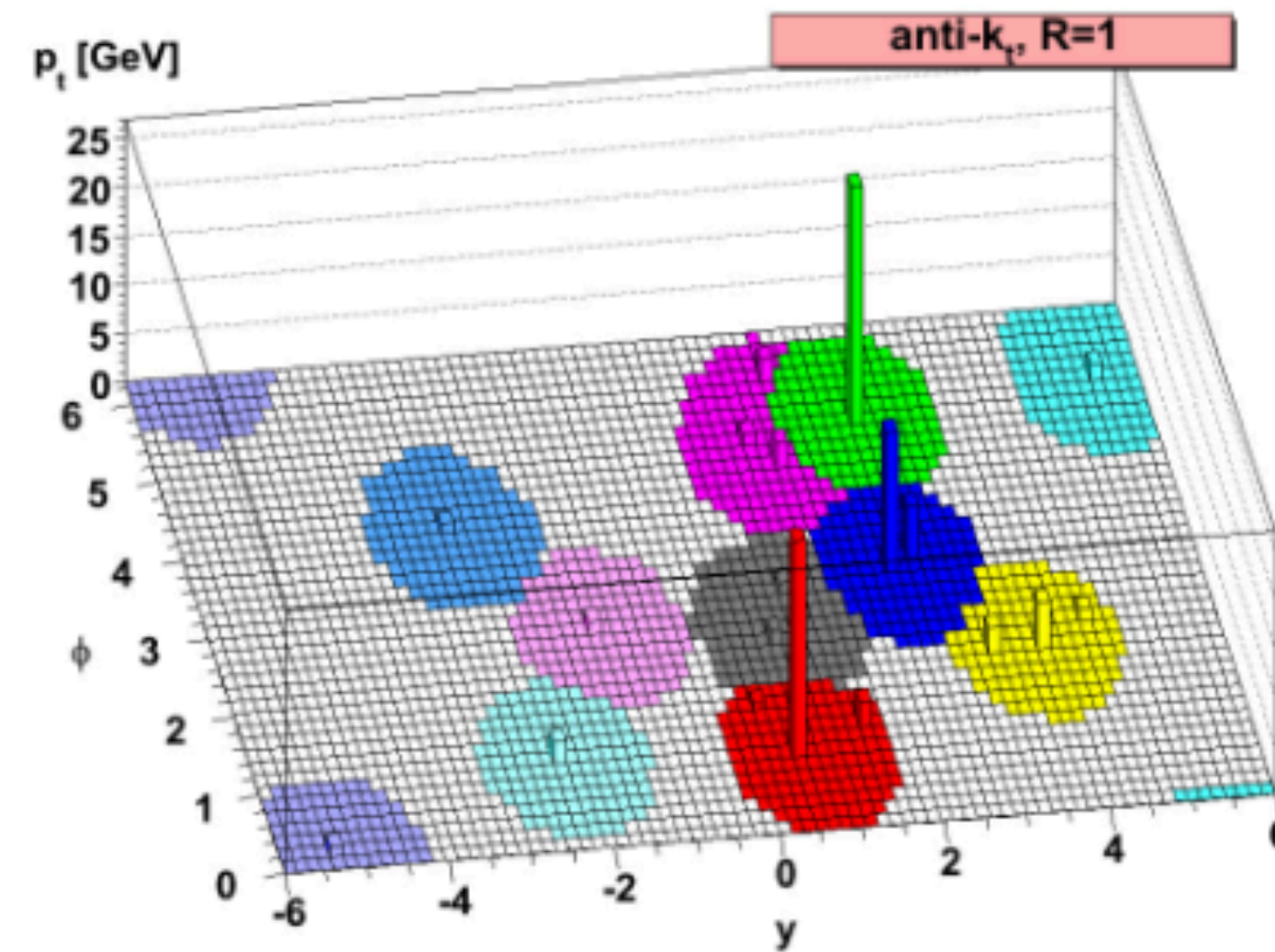
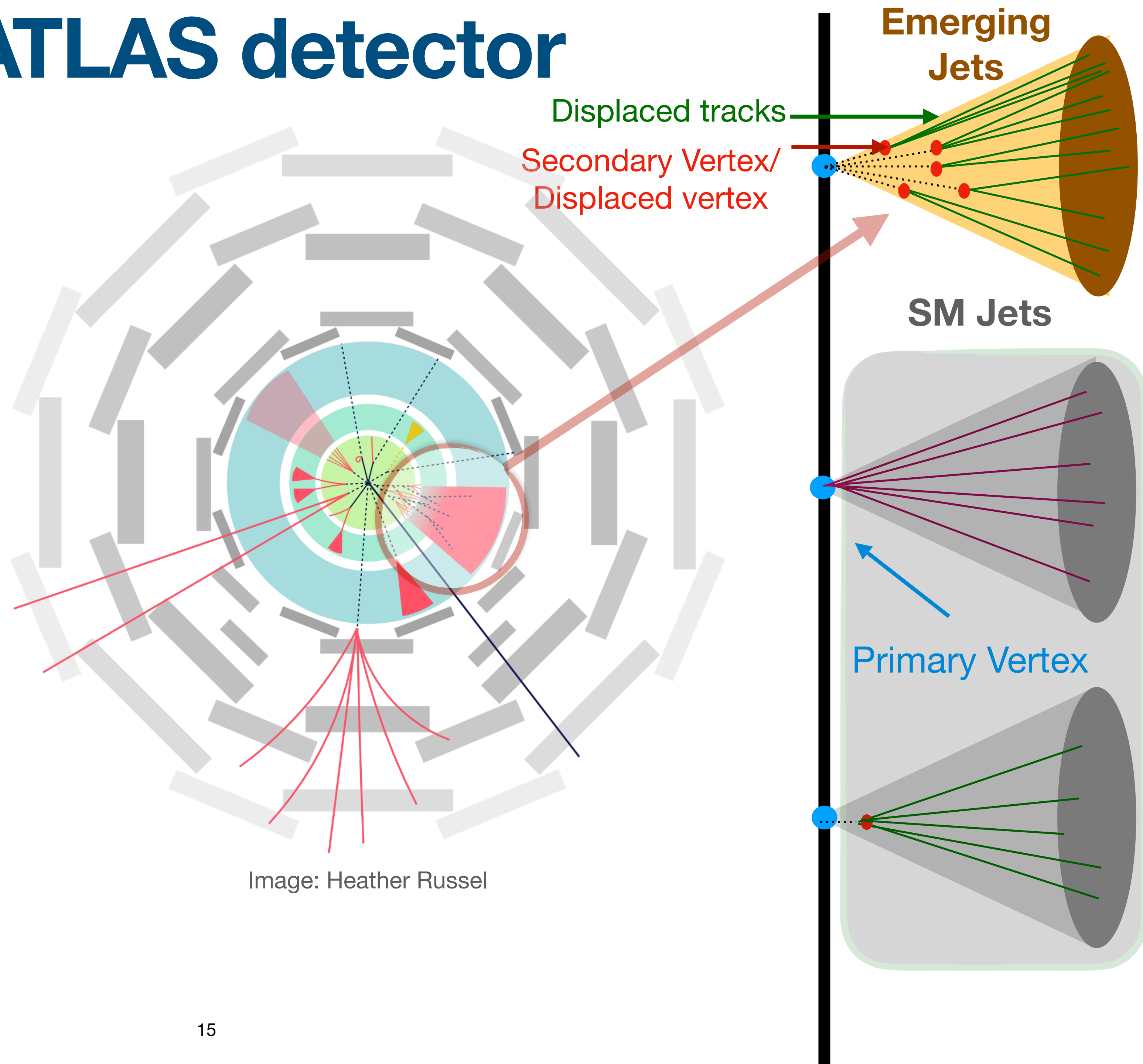


Figure A sample parton-level event clustered with the anti-kt algorithm used to reconstruct jets with  $R=1$ .

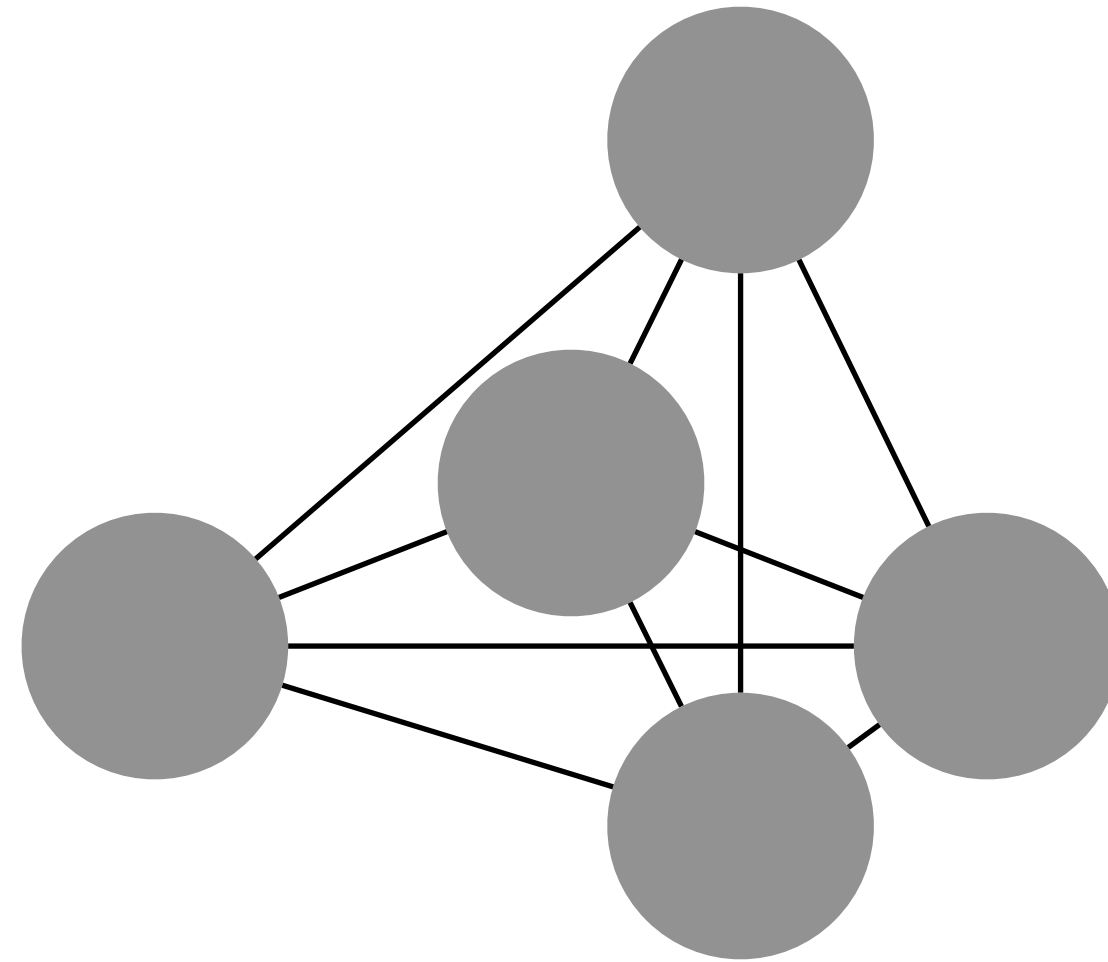
- First, calorimeter cells are grouped into three-dimensional clusters (topo-clusters) using the nearest-neighbour algorithm.
- Then clusters are merged based sequential recombination algorithm (anti-kt), meaning it builds jets by iteratively merging particles based on a specific distance metric.

# Emerging Jets in ATLAS detector

- EJ's are BSM LLP signature!
- **EJs are jets with many displaced tracks and displaced vertices.**
- Difficult to identify!
  - Calorimeter signature looks similar to a QCD jet
  - Need to use the displaced tracks and vertices to identify the EJ using conventional methods



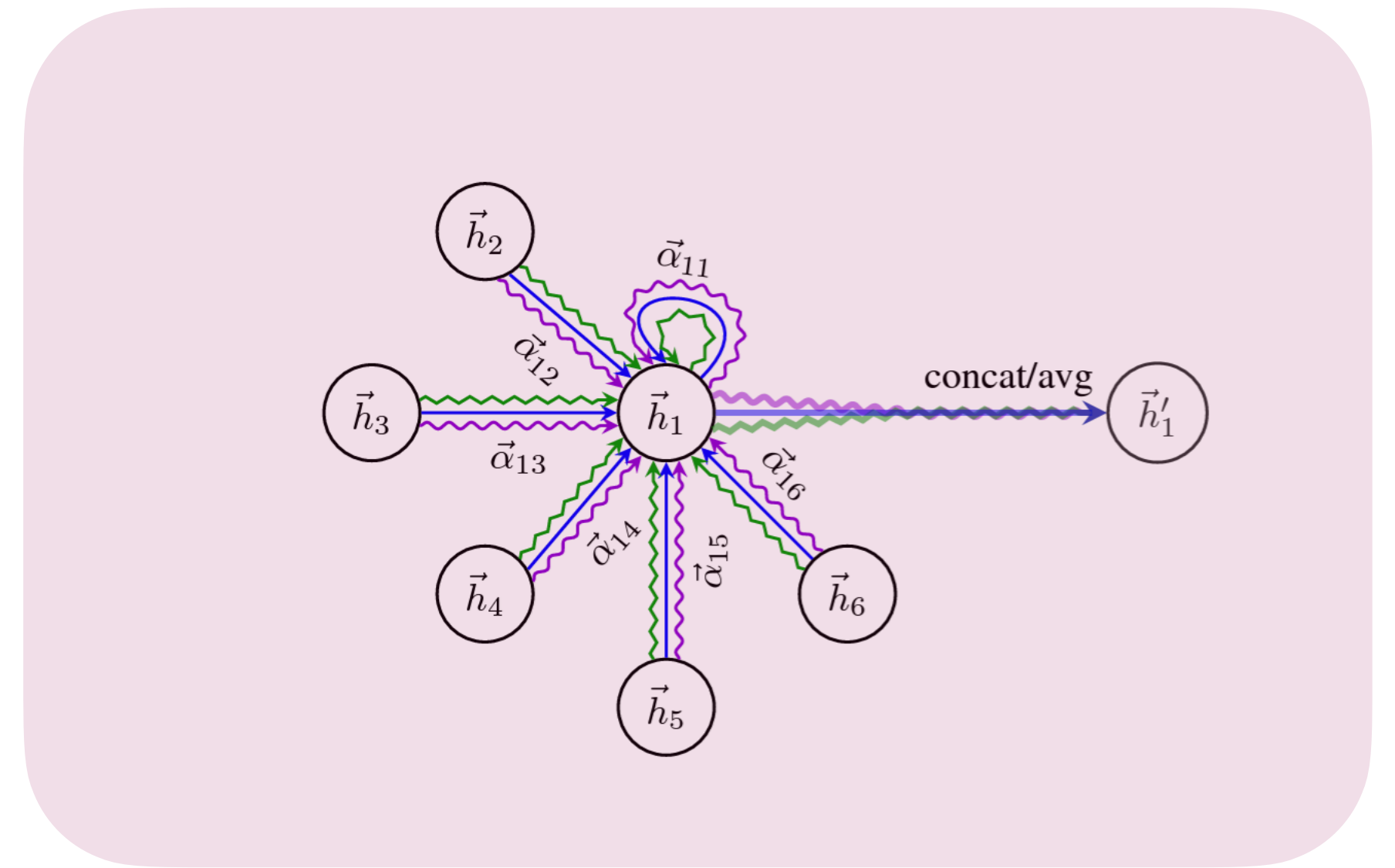
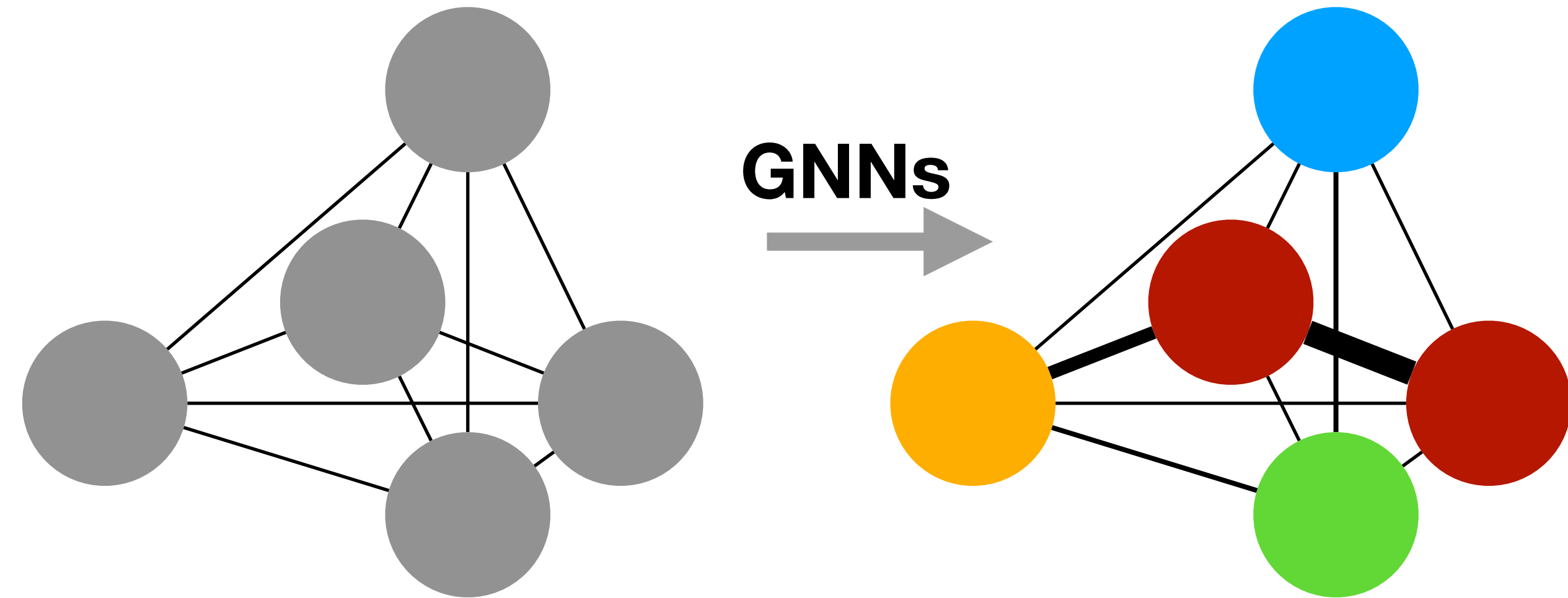
# Graphs



- A graph,  $\mathcal{G} = (\mathcal{V}, \mathcal{E})$  is COLLECTION of nodes  $\mathcal{V} = \{v_1, v_2, \dots, v_n\}$  and edges  $\mathcal{E} \subseteq \mathcal{V} \times \mathcal{V}$ .
- Nodes are often used to represent multi-dimensional feature-vectors. Feature vectors are numerical representations of data entities and denoted as  $\mathbf{x}_u$  for  $u \in \mathcal{V}$



# GNNS



Transformation of node feature vector  $\vec{h}_1$  into  $\vec{h}'_1$  by using neighbourhood feature vectors .

- Optimizable transformation on graph attributes such as nodes and edges.
- For example, transformation's of node representation  $\vec{h}_1$  to  $\vec{h}'_1$  through a weighted aggregation of its neighbour's representation, where the weights are derived from attention mechanism,  $a(\mathbf{x}_u, \mathbf{x}_v)$ .
  - $\mathbf{h}_u = \phi \left( \mathbf{x}_u, \square_{v \in \mathcal{N}_u} a(\mathbf{x}_u, \mathbf{x}_v) \psi(\mathbf{x}_v) \right)$ , where  $\psi(\mathbf{x}_v) = \mathbf{W} \mathbf{x}_v$

# GNNs for Emerging Jets Analysis (Run 03)

- GNNs can handle large sized inputs because of permutation symmetry.

- EJs have large number of tracks inside them

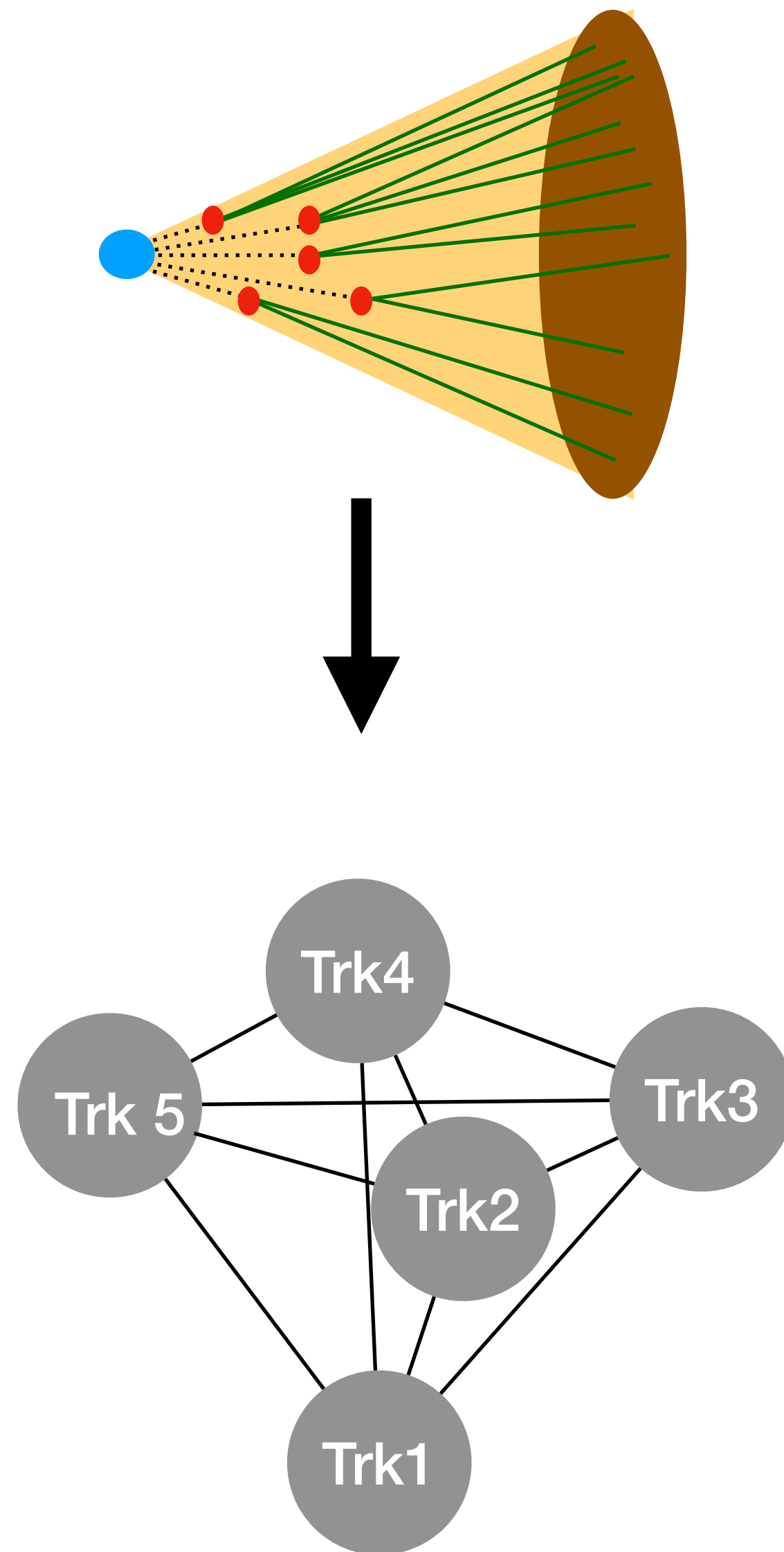
- As EJs are difficult to identify using conventional methods, GNNs facilitate the use of several low level track input variables.

- GNNs handle irregular sized inputs

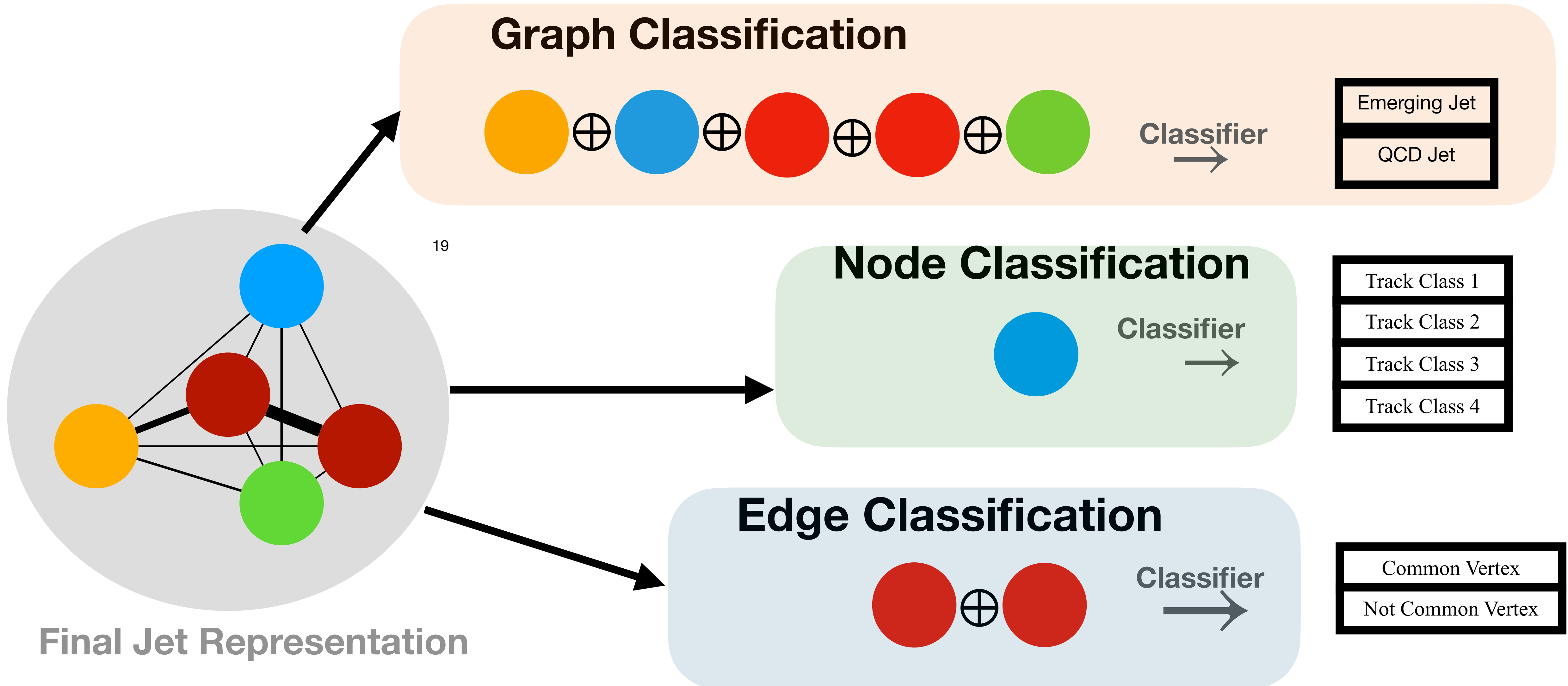
- Number of tracks in EJ is not fixed, therefore well suited

- GNNs exploit relationship between data entity

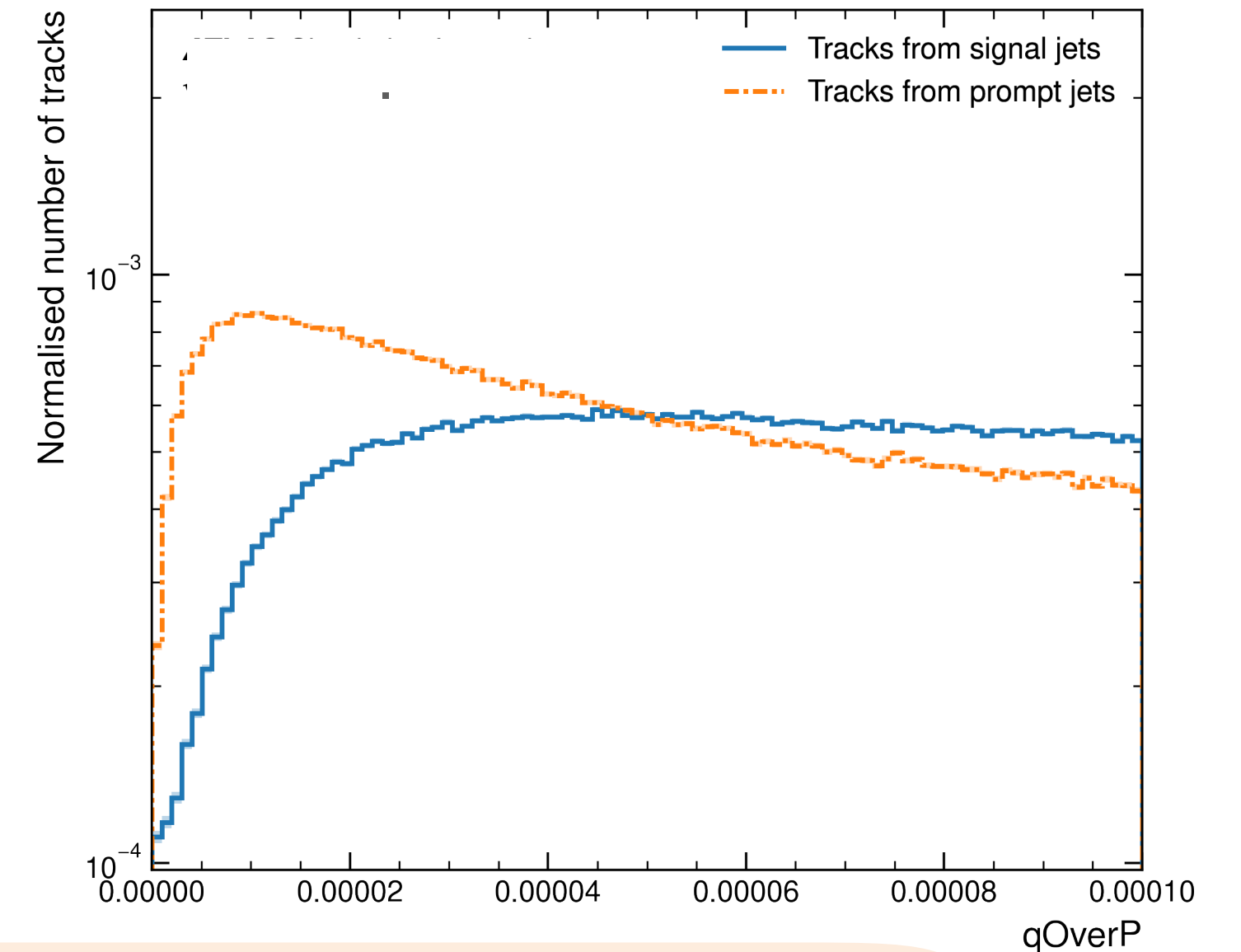
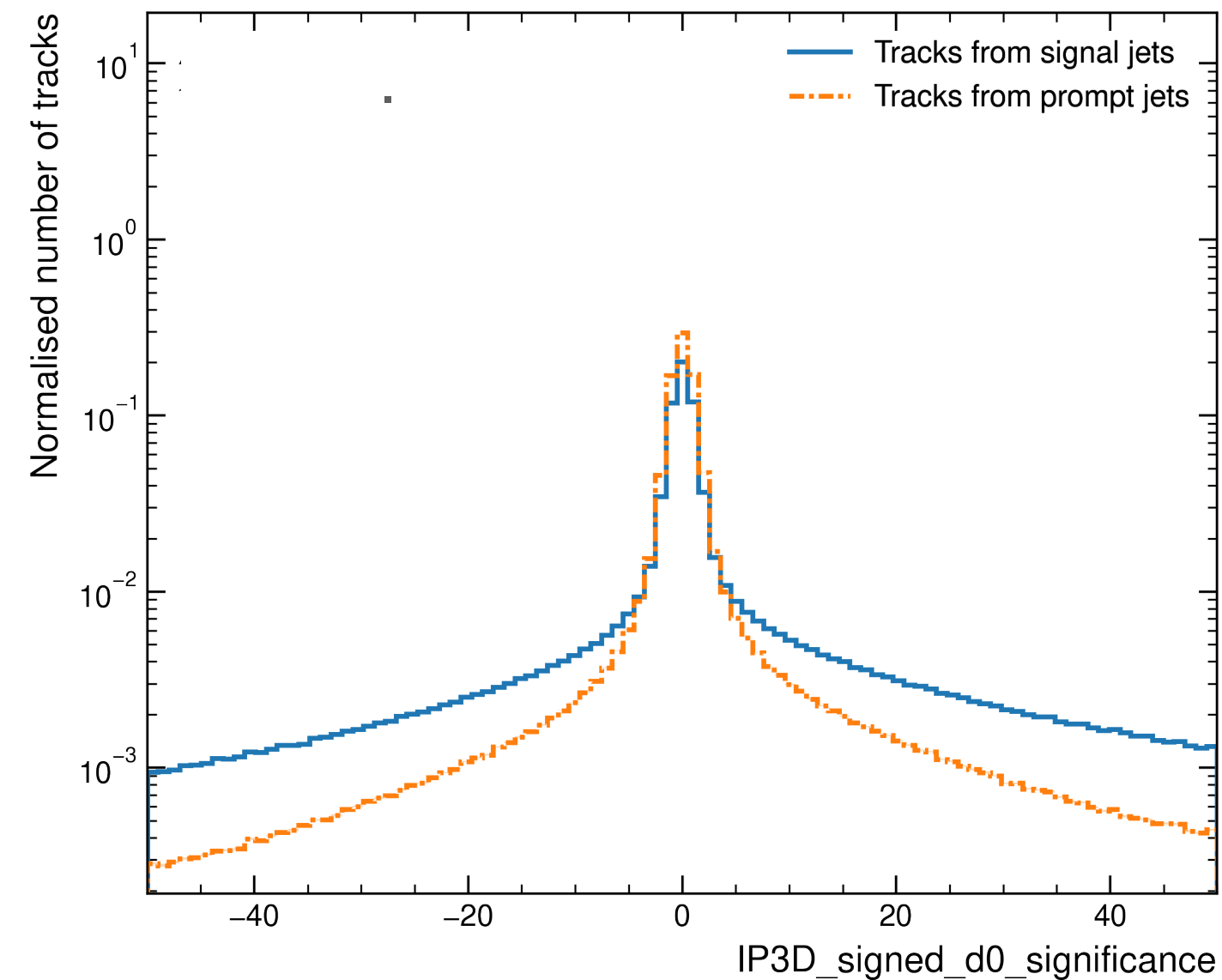
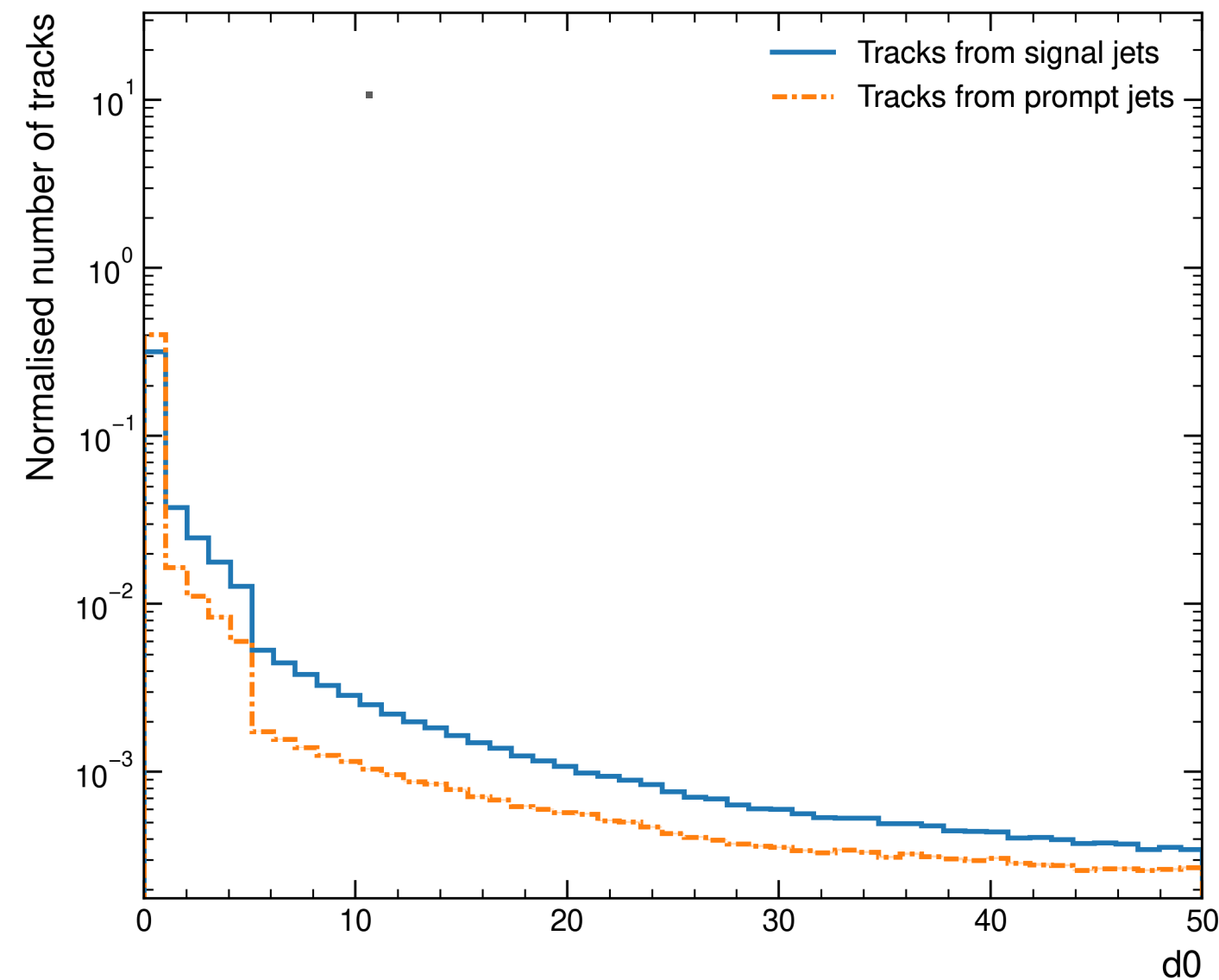
- Tracks in EJ exhibit rich relations due to the presence of multiple displaced vertex and displaced tracks



# Classification tasks



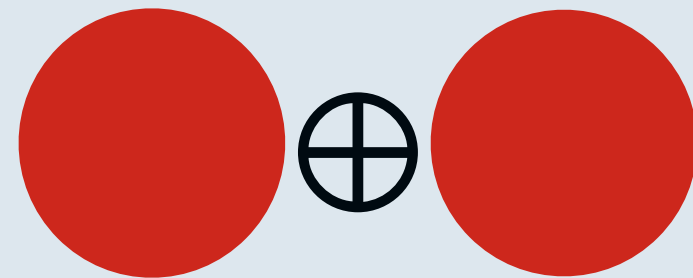
# Input Variables



- 16 track variables including track parameters in ATLAS tracking system, detector hits and holes variables, uncertainty in track parameters ... (detailed in backup slides)
- Most discriminating ones include
  - -  $d_0$ : Distances of closest approach between the track
  - - IP3D\_signed\_d0\_significance: Ratio of  $d_0$  and  $\sigma(d_0)$  defined for both positive and negative scale with reference to the primary interaction point of the ATLAS detector
  - -  $\frac{q}{p}$  Track charge divided by momentum (measure of curvature)

# Results from Performance of GNNS in Vertex Classification

## Edge Classification

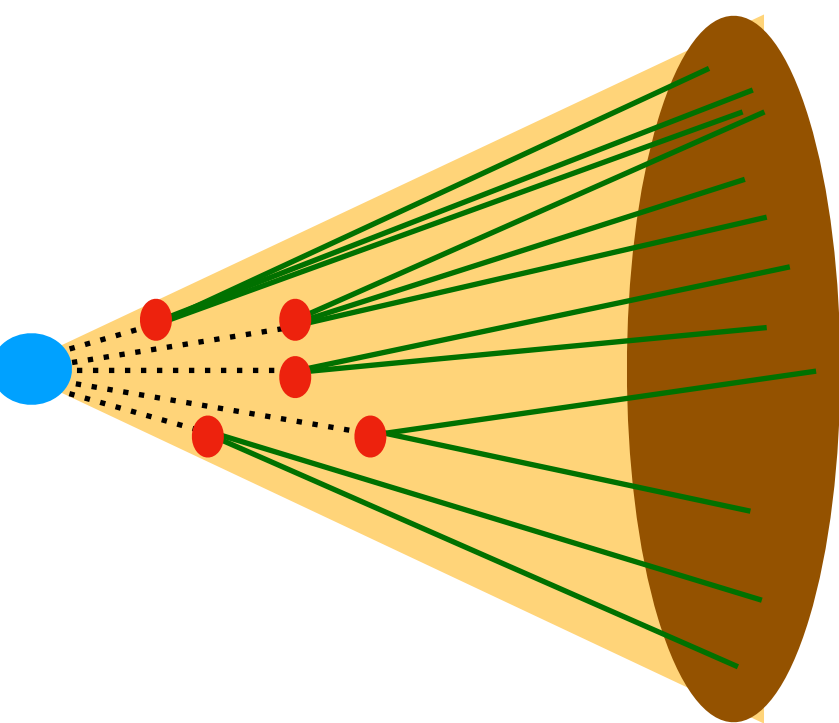


Classifier  
→

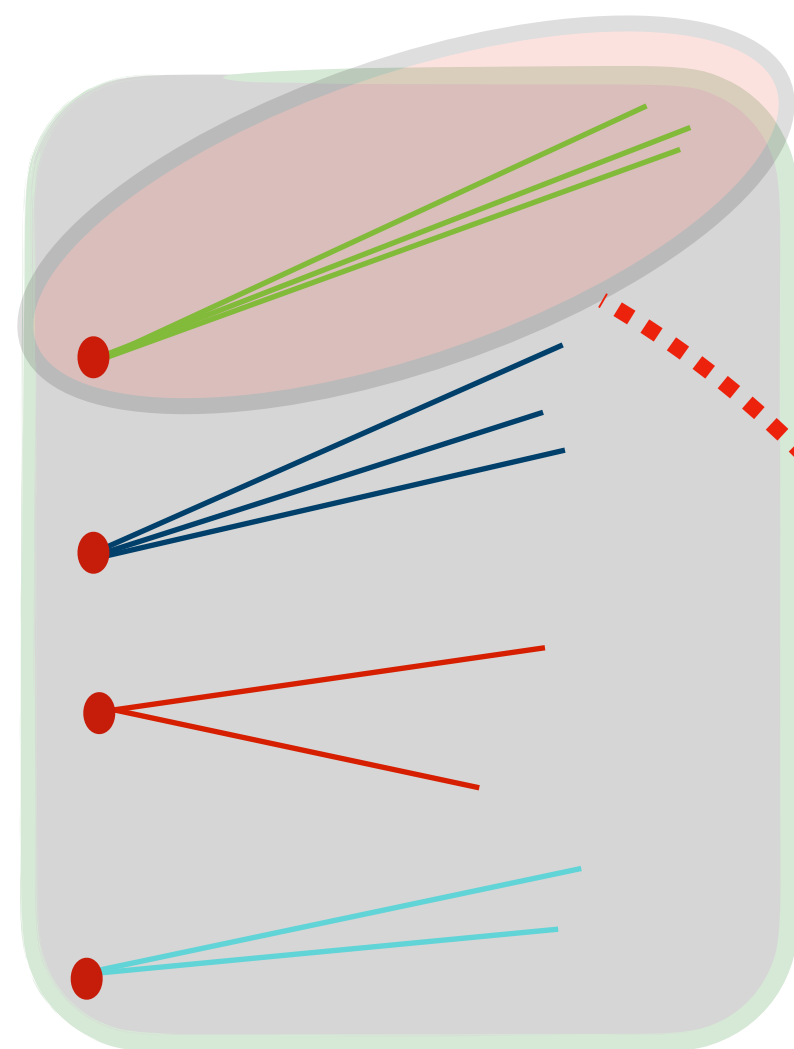
Probability of having common vertex

# Vertex Performance: Efficiency

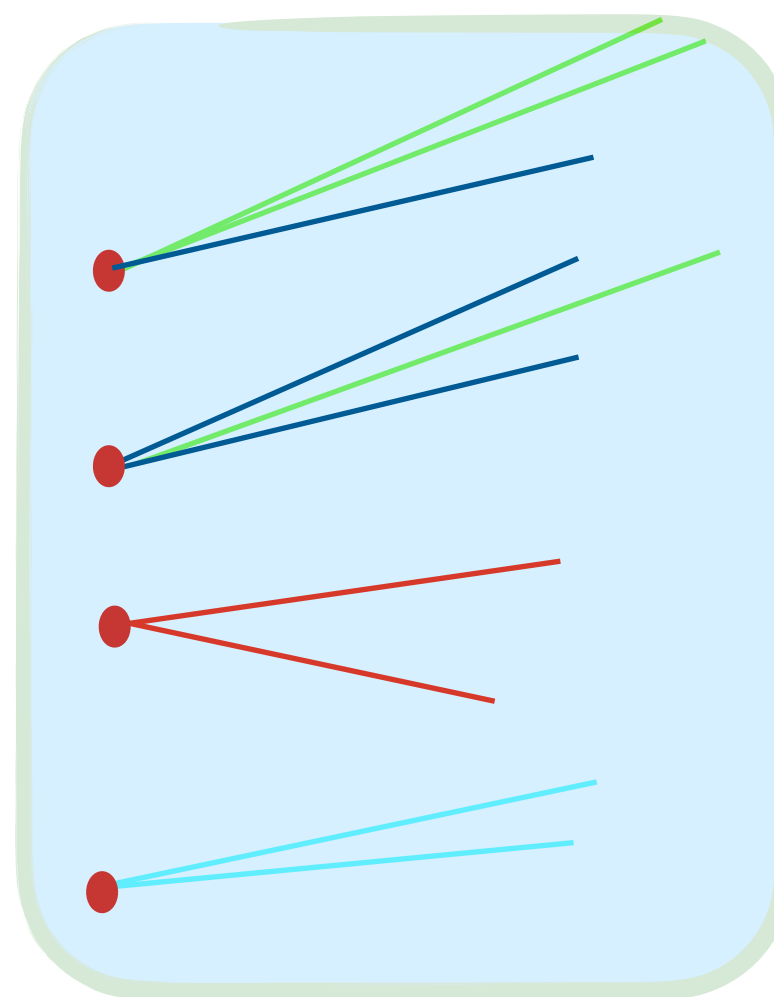
Emerging Jet



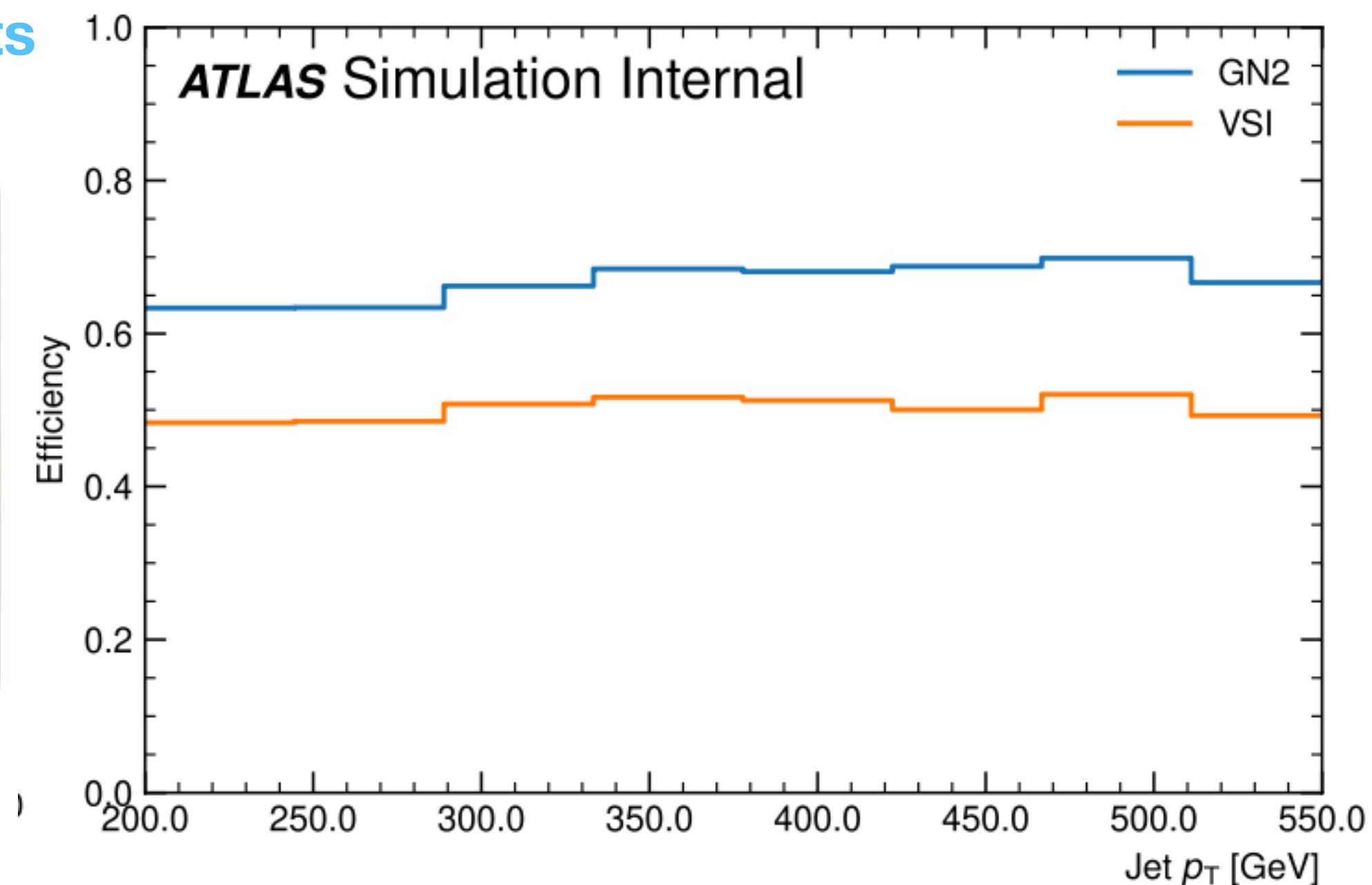
True track sets



Predict. track sets



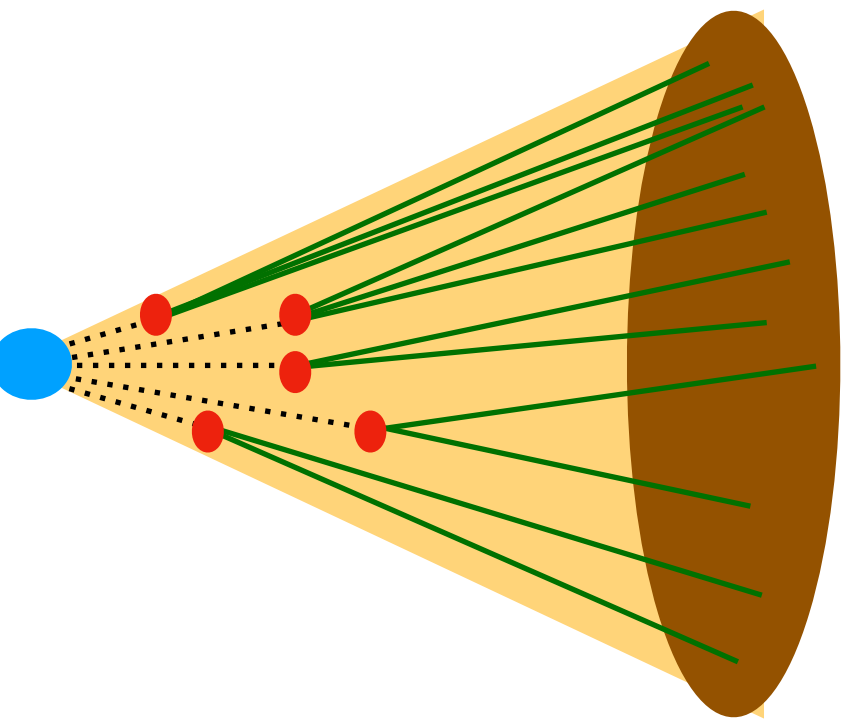
*Are these vertex efficiently reconstructed?*



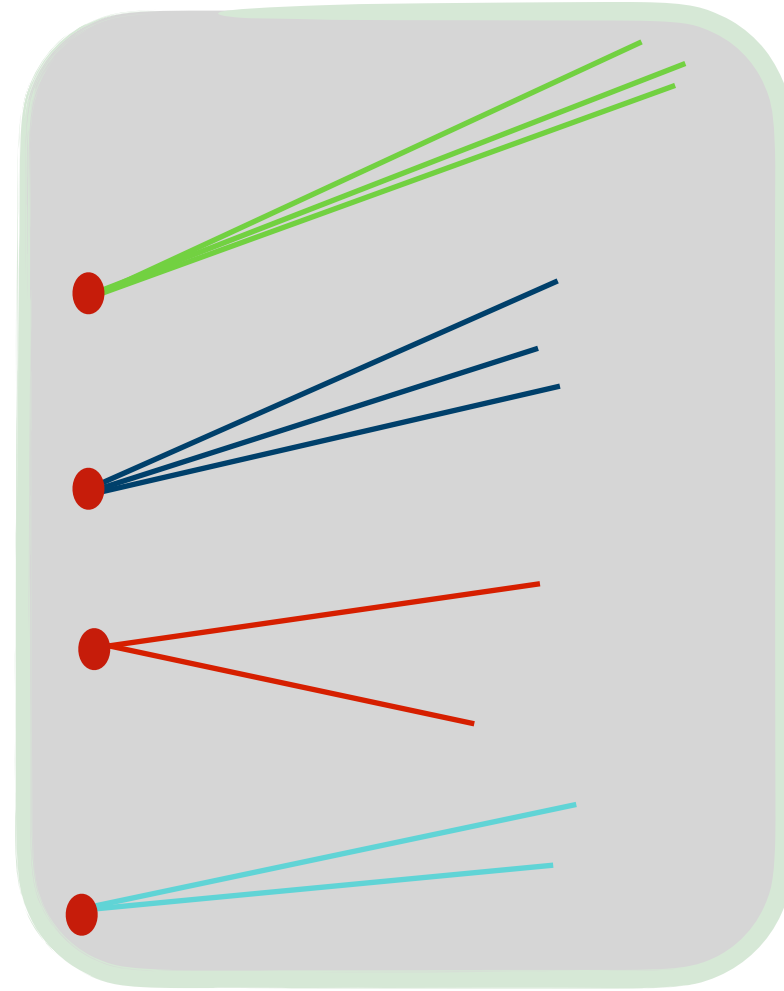
- Efficiency: Per-vertex fraction of tracks in the truth-vertex which are included in a common reco-vertex!
- GNNs have higher efficiency than VSI

# Vertex Performance: Purity

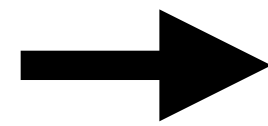
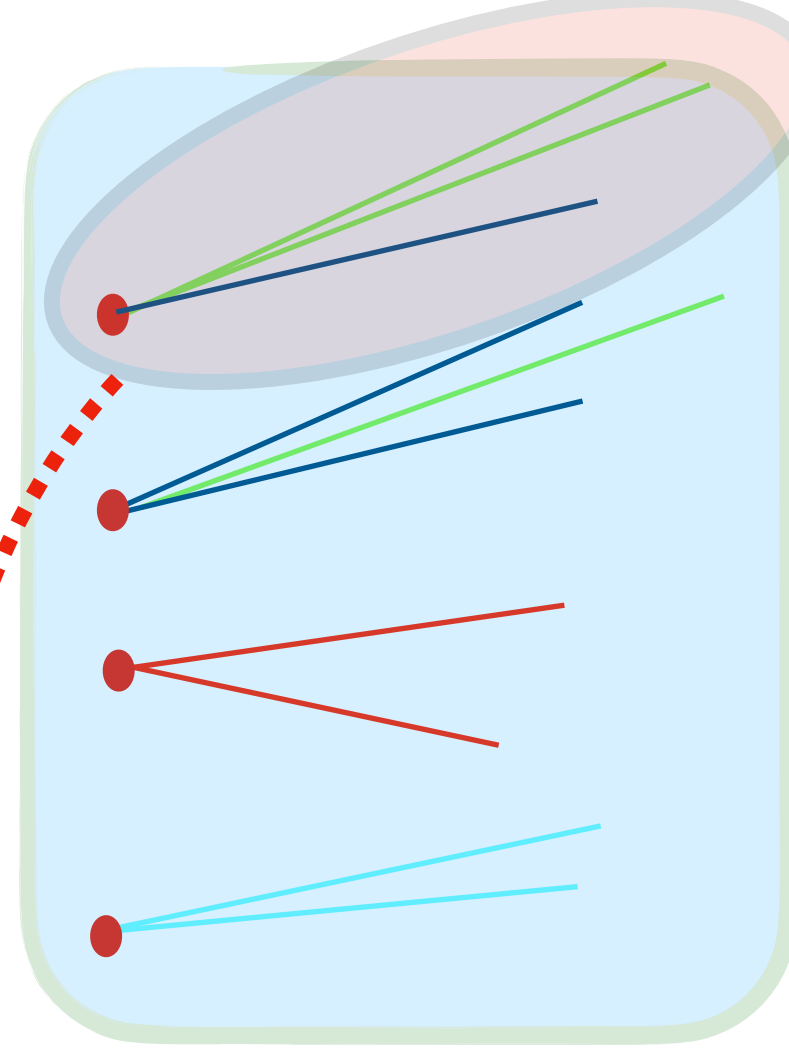
Emerging Jet



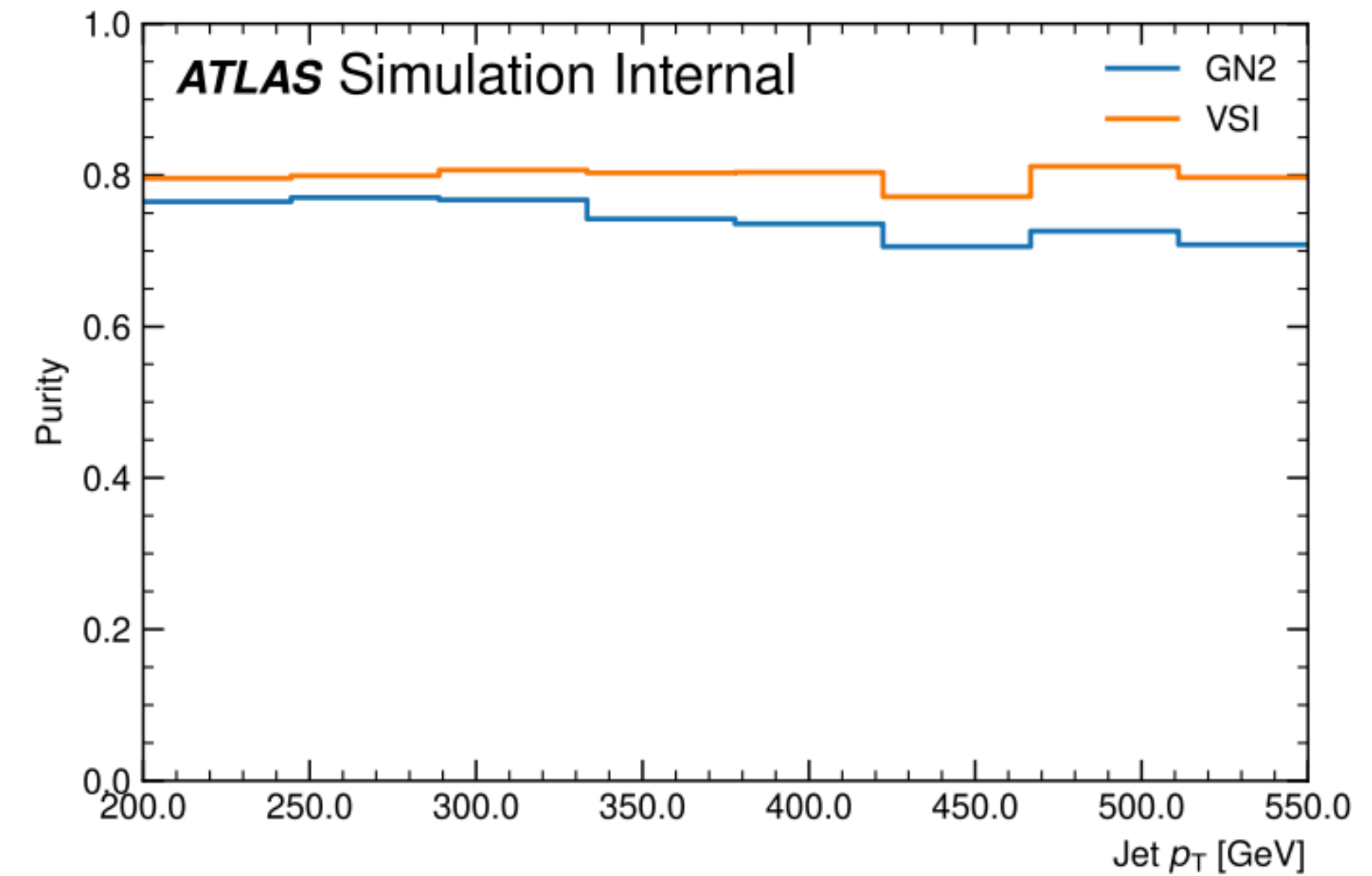
True track sets



Predict. track sets



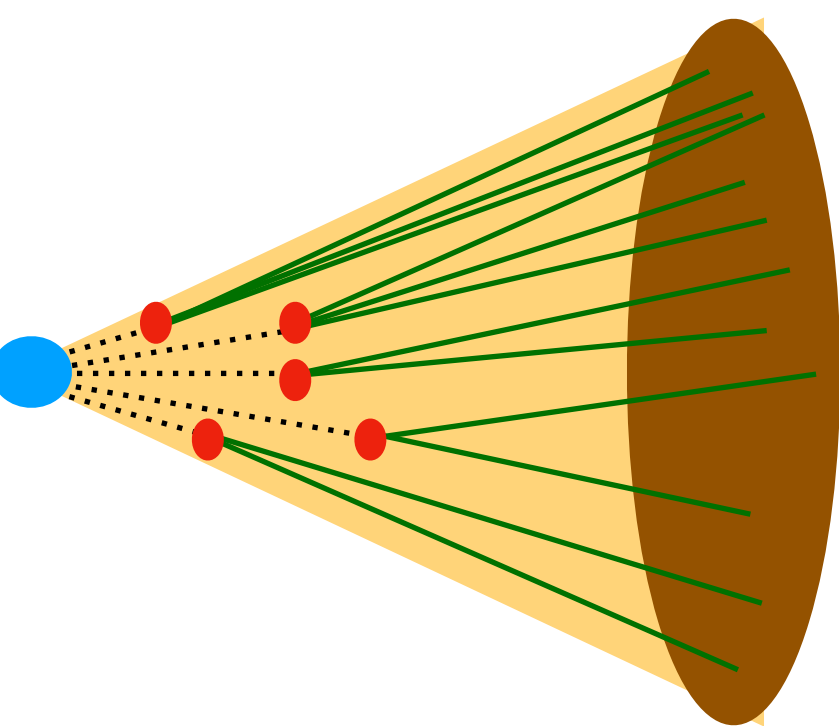
*How "PURE" are these groupings?*



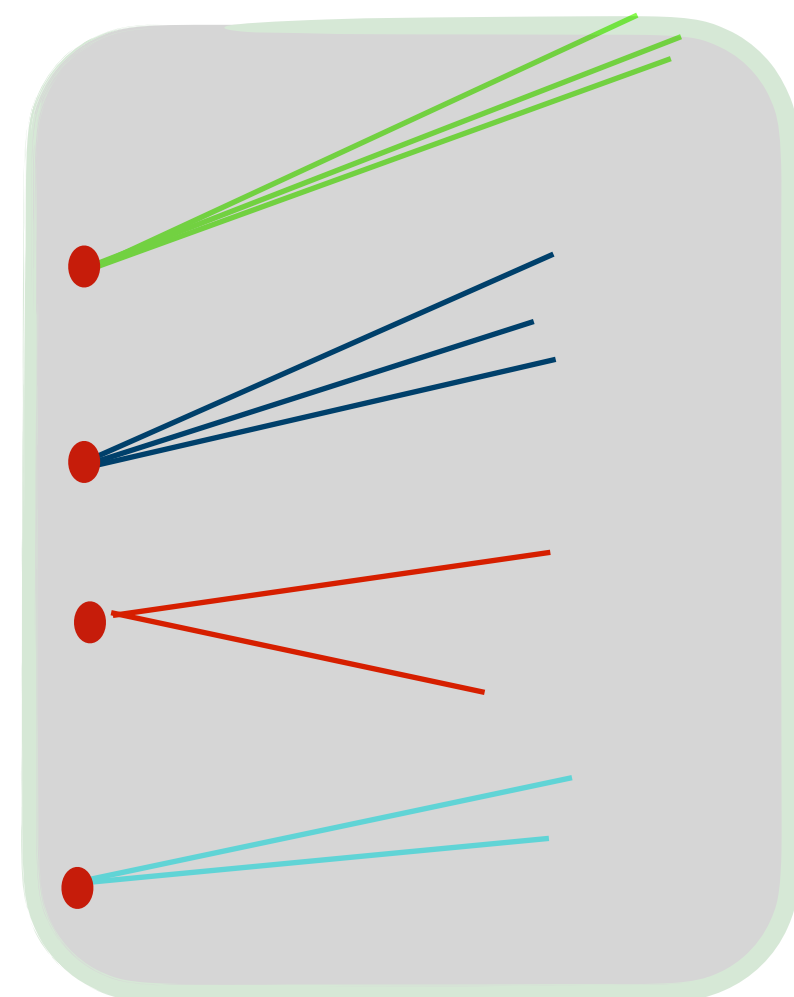
- Purity: Per-vertex fraction of tracks in the reconstructed vertex which are from the same truth vertex.
- GNN predicted vertex and VSI have similar purity.

# Vertex Performance: NumVertex Dist.

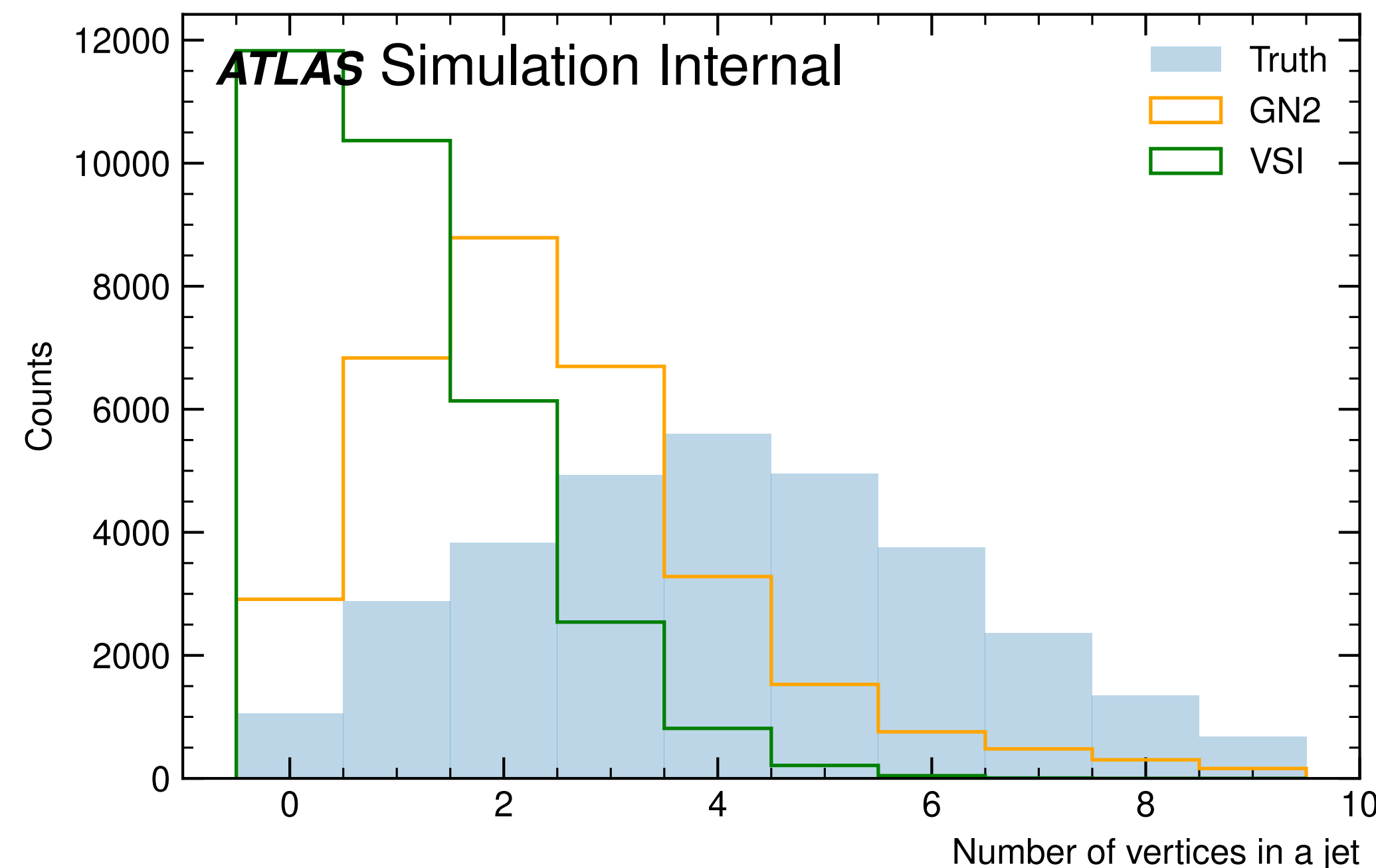
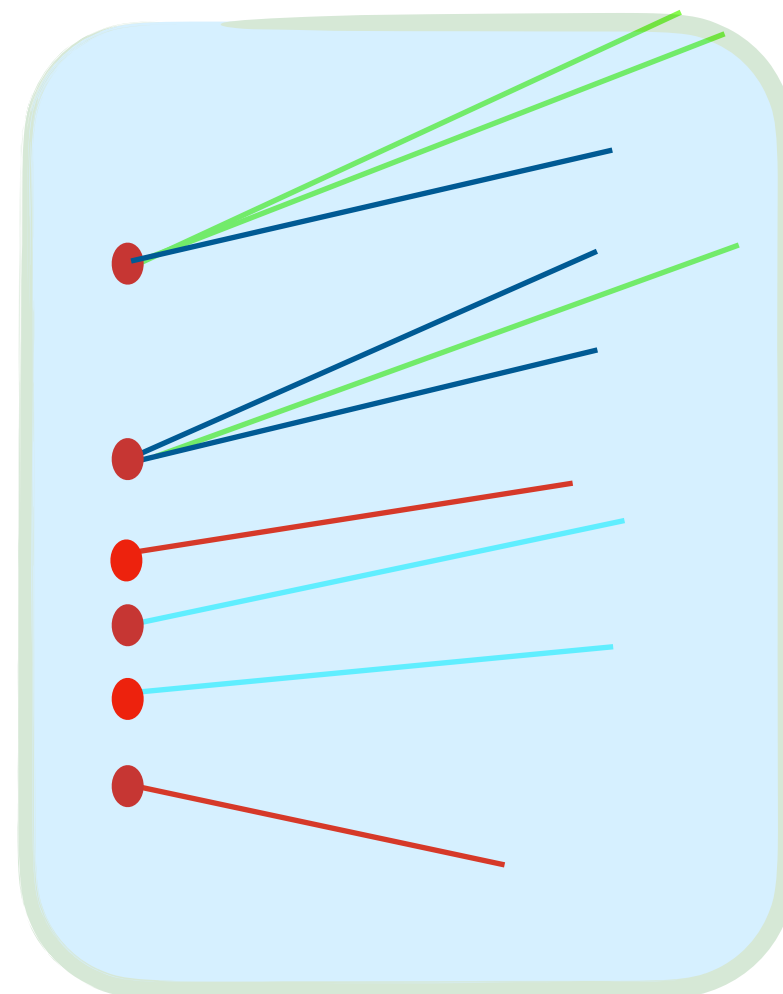
Emerging Jet



True track sets



Predict. track sets

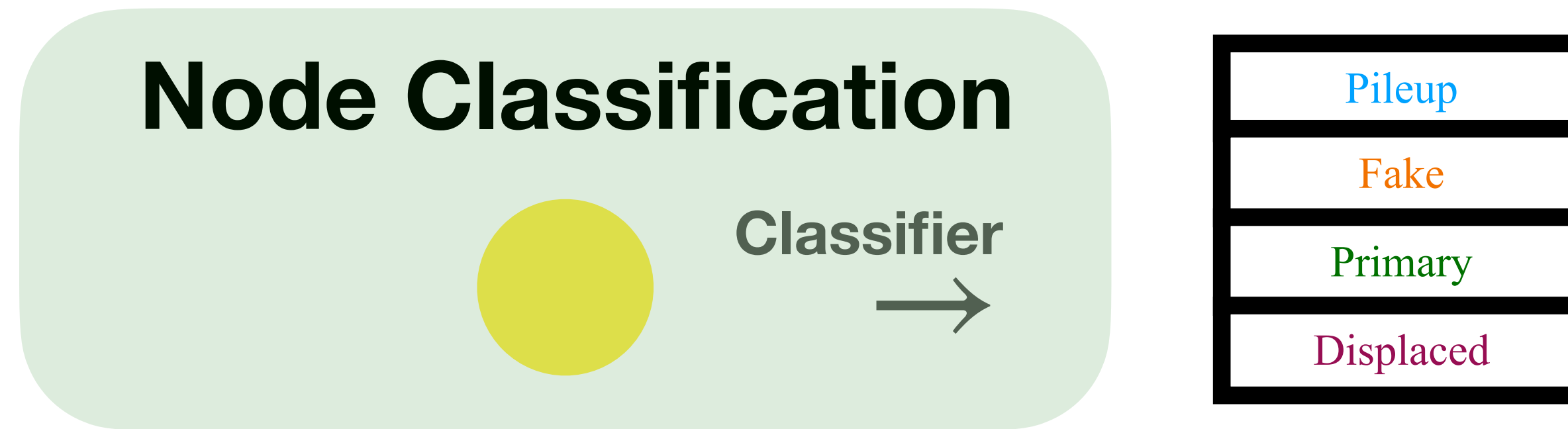


*How many vertex identified?*

- Emerging jets, by definition, has multiple vertices in a jet.
- Number of vertex in per jet distribution shows jet topology identified by GNN closer to the truth.

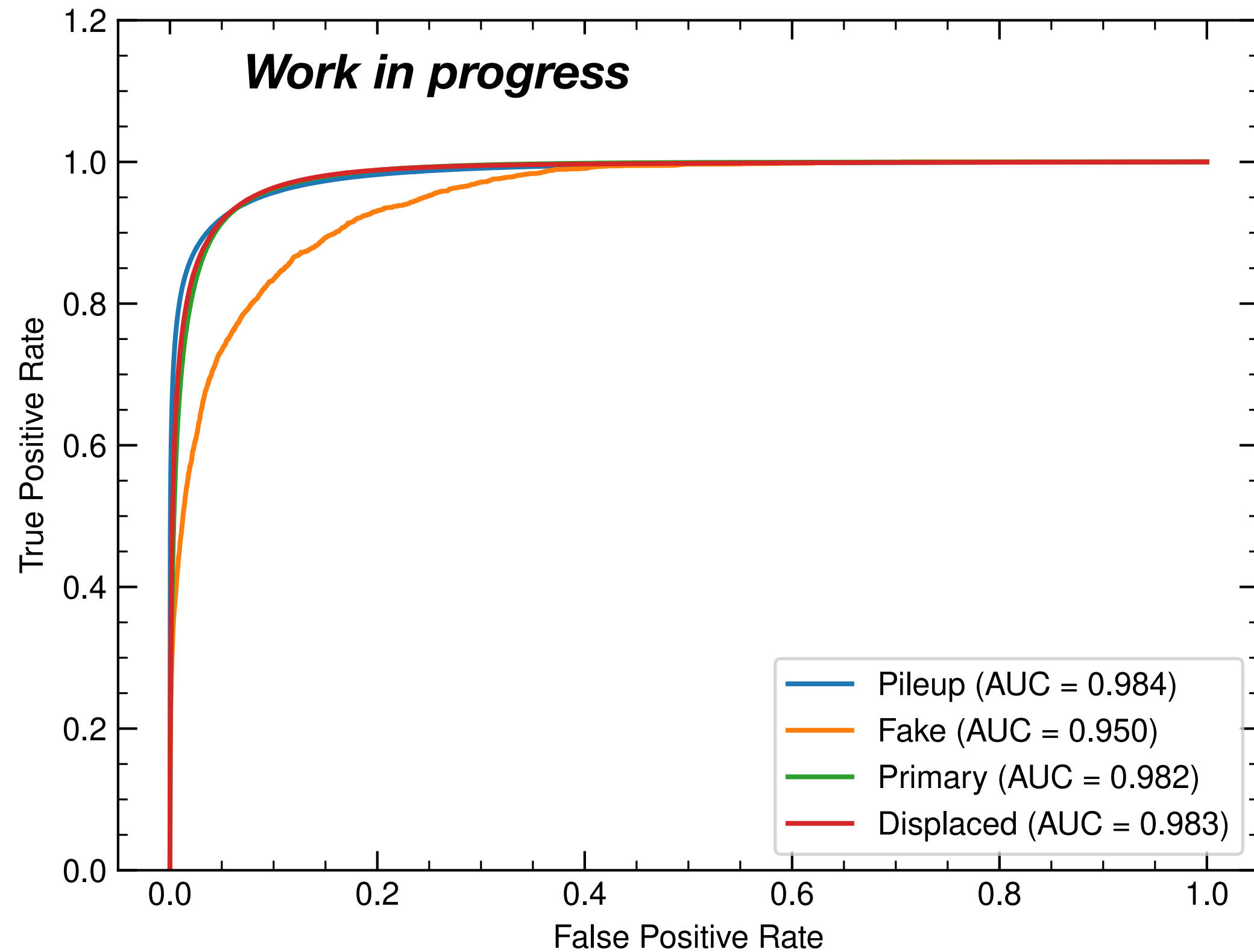


# Results from Performance of GNNS in Track Classification



- Pileup: From additional proton-proton interactions that occur within the same bunch crossing
- Fake: From purely combinatorial collections of hits
- Primary: From Primary Vertex
- Displaced: From Secondary vertices

# GNNs Performance: Track Origin Classification (ROC)

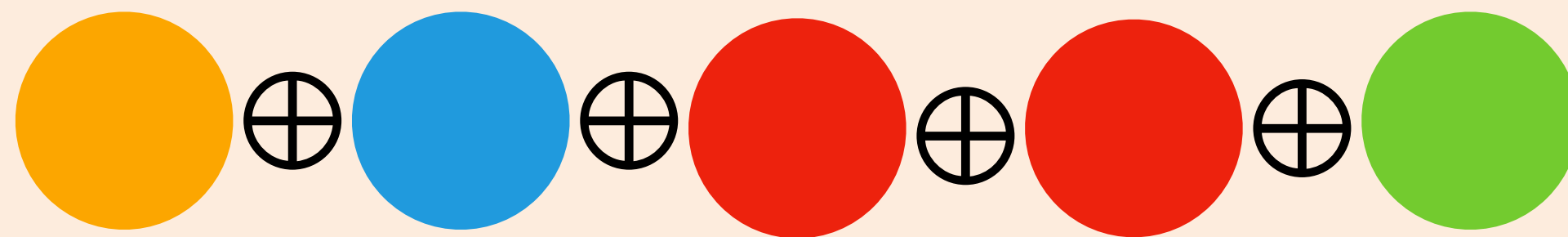


- FPR: proportion of actual negatives that are incorrectly identified as positives
- TPR: proportion of actual positives that are correctly identified

- Highly effective in classifying tracks!
- Displaced tracks classification AUC: 0.983!

# Results from Performance of GNNS in EJ Classification

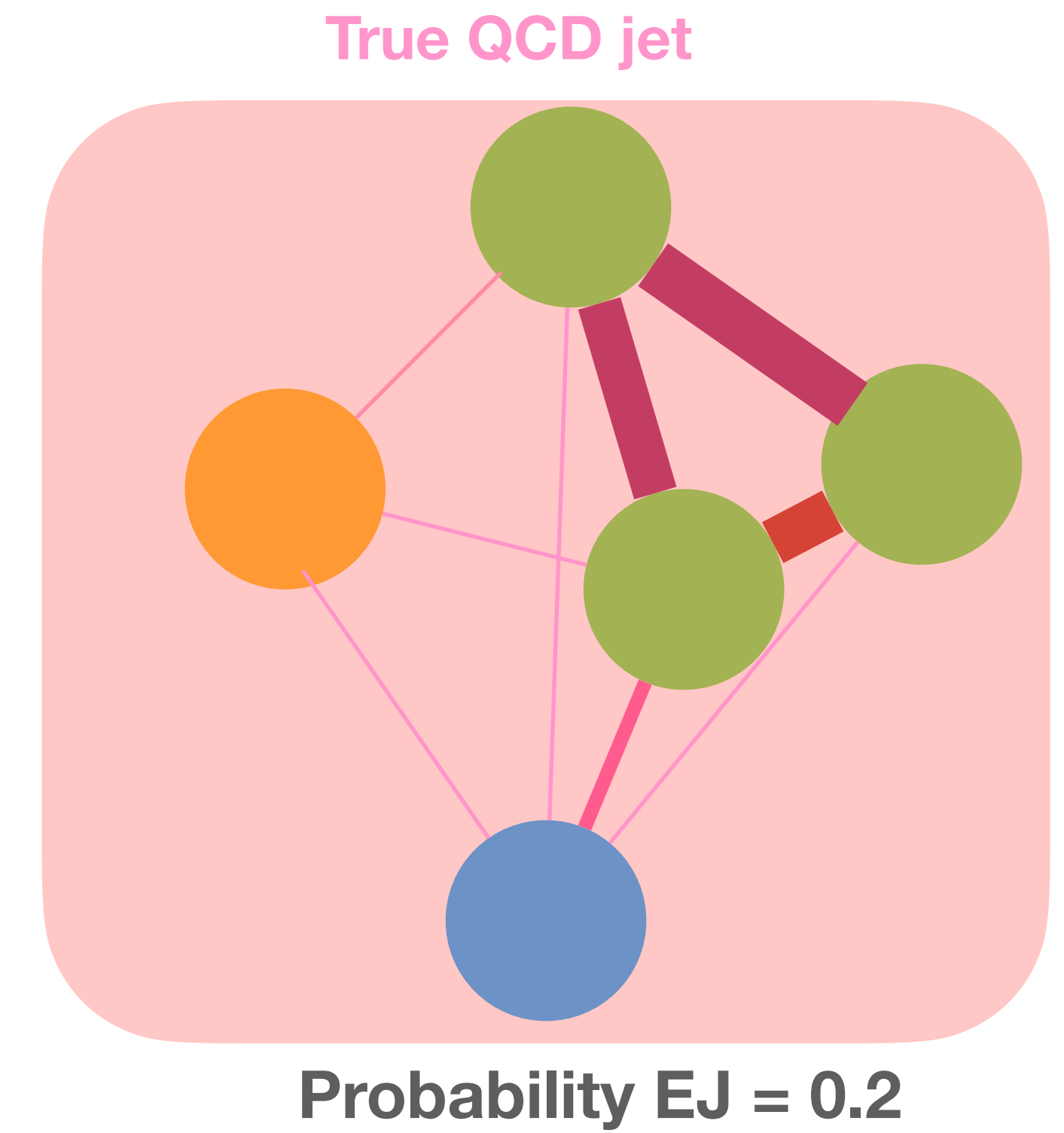
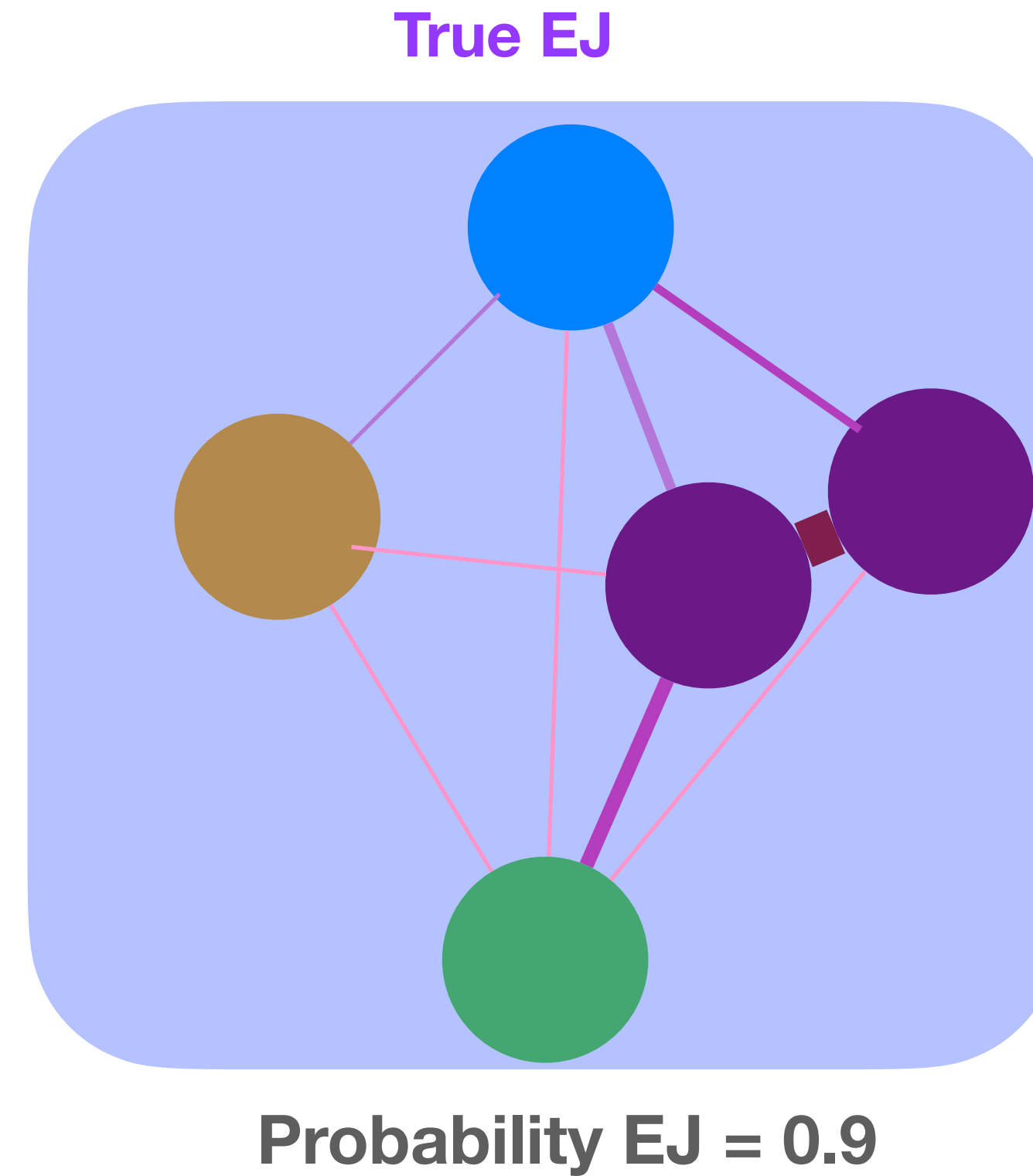
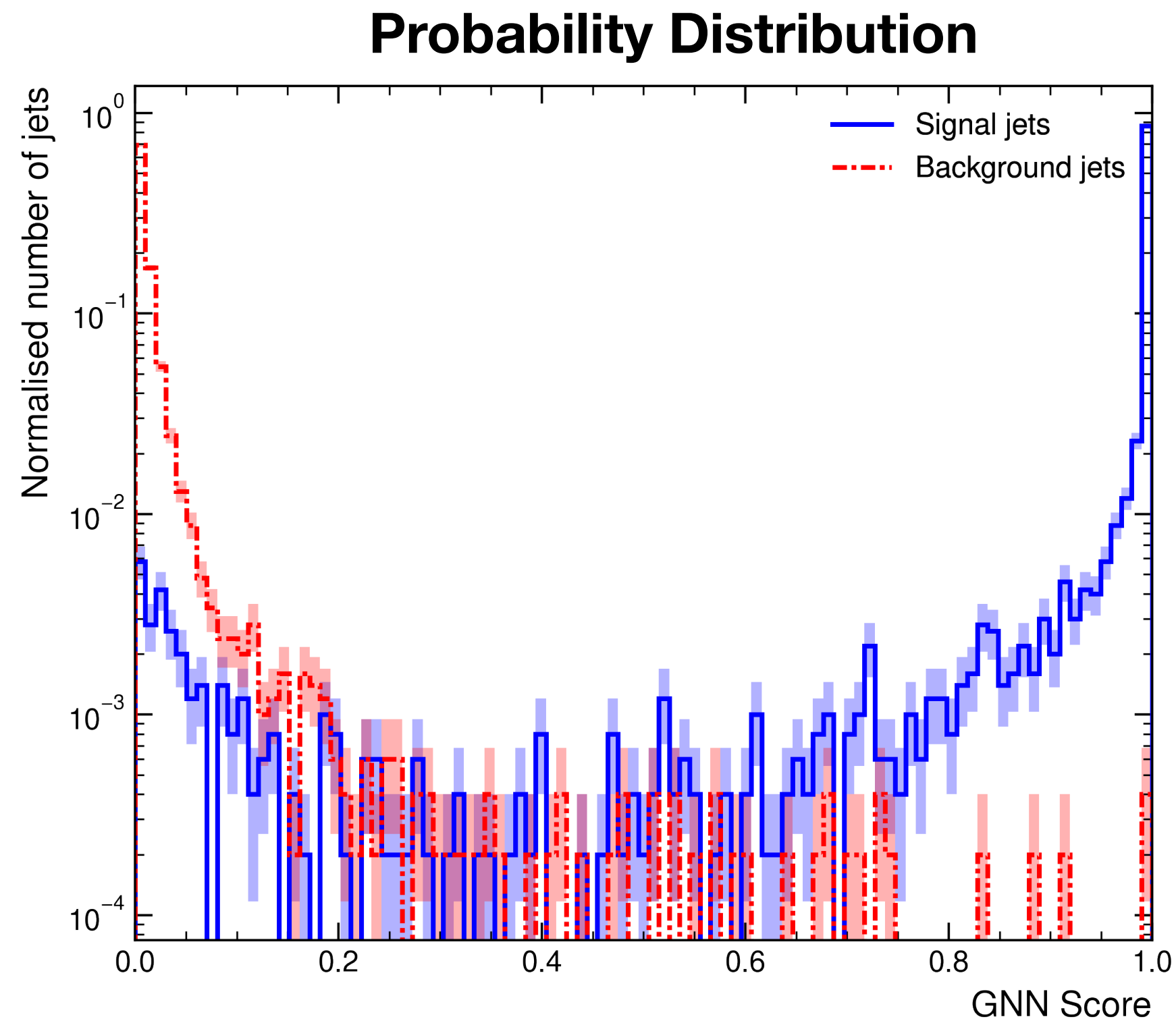
## Graph Classification



Classifier  
→

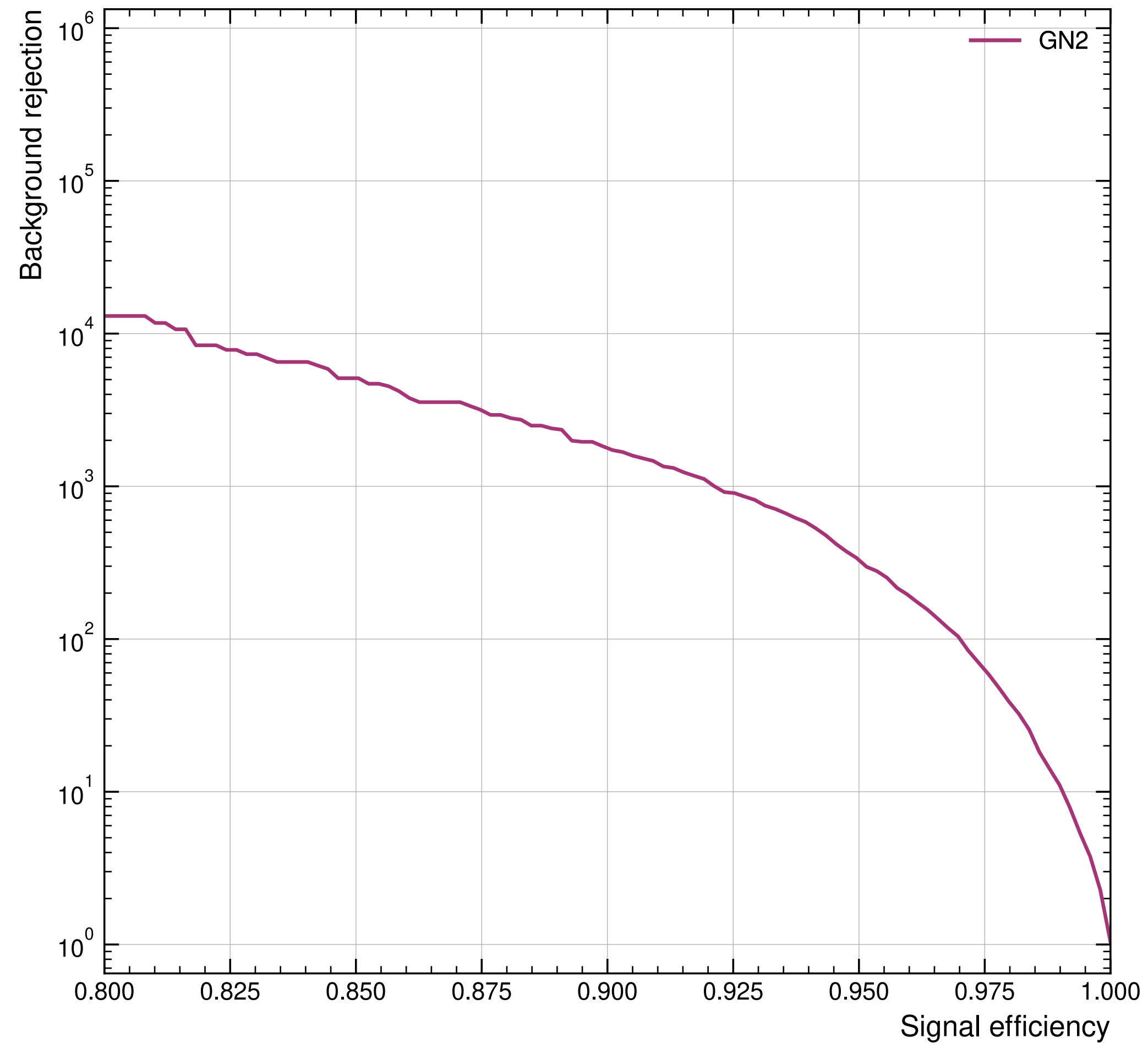
Emerging Jet
QCD Jet

# Jet Classification: Probability Distribution



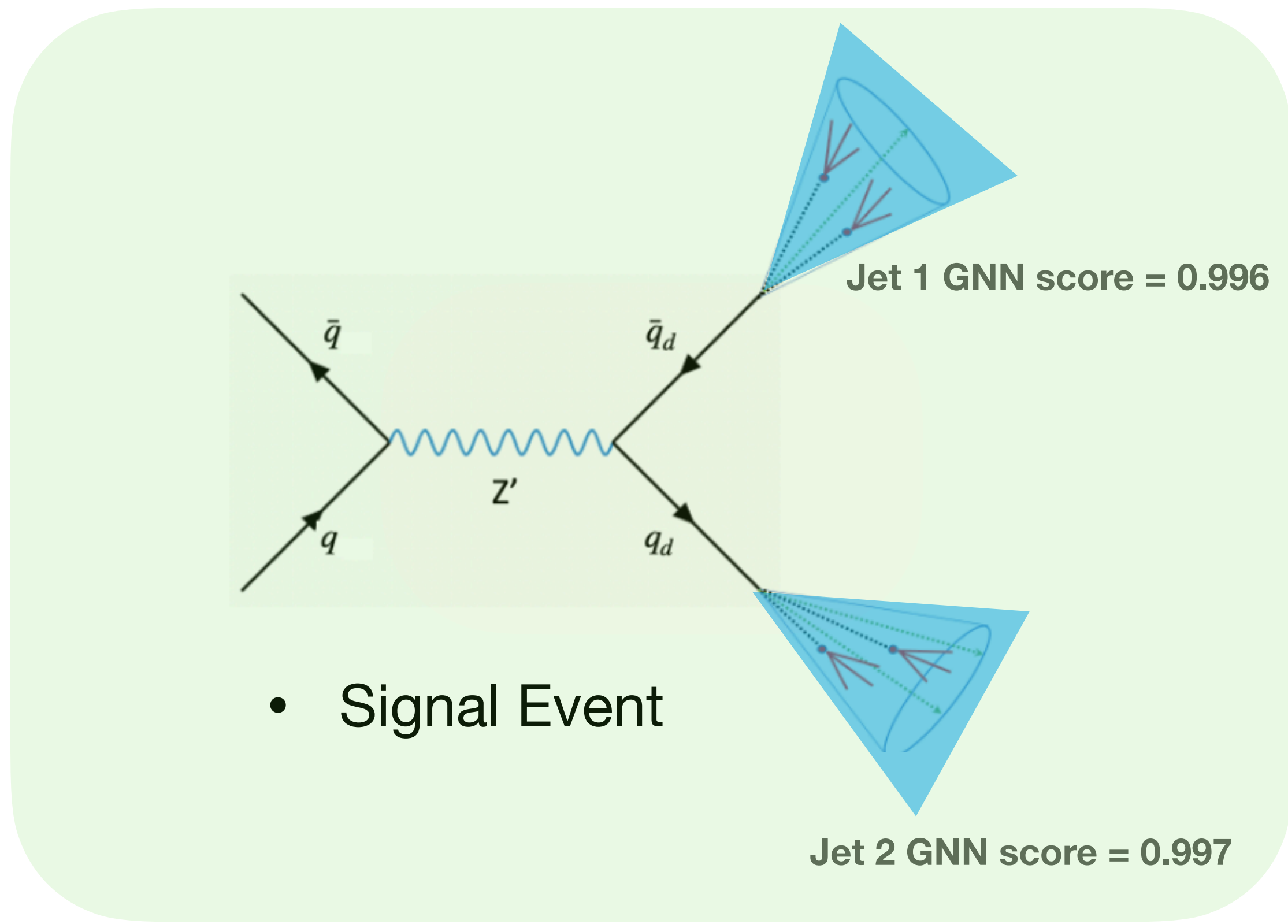
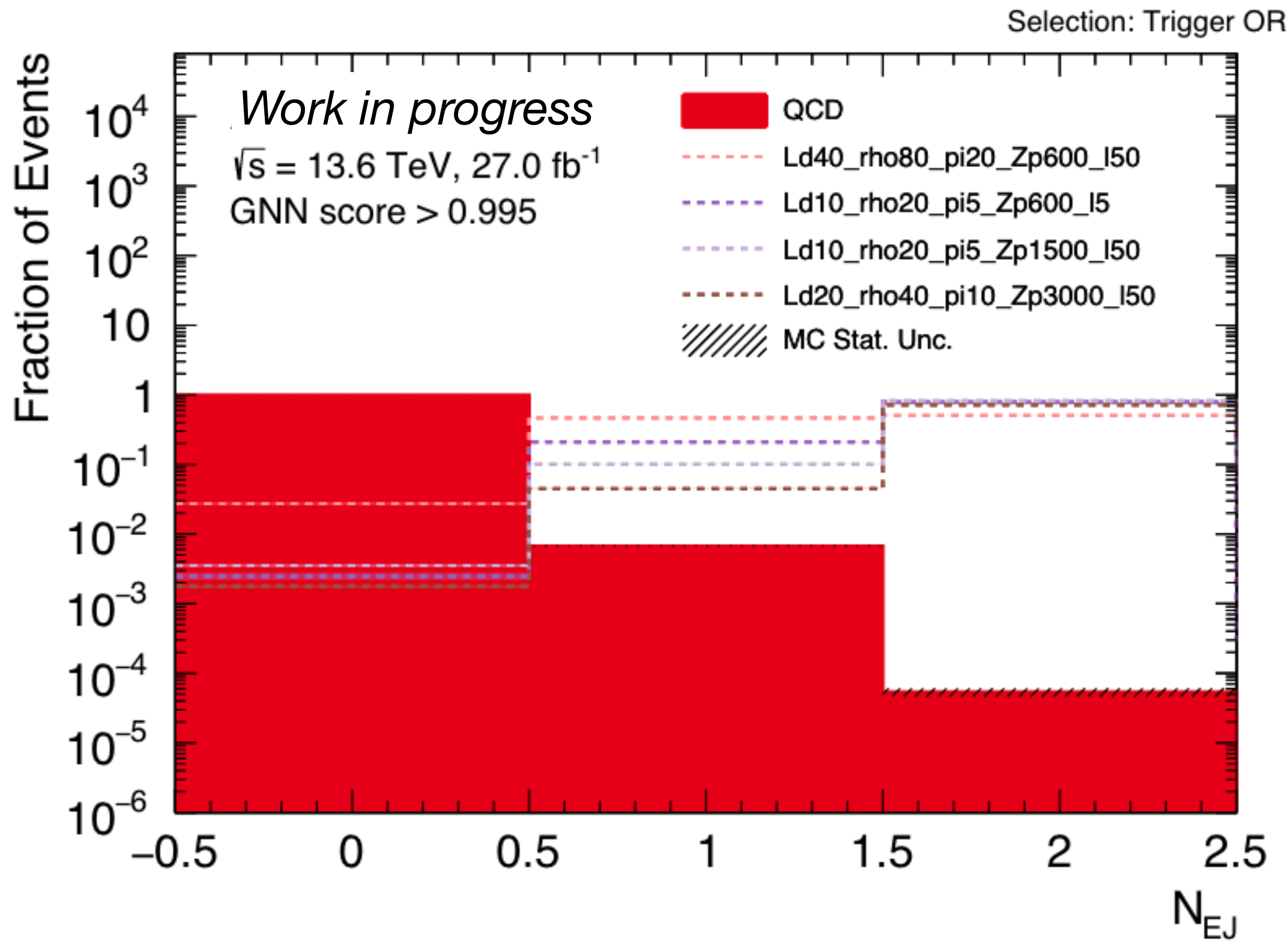
- Two categories: Signal Jets (*E*s) from long lived dark mesons and background Jets from QCD background process!
- EJ probability(GNNScore) distribution.
- Signal jets peaks at last bin suggesting extremely high likelihood for majority of signal jets to be correctly identified!

# Jet Classification: ROC



- Extremely good classifier with great background rejection while retaining majority of the signal.
- This implies that within a threshold where 80 % of the signal jets are accurately identified, there is a misclassification of 1 jet for every  $\sim 10^4$  jets.

# GNN in EJ (Run 03) Analysis



o Requiring two jets to have GNN score > 0.995 gives significant background reduction with high signal efficiency!

# Conclusion

- Use of GNNs are very effective in classifying atypical LLP signature- emerging jets.
- Additionally GNNs were also able to perform classification of tracks inside the jet and find of pair of tracks belong to the same vertex.

*Thank You!*

# Backup

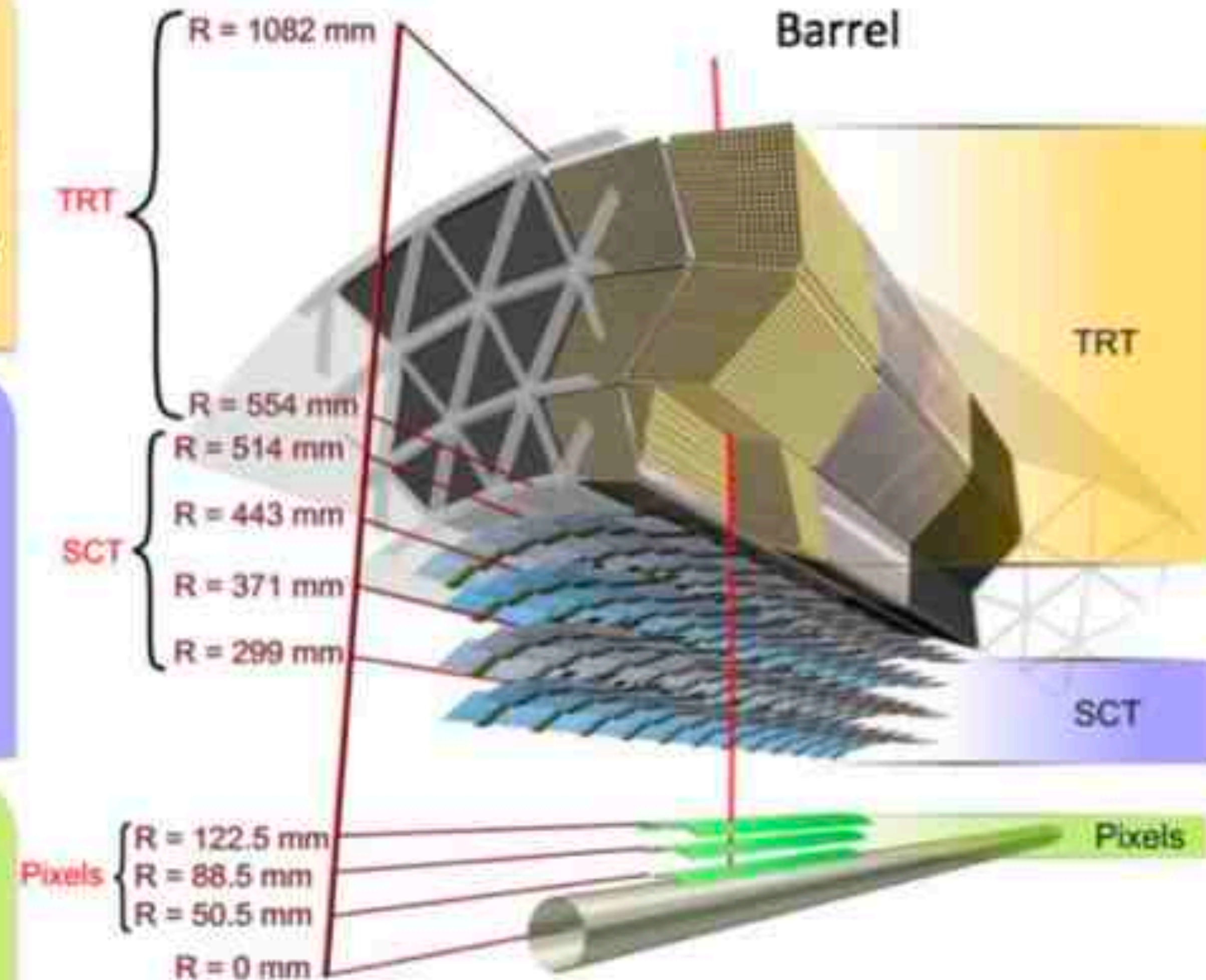


# ATLAS Detector

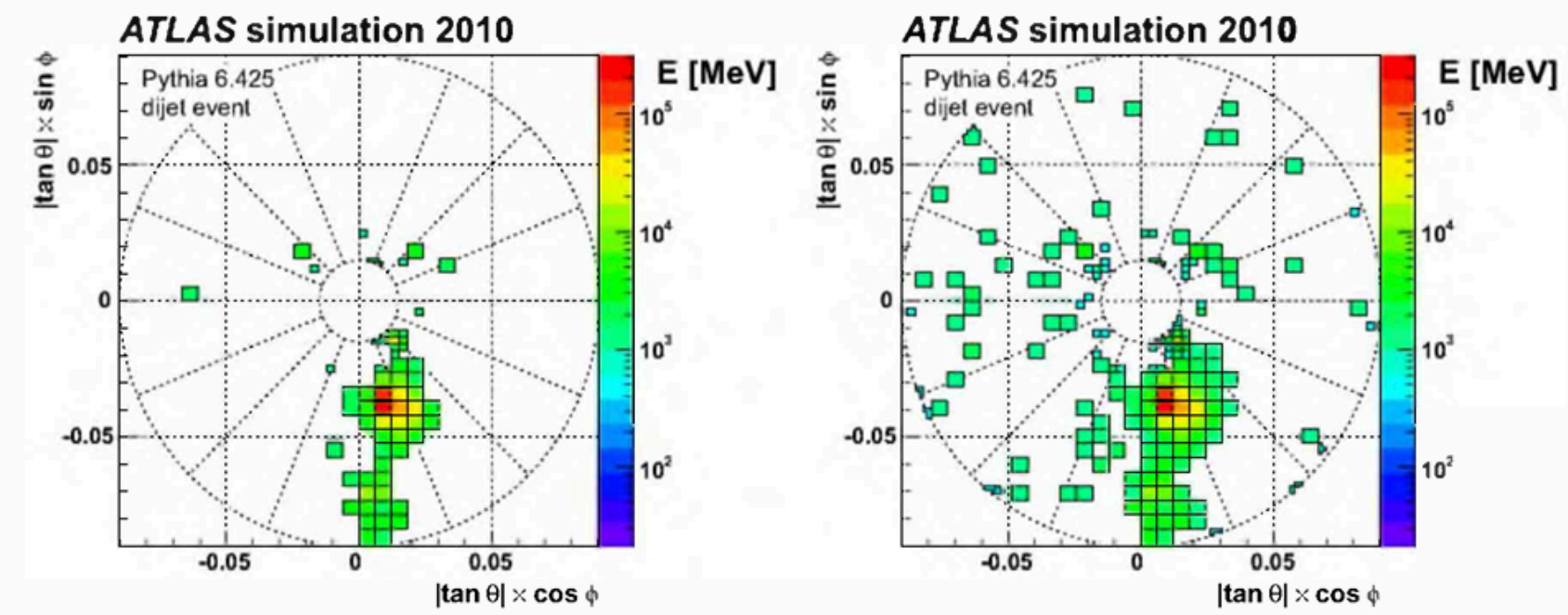
- Straw tracker + Transition Radiation
- 4mm diameter straws with 35  $\mu\text{m}$  anode wire
- Layers: 73 in Barrel (axial) 2x160 in Endcap (radial)

- 4(9) double layers in Barrel/Endcap
- 4088 modules, 6M chan., strips 80  $\mu\text{m}$
- Resolution 17 x 580  $\mu\text{m}$

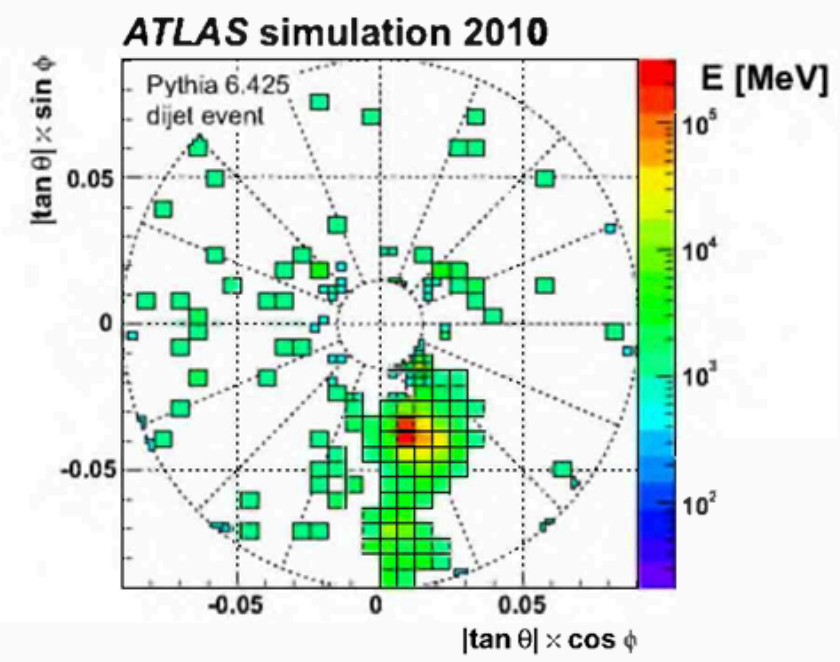
- 3 layers in Barrel and Endcap
- Pixel size 50 x 400  $\mu\text{m}$
- Resolution 10 x 110  $\mu\text{m}$
- 80 M channels



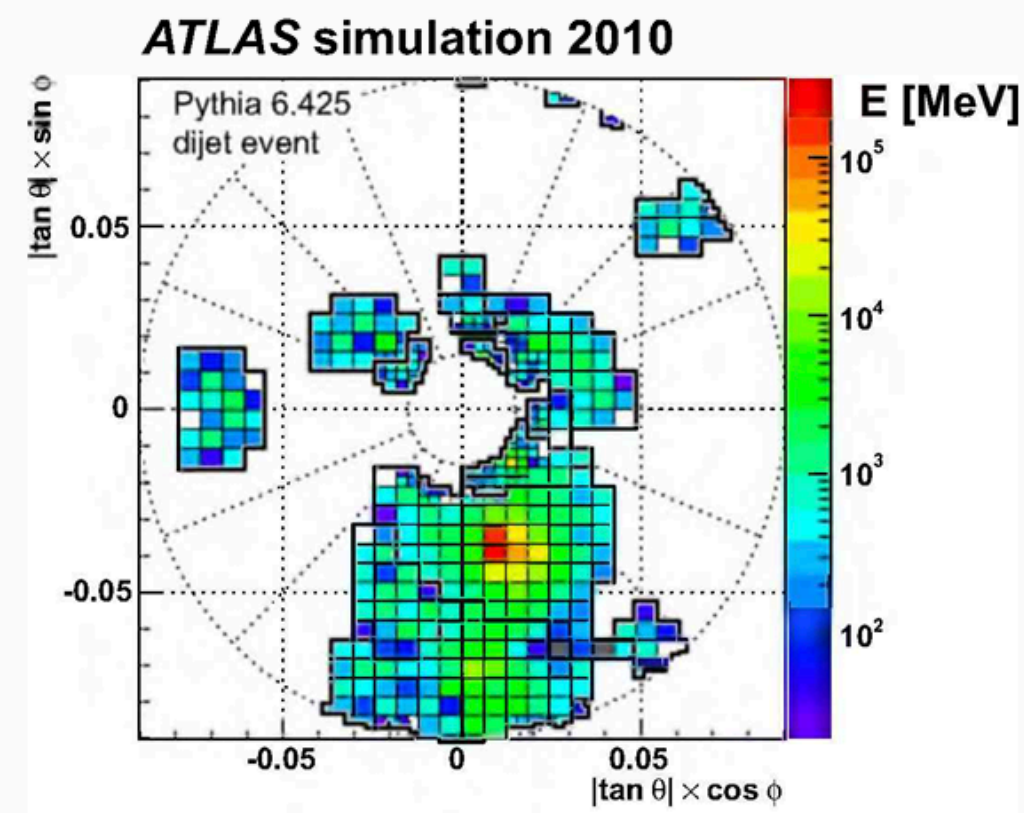
# Jet cluster



(a) Cells passing selection in Eq. (3)



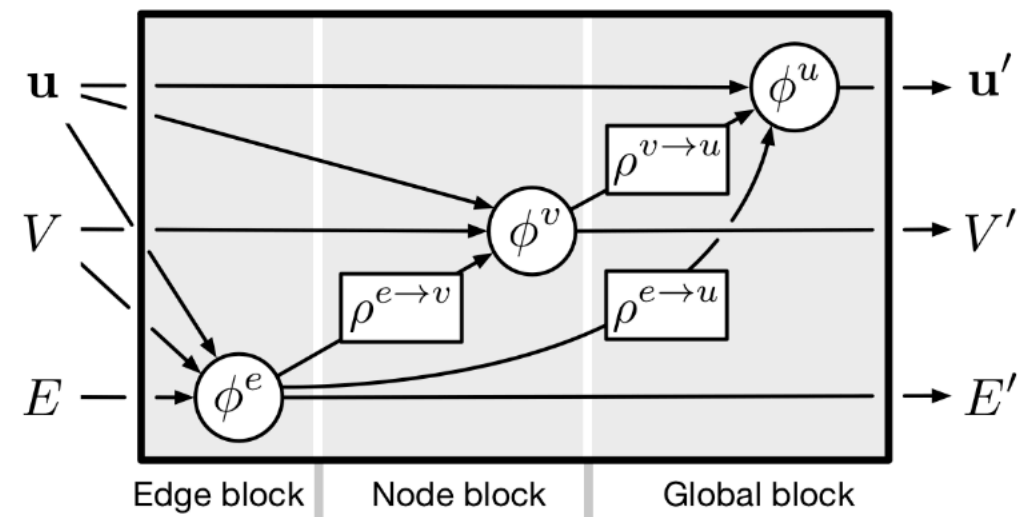
(b) Cells passing selection in Eq. (4)



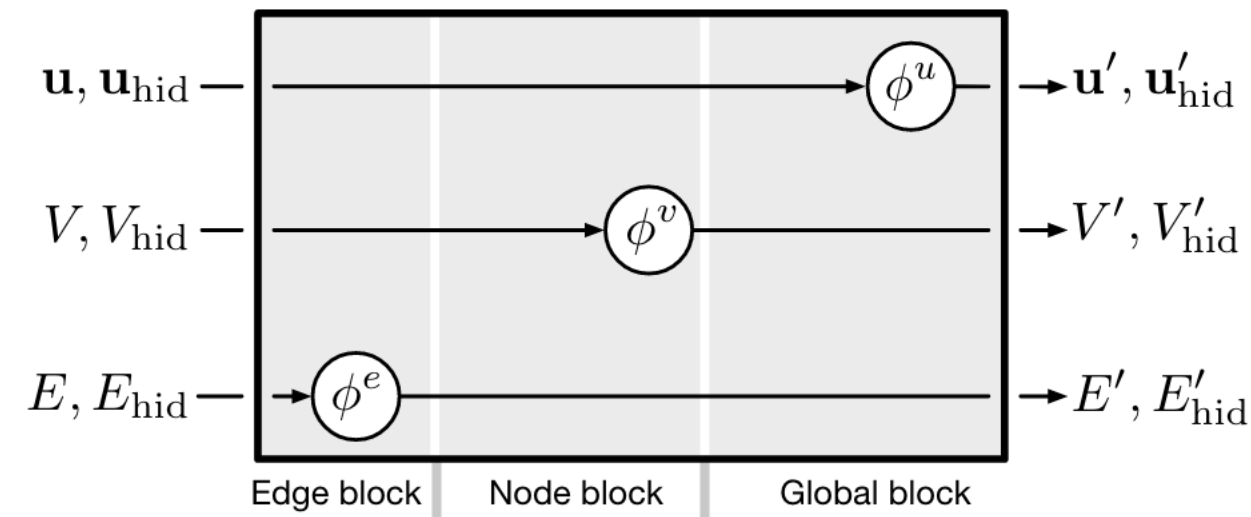
(c) All clustered cells

- Image: <https://arxiv.org/abs/1603.02934>

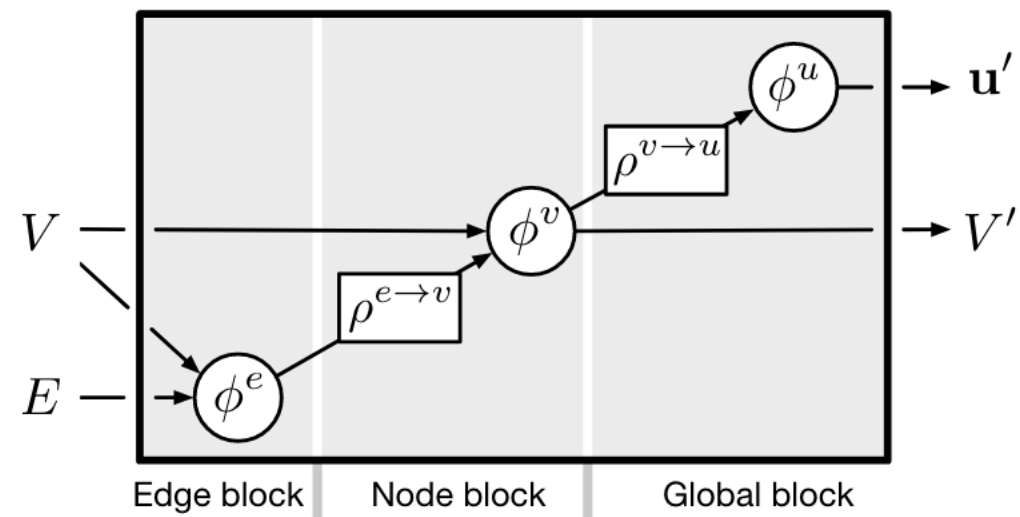
# GNN generalizations



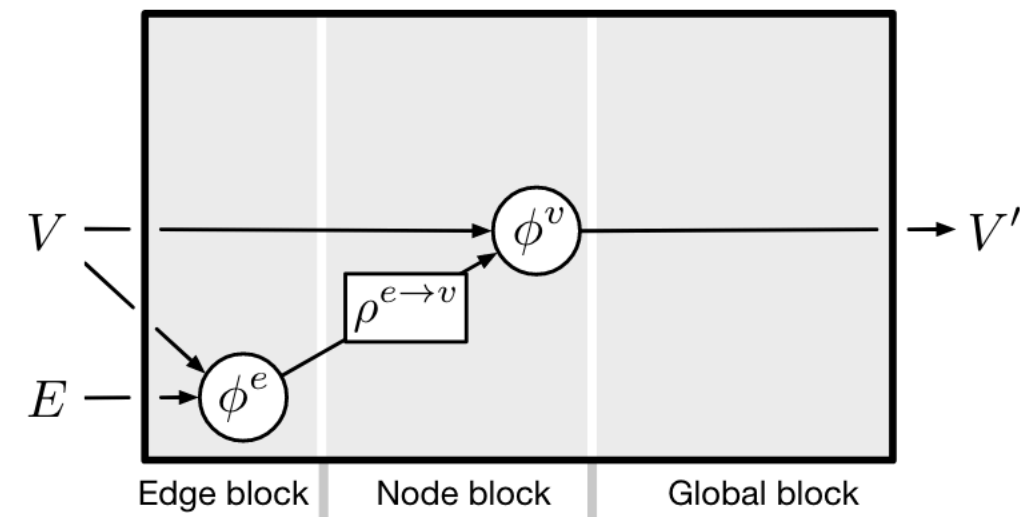
(a) Full GN block



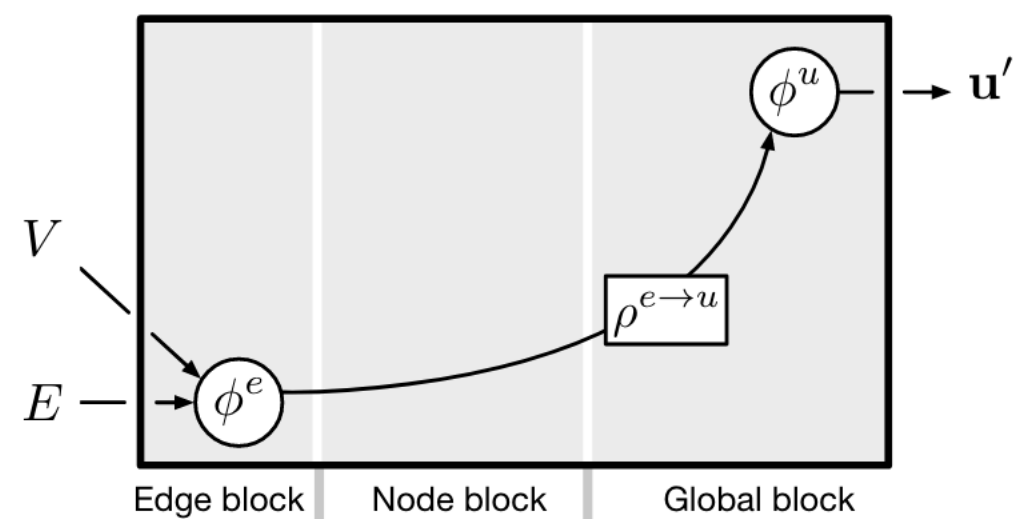
(b) Independent recurrent block



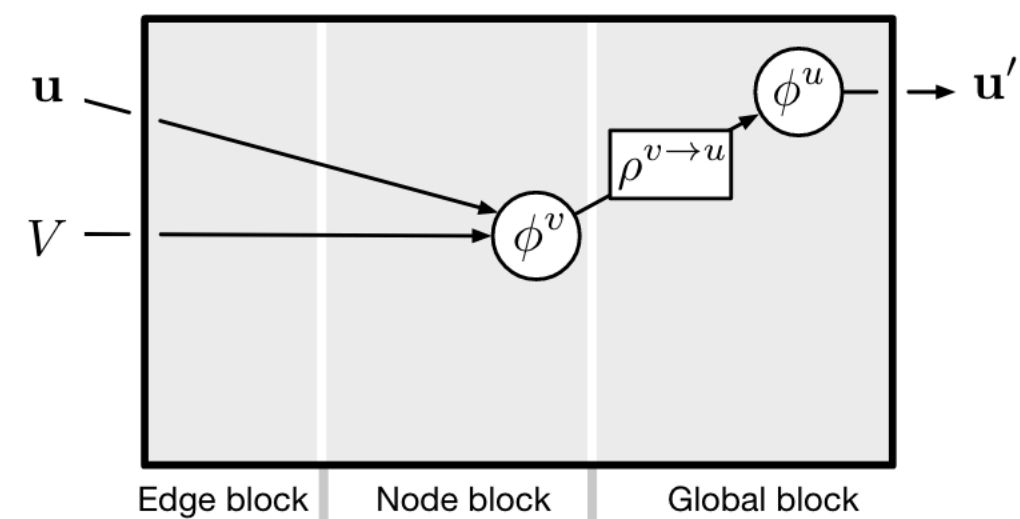
(c) Message-passing neural network



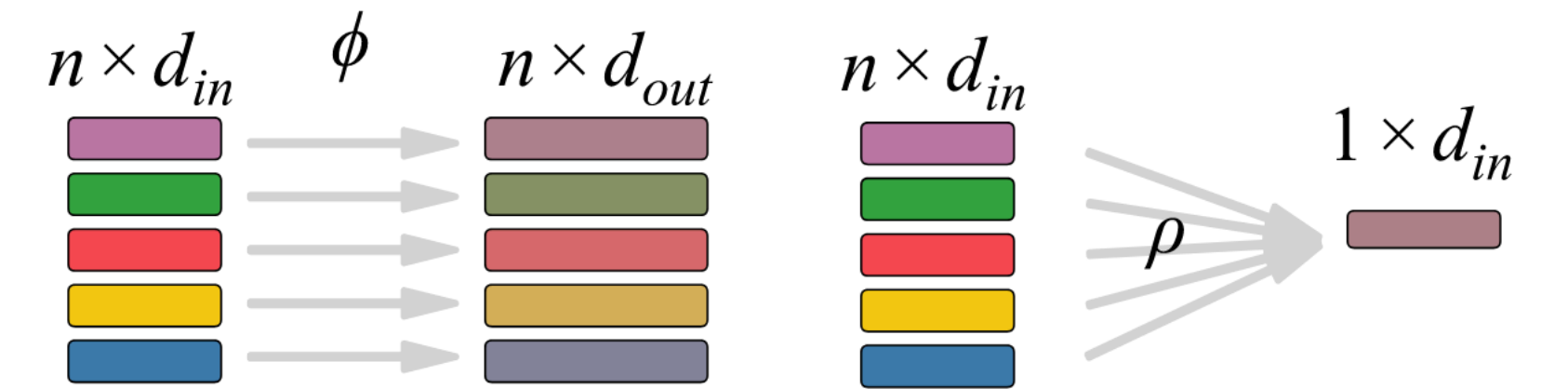
(d) Non-local neural network



(e) Relation network



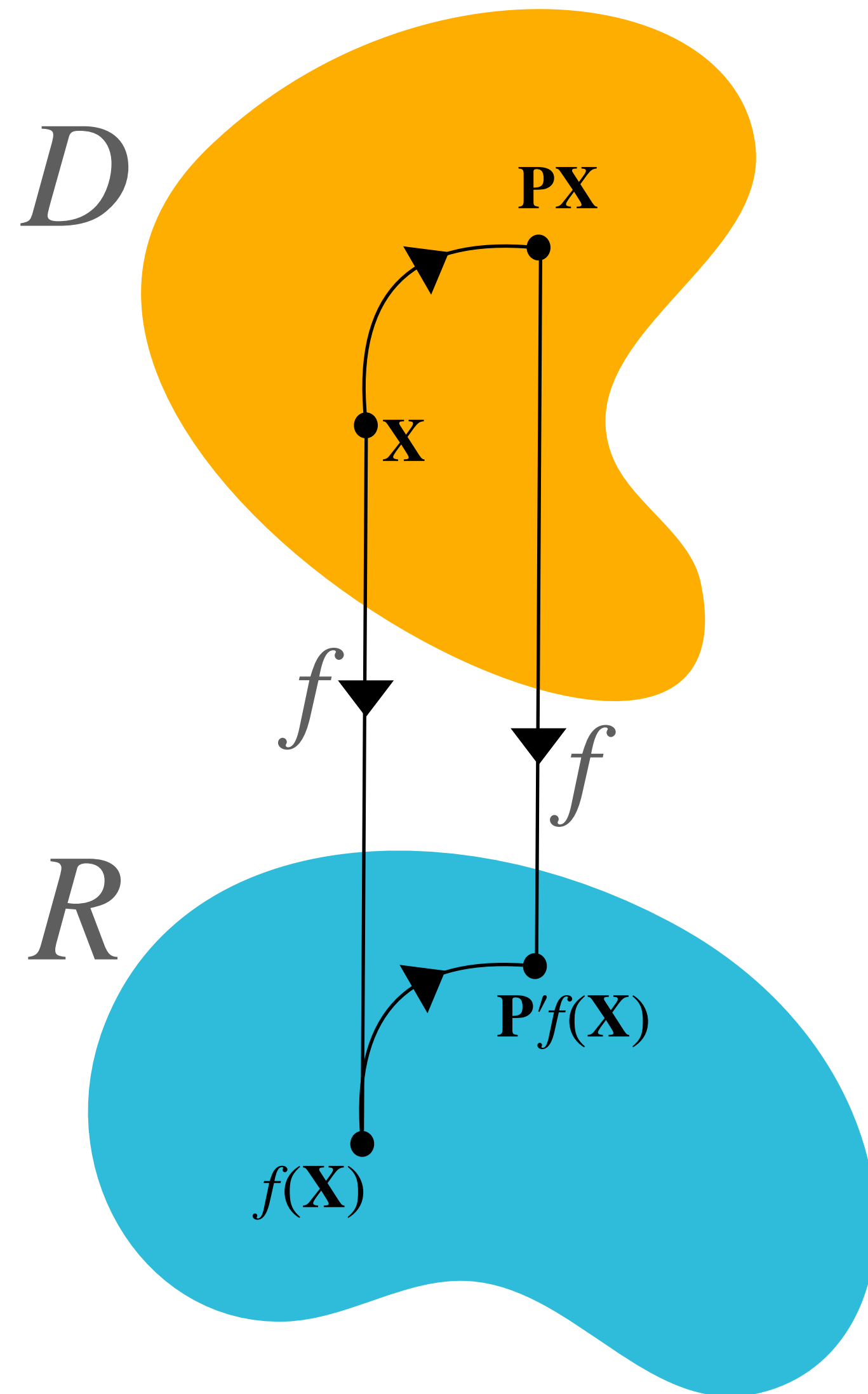
(f) Deep set



## Internal component of GNNs

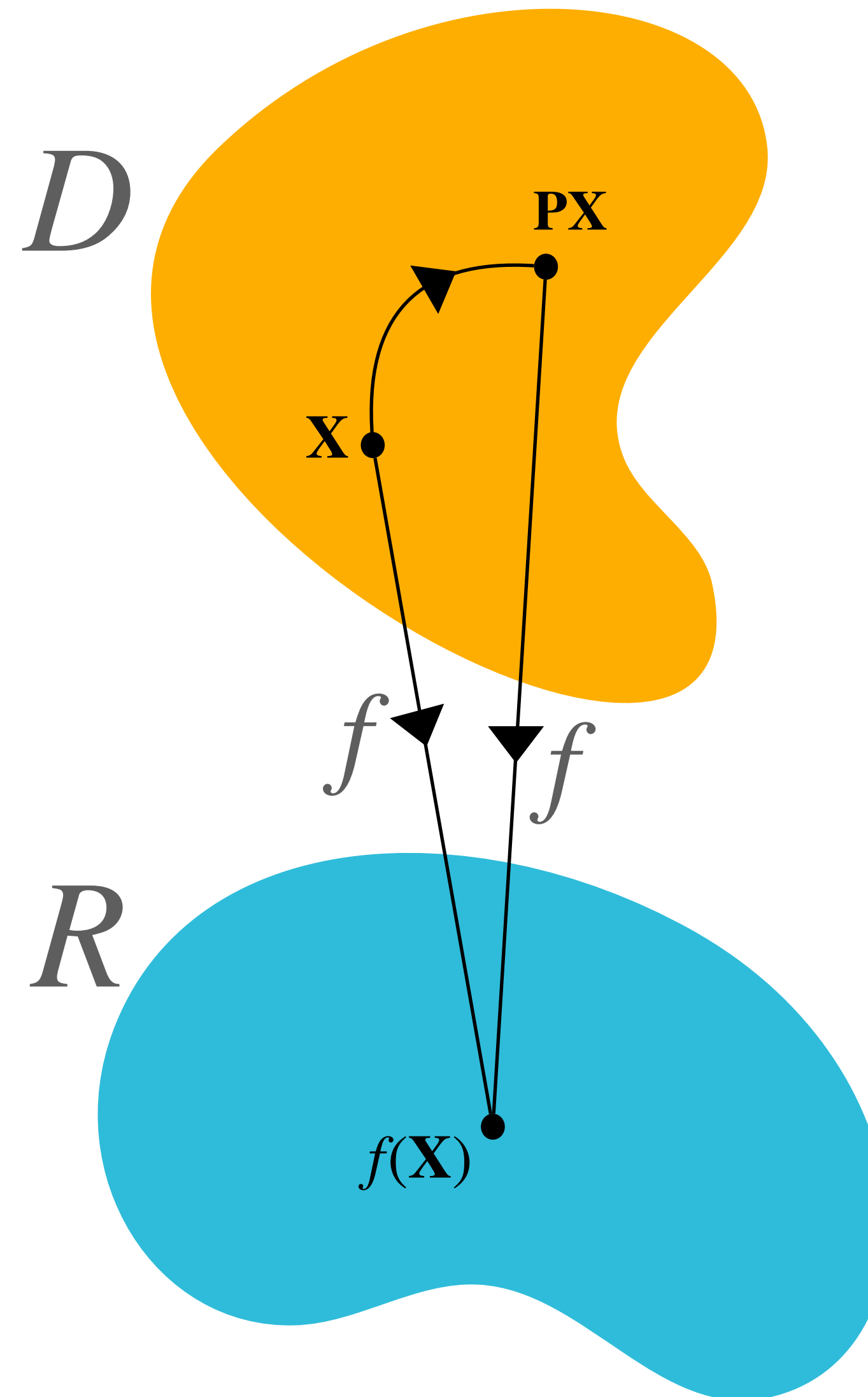
## Equivariance

$$f(\mathbf{P}\mathbf{X}) = \mathbf{P}'f(\mathbf{X})$$

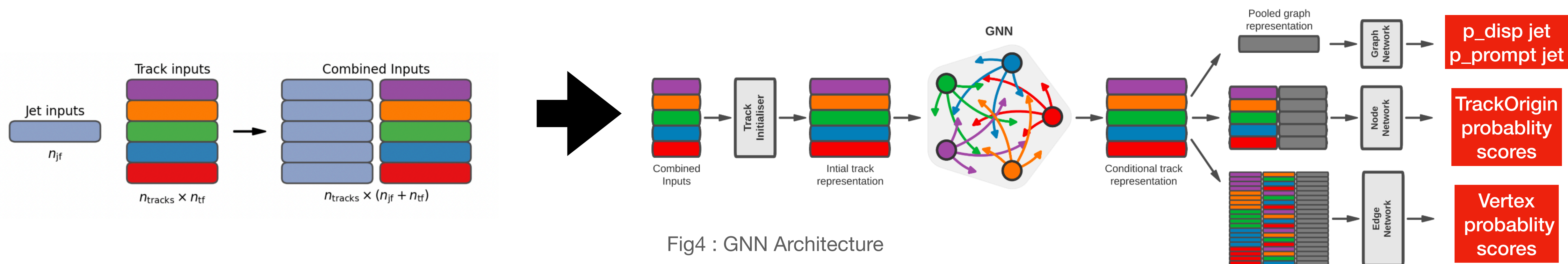


## Invariance

$$f(\mathbf{P}\mathbf{X}) = f(\mathbf{X})$$



# GNN Architecture



- Combined input prepared and fed into network architecture (2 jet variables 16 track variables)
- Initial latent representation for each track created. These representations are then used to populate the node features of a fully connected graph network
- Message passing graph neural network's loss function also accounts node and vertex classification loss function.
- After the graph network, the resulting node representations used to predict Track Label (truthOriginLabel), JetLabel (isDisplaced) probability score.
- Architecture based on the ATLAS Flavour tagging software!



# Samples Used for Training EJ classifier

QCD

Ld40\_rho80\_pi20\_Zp600\_I50

Ld10\_rho20\_pi5\_Zp600\_I5

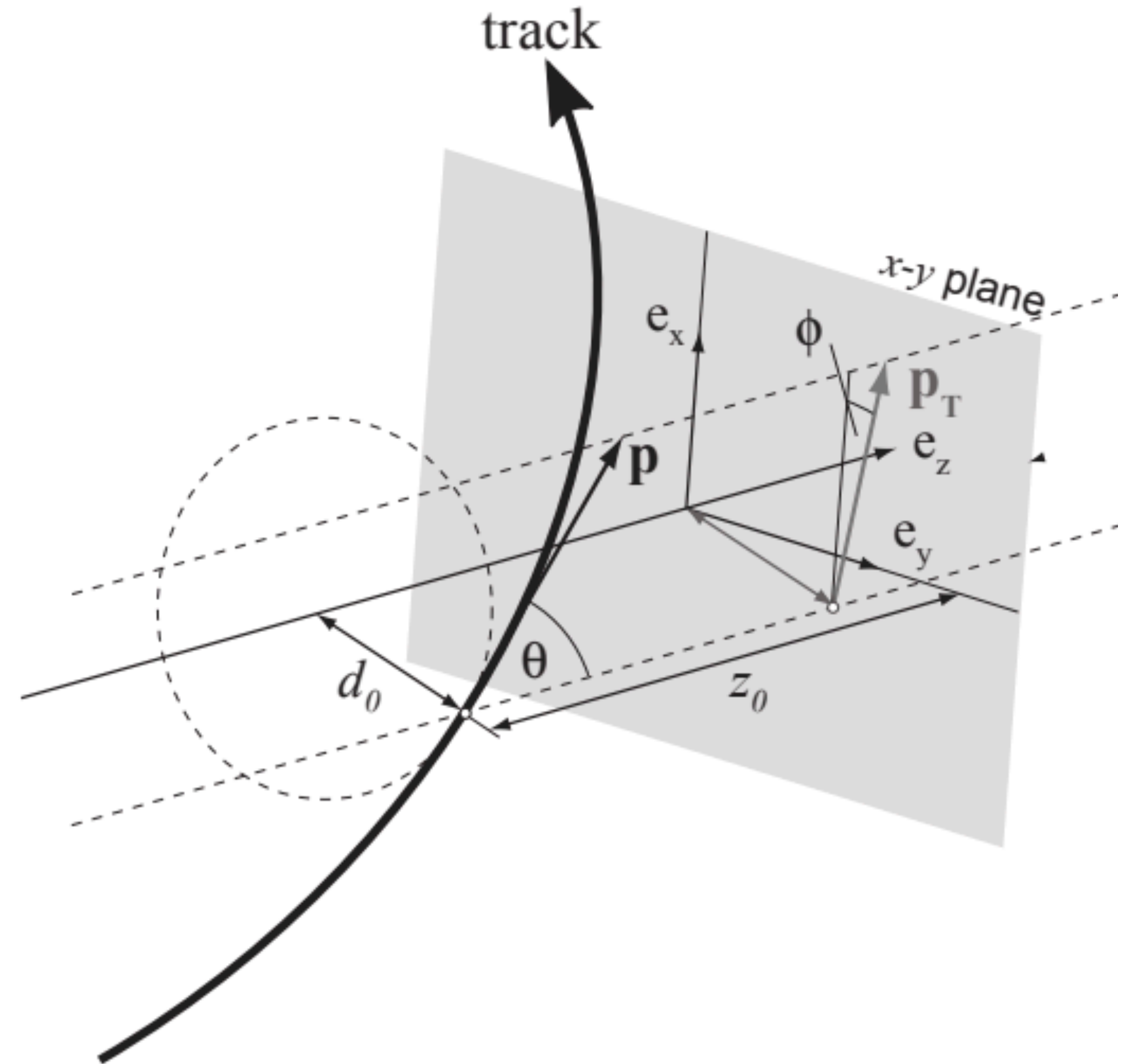
Ld10\_rho20\_pi5\_Zp1500\_I50

Ld20\_rho40\_pi10\_Zp3000\_I50

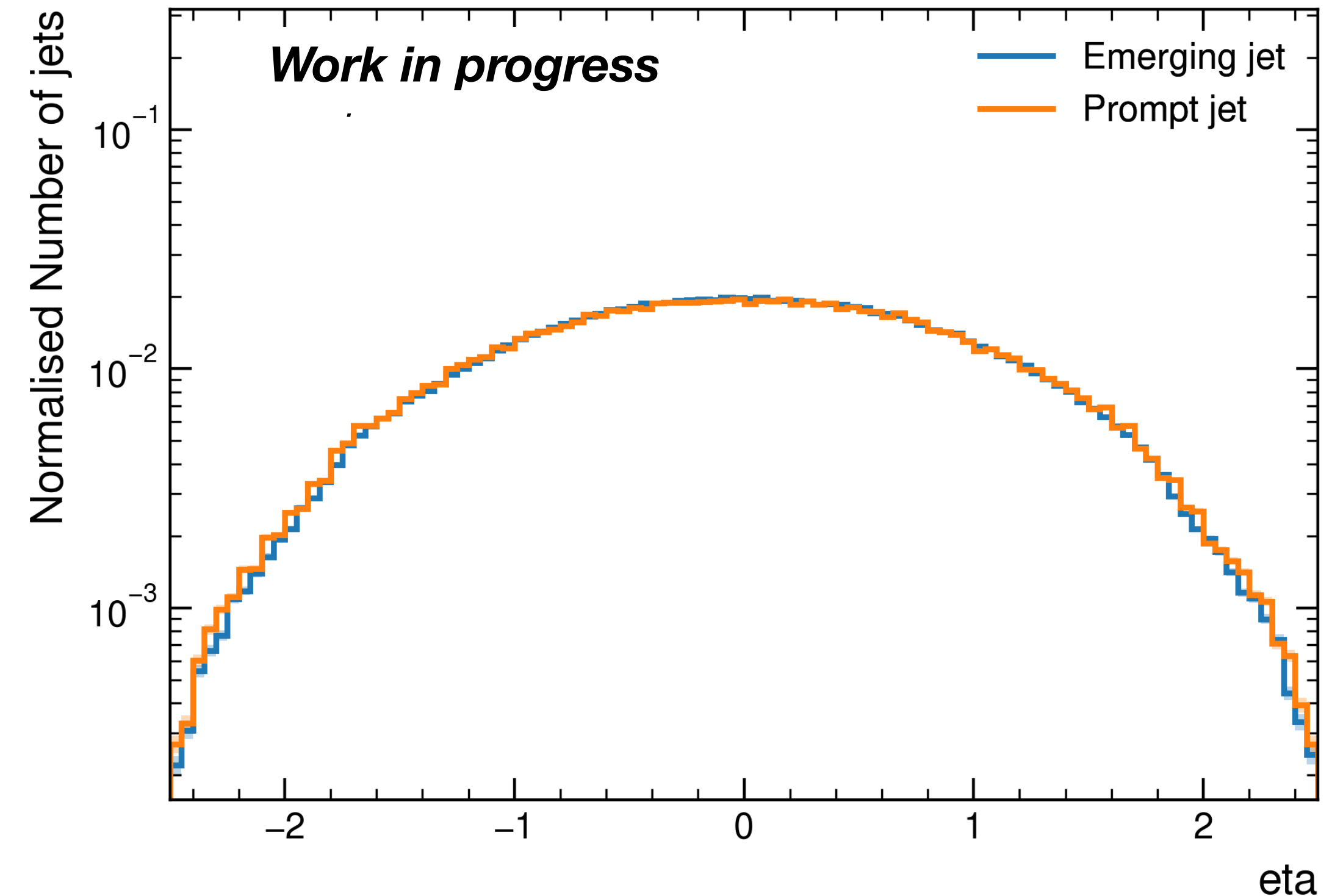
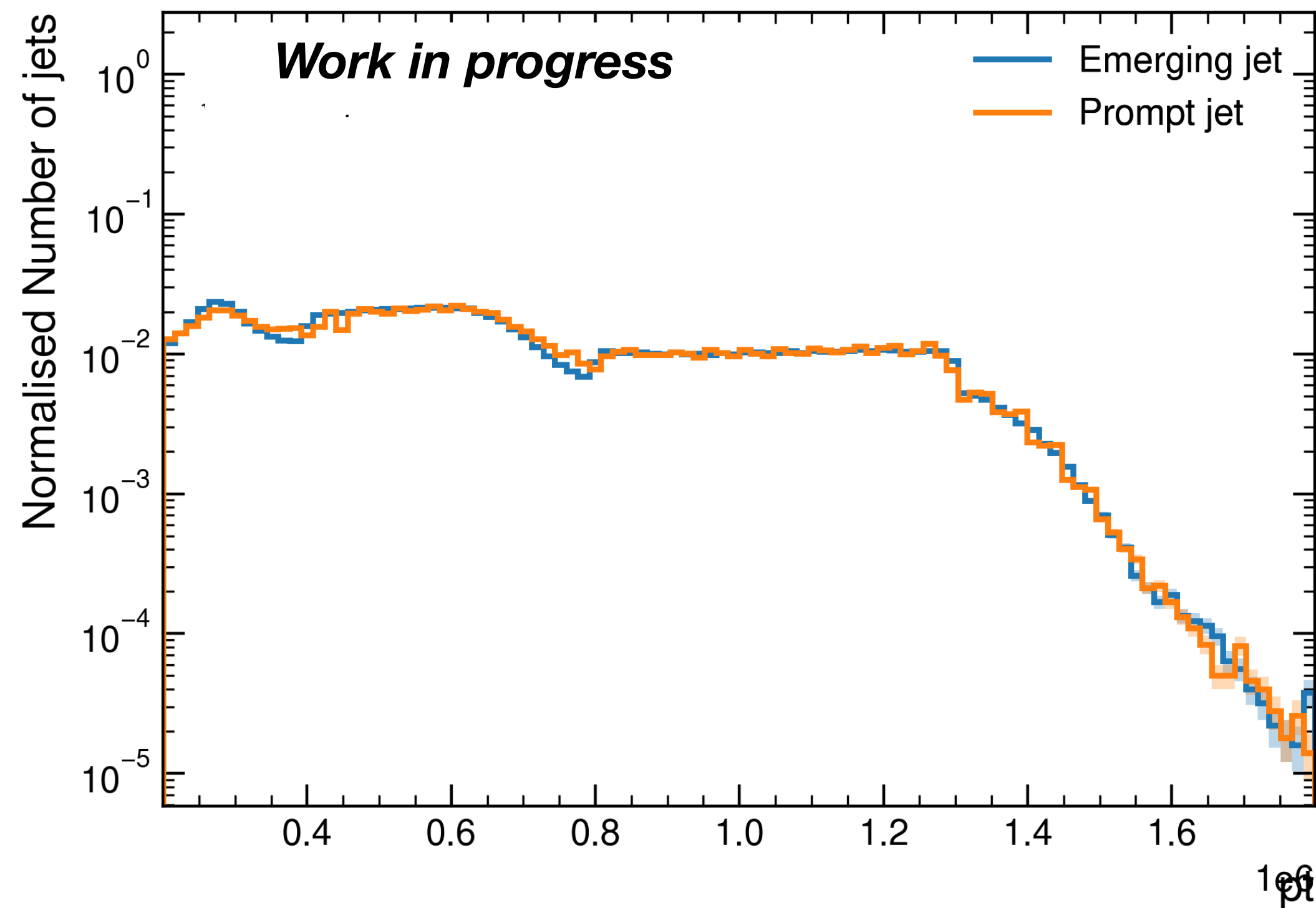
- Ld = dark confinement scale [GeV]
- rho = mass of rho meson [GeV]
- pi = mass of dark pion [GeV]
- Zp = mass of Z' [GeV]
- I = lifetime [mm]

# Jet-Track Inputs

Category	Variable	Description
Jet	$p_T$	Jet transverse momentum
	$\eta$	Signed jet pseudorapidity
Track	$d_0$	Distances of closest approach between the track and beamline in the transverse plane
	$z_0 \sin \theta$	Closest distance from the track to the primary interaction point in the transverse plane
	$d_\phi$	Azimuthal angle of the track, relative to the jet $\phi$
	$d\eta$	Pseudorapidity of the track, relative to the jet $\eta$
	$\frac{q}{p}$	Track charge divided by momentum (measure of curvature)
	$\sigma(\phi)$	Uncertainty on track azimuthal angle $\phi$
	$\sigma(\theta)$	Uncertainty on track polar angle $\theta$
	$\sigma(\frac{q}{p})$	Uncertainty on $\frac{q}{p}$
	nPixHits	Number of pixel hits
	nSCTHits	Number of SCT hits
	nPixShared	Number of shared pixel hits
	nSCTShared	Number of shared SCT hits
	nPixHoles	Number of pixel holes
	nSCTHoles	Number of SCT holes
	IP3D_signed_d0_significance	Ratio of $d_0$ and $\sigma(d_0)$ defined for both positive and negative scale with reference to the primary interaction point.
	IP3D_signed_z0_significance	Ratio of $z_0 \sin(\theta)$ and $\sigma(z_0 \sin(\theta))$ defined for both positive and negative scale with reference to the primary interaction point



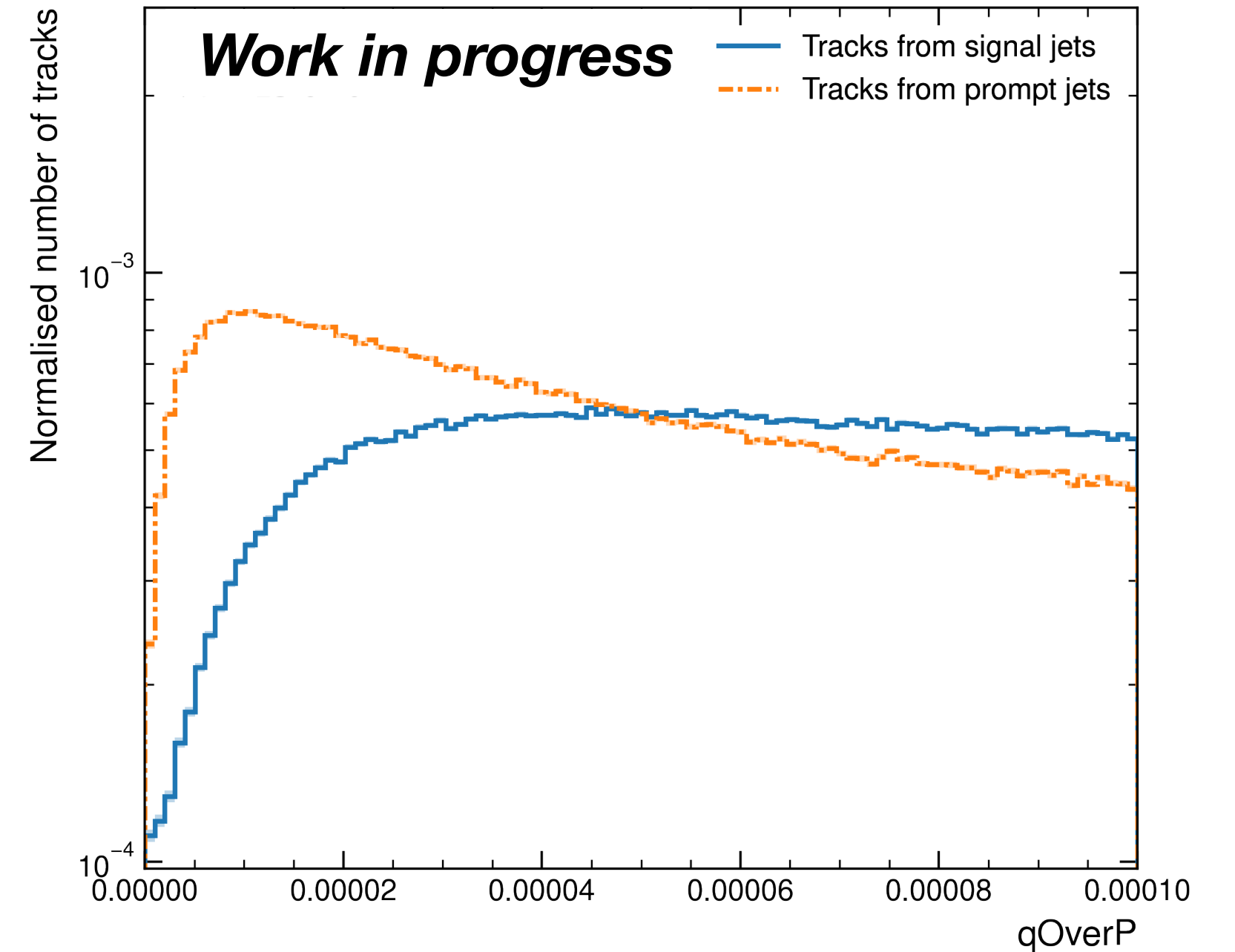
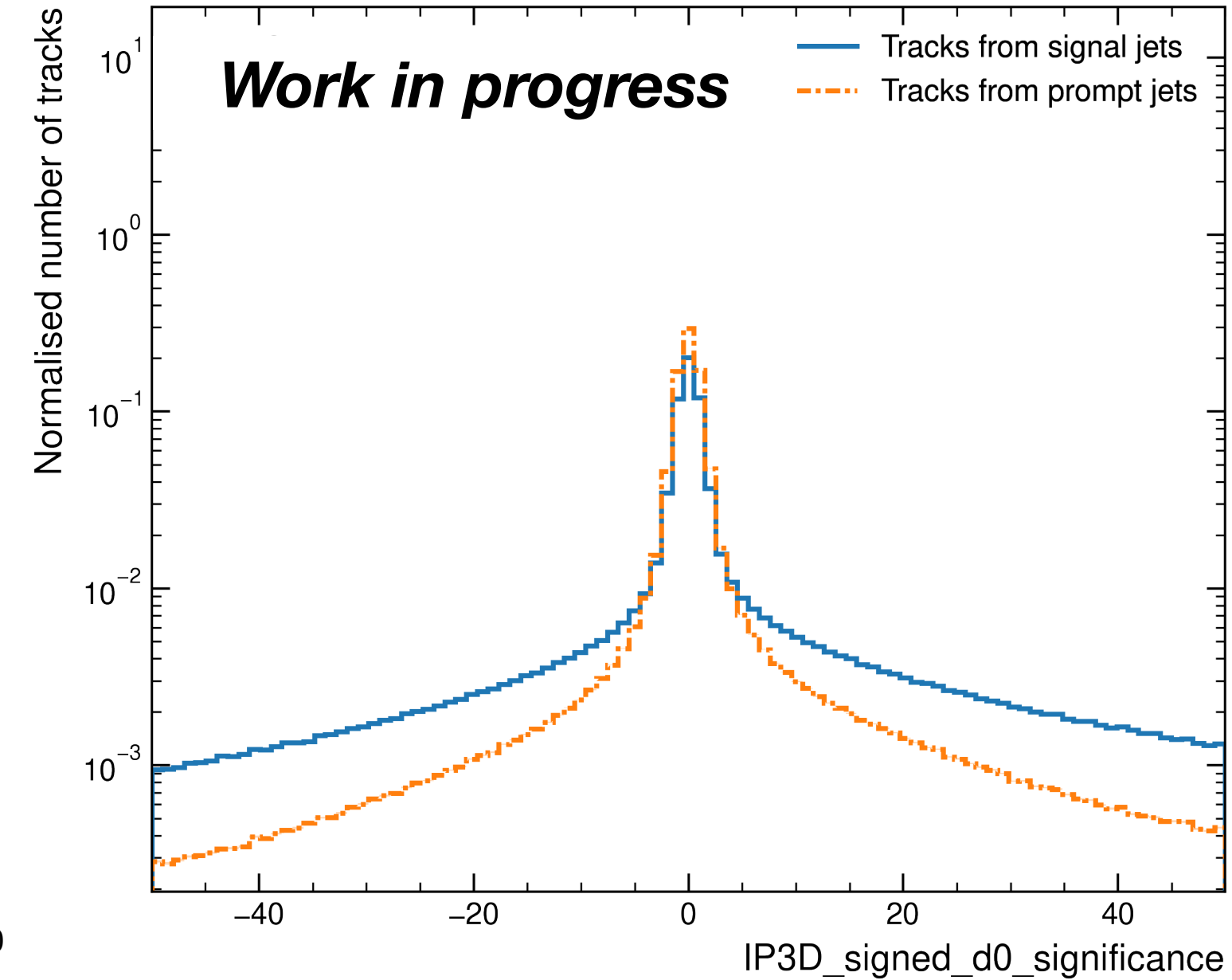
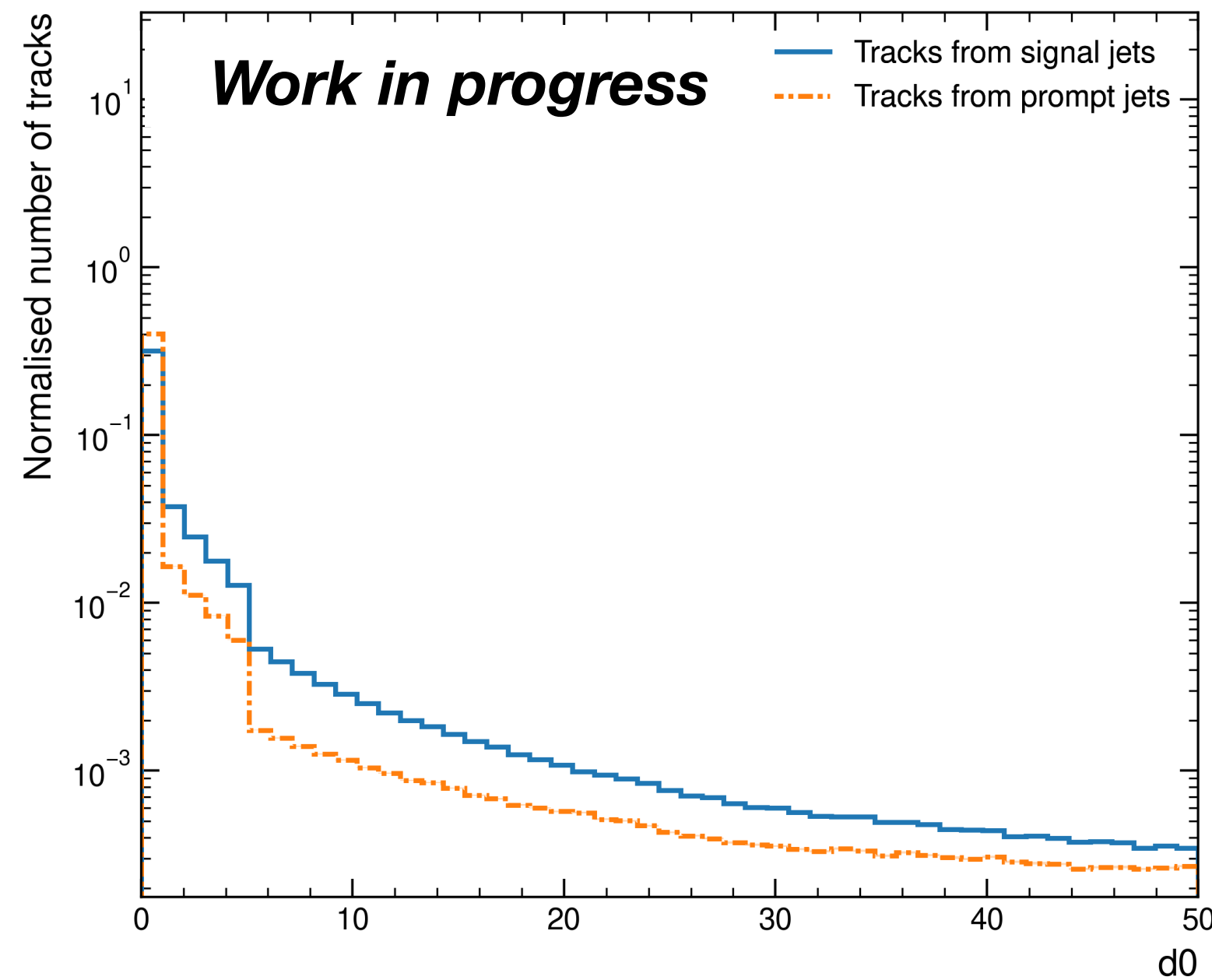
# Input Variables: Jets



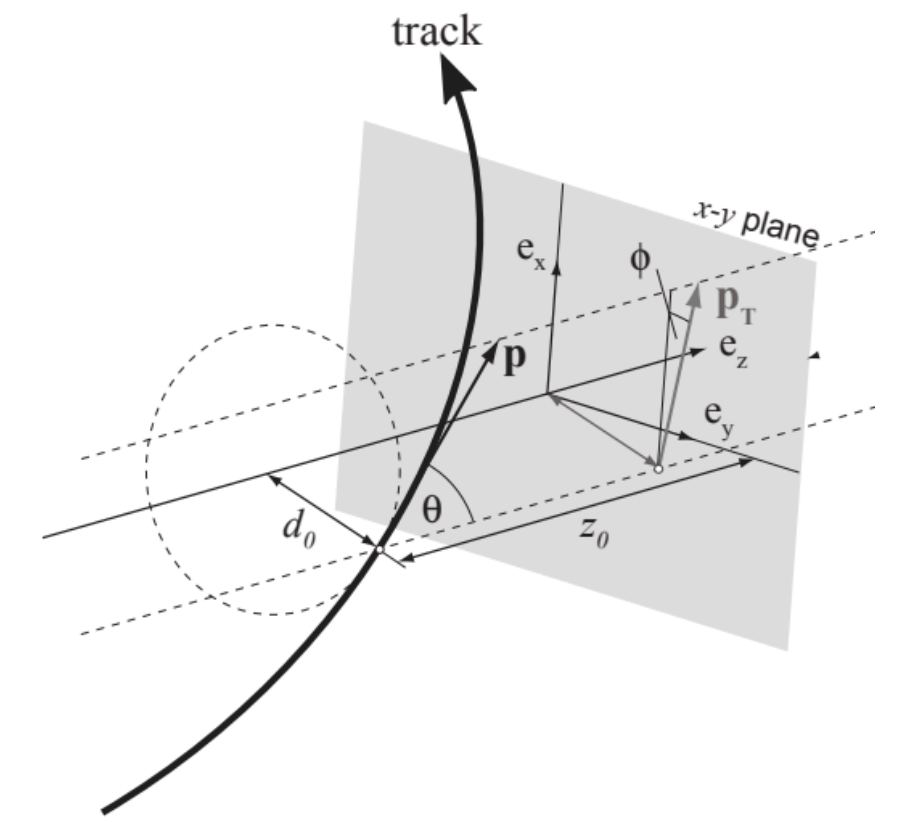
- Two jet variables that constitute the basic kinematics of a jet  $p_T, \eta$
- To avoid avoid kinematic biases for jet tagger, the distributions are “resampled”, i.e ensure uniformity in the kinetic distribution!



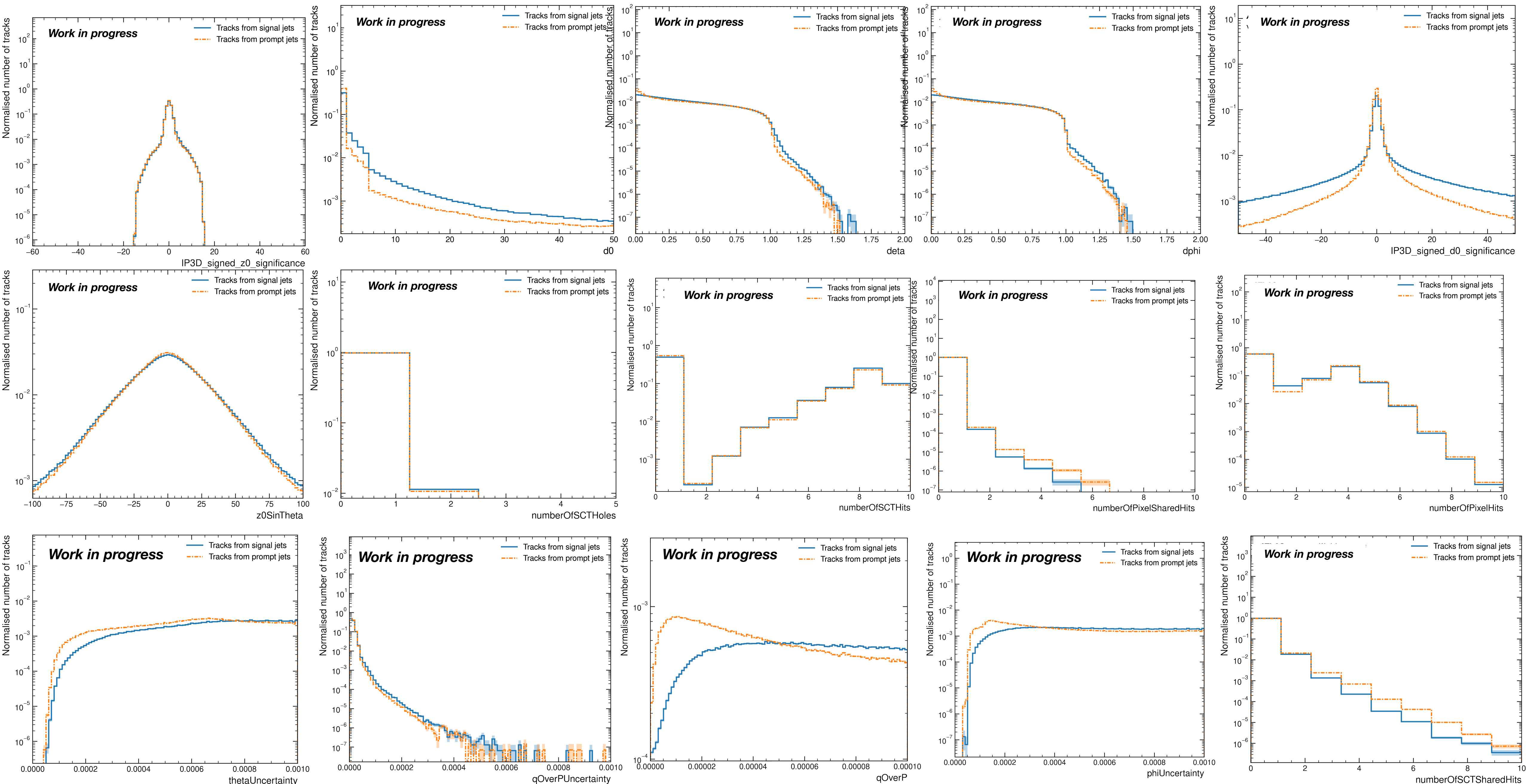
# Input Variables: Tracks



- 16 track variables including track parameters in ATLAS tracking system, detector hits and holes variables, uncertainty in track parameters ... (detailed in backup slides)
- Most discriminating ones include
  - $d_0$ : Distances of closest approach between the track
  - IP3D\_signed\_d0\_significance: Ratio of  $d_0$  and  $\sigma(d_0)$  defined for both positive and negative scale with reference to the primary interaction point of the ATLAS detector
  - $\frac{q}{p}$  Track charge divided by momentum (measure of curvature)



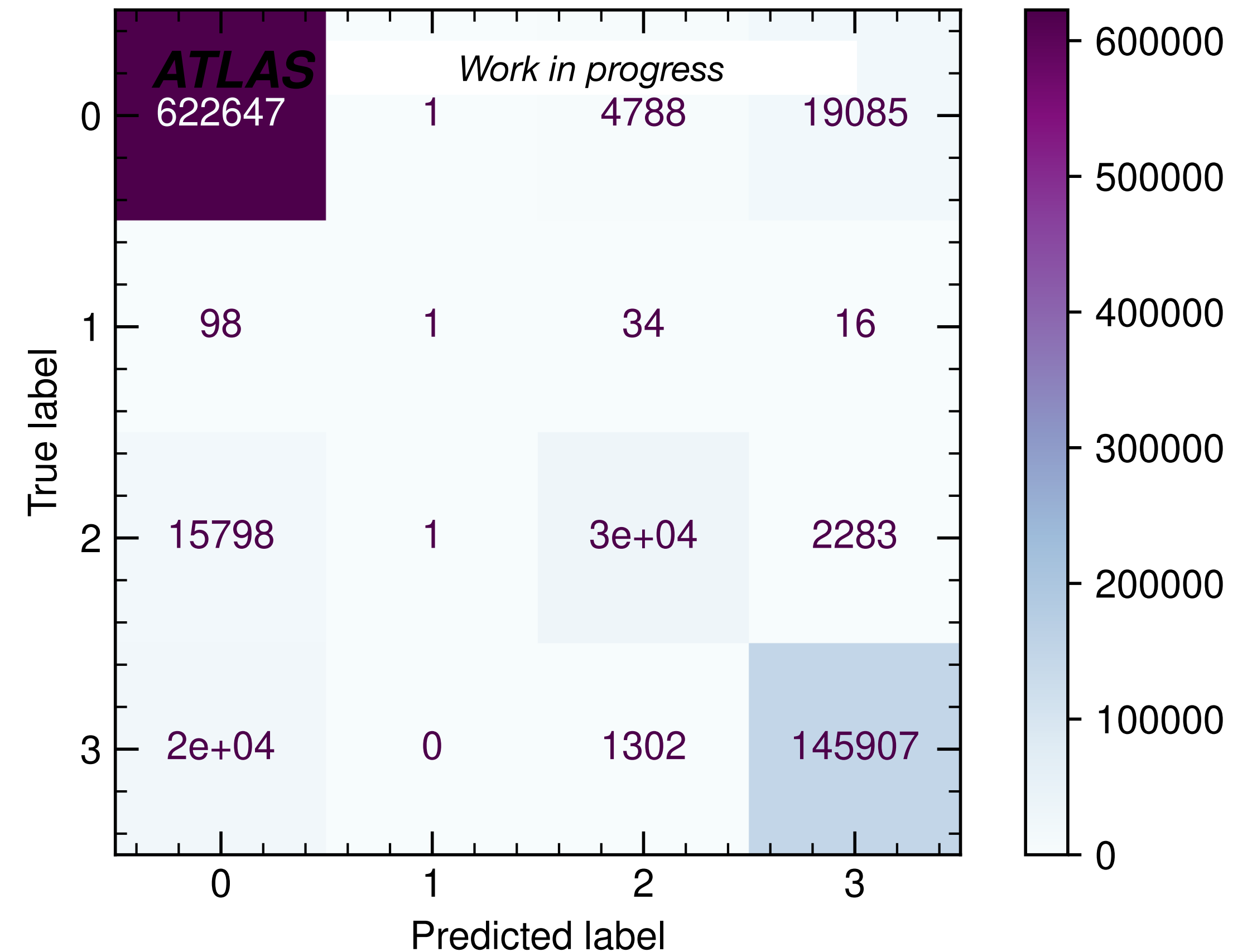
# Input Distribution (Tracks)



# Track Origin Identification: Performance

## Confusion Matrix

- The diagonal elements of the matrix represent correct classification!
- Pileups and Displaced tracks most accurately classified
- ~20k “true” displaced tracks classified as pileups and vice versa!
- ~16k “true” primary tracks classified as pileups

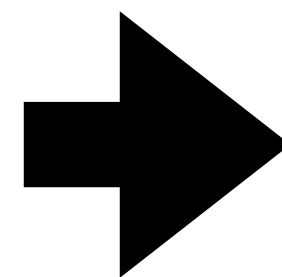


# JetMatrixView

- 40 tracks x 40 tracks confusion matrix
  - Instead of being sorted by trackID's its sorted by truthVertexId of each track
  - For example {TrackId(VertexId)} in a Jet is {2223(1),2224(3),2225(1),2226(2)}

## Track ID Based Sort

	2223	2224	2225	2226
2223	1	0	1	0
2224	0	1	0	0
2225	1	0	1	0
2226	0	0	0	1



## VertexID Based Sort

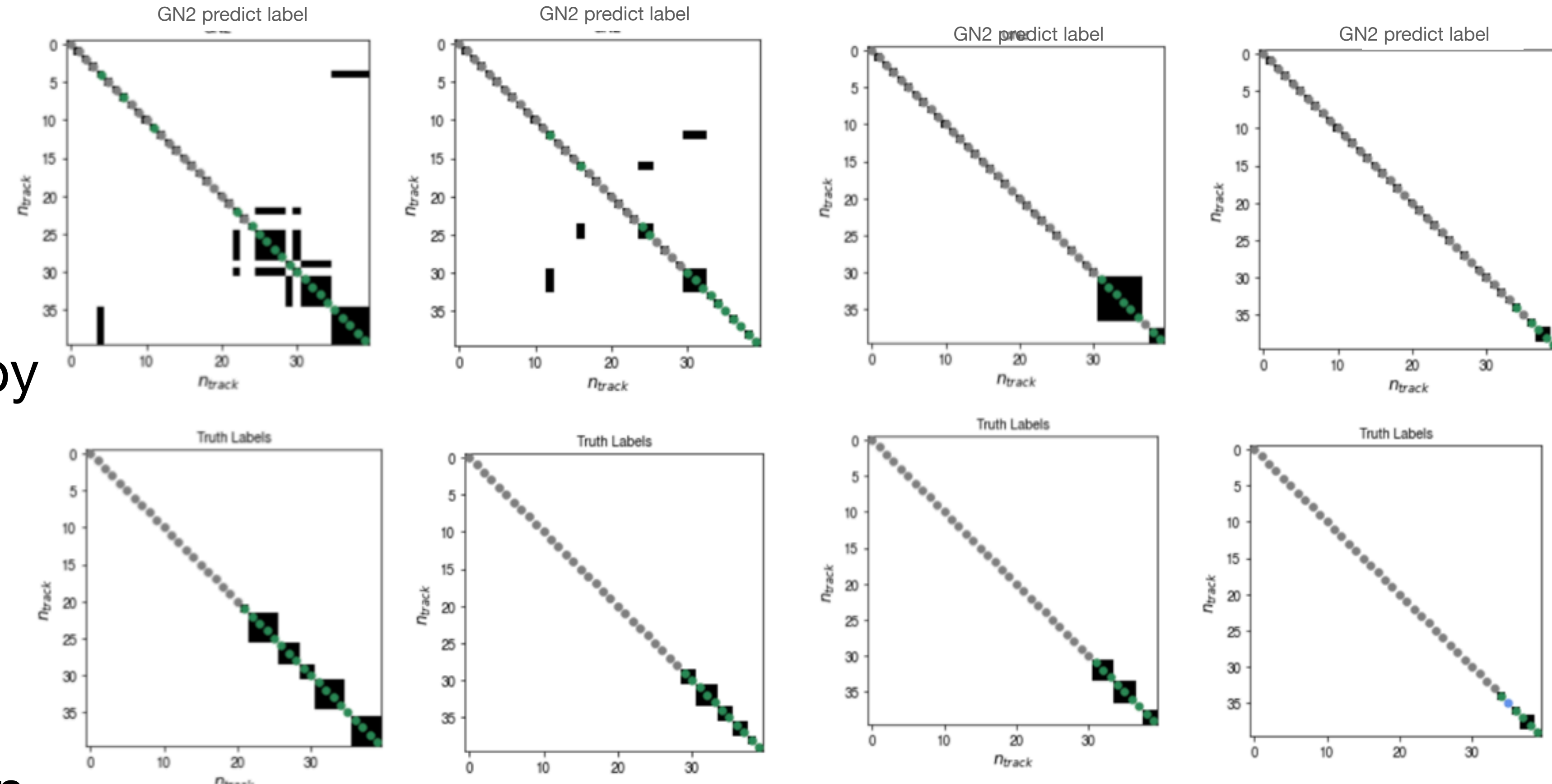
	2223	2225	2226	2224
2223	1	1	0	0
2225	1	1	0	0
2226	0	0	0	0
2224	0	0	0	0

# Jet View from Classifiers!

## Use GNN to classify events?

ATLAS Work in progress

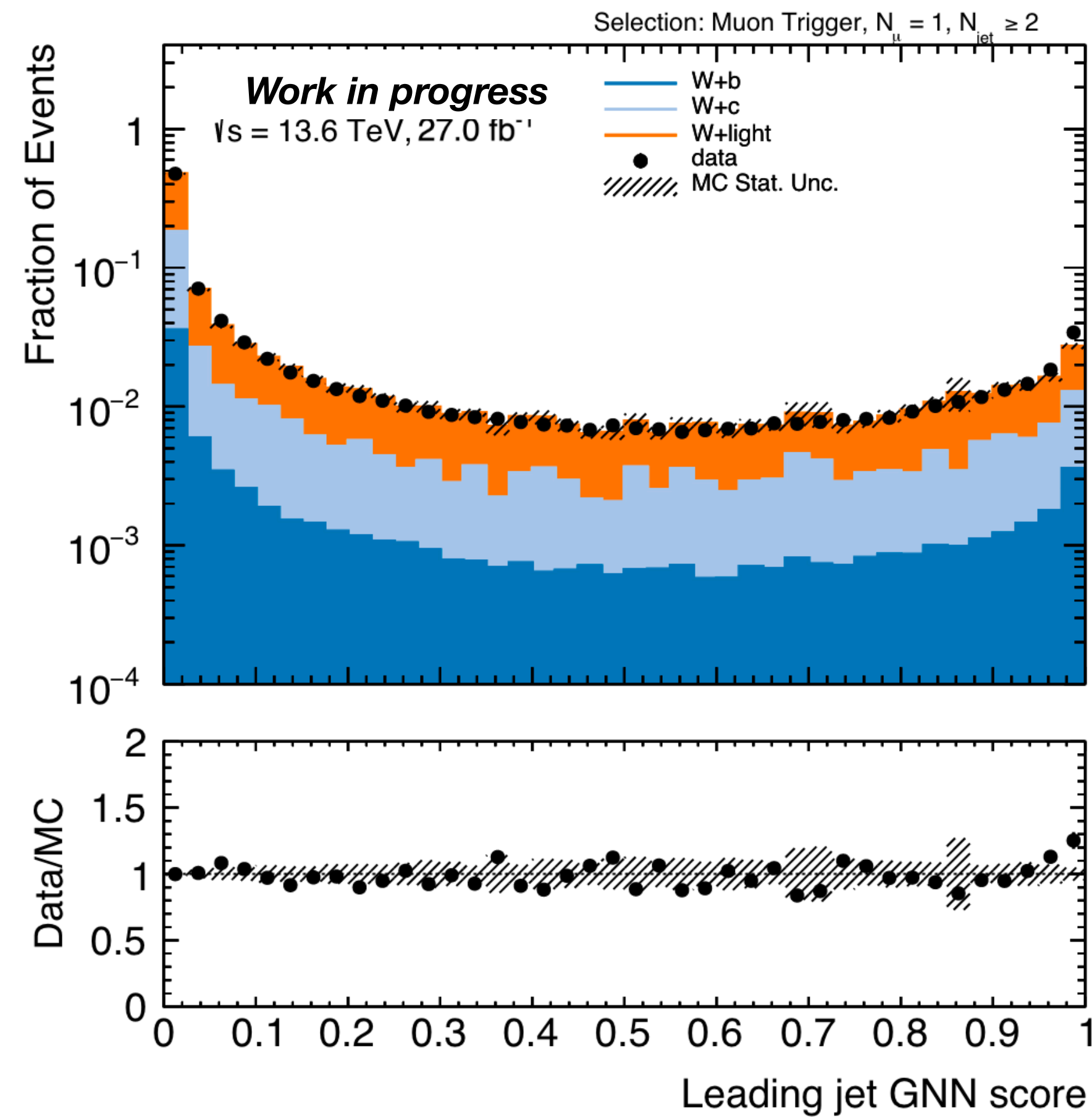
- True labels vs GNN predicted labels visualization for jet, track and vertex prediction
- $n_{trk} \times n_{trk}$  matrix sorted by TruthVertID
  - 1 (Black) if two tracks share the same vertex
  - 0 (White) if two tracks do not share a common vertex



### Track Labels

- Pileup ●
- Fake ●
- Primary ●
- Displaced ●

# GNN Validation



- First looks at 2022 data validate GNN performance on real data!