Framing secondary vertexing as a clustering problem: First results with Point Cloud and HyperGraph

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STAR Sensing and Sensibility
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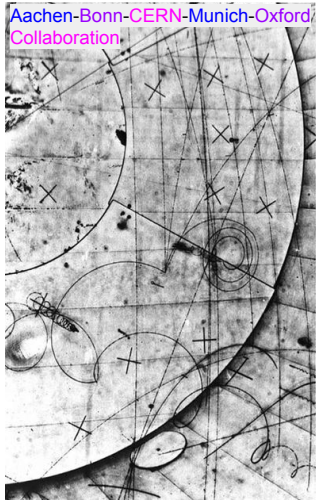
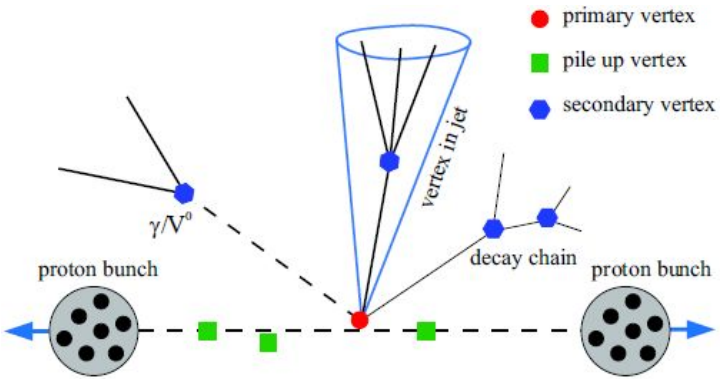
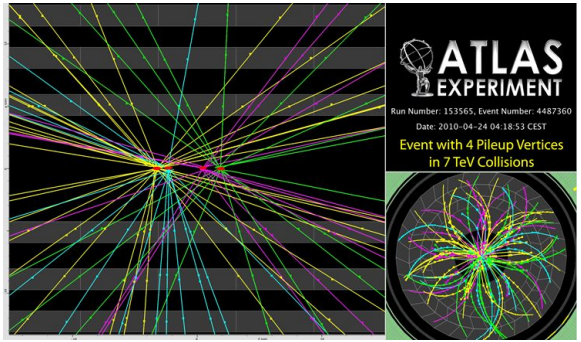
Vertexing and the HL–LHC

- Vertexing: Reconstructing particle interaction or decay points.
  - ➢ Crucial for identifying primary and secondary vertices.
  - ➢ Essential for flavor tagging (b/c quarks) and LLP searches.
- HL–LHC: Significant luminosity increase for precision studies.
  - ➢ Increased luminosity = increased challenges for vertexing.
  - ➢ Dramatic rise in pile-up (140-200 collisions/bunch crossing).



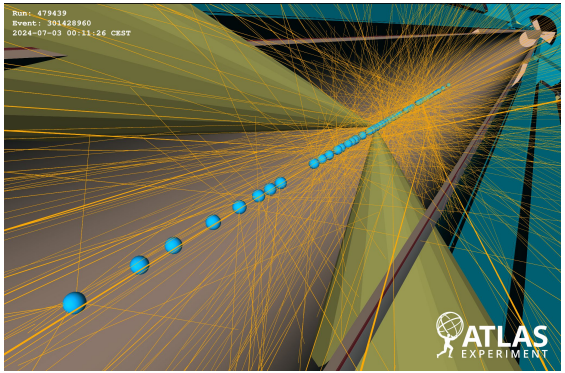


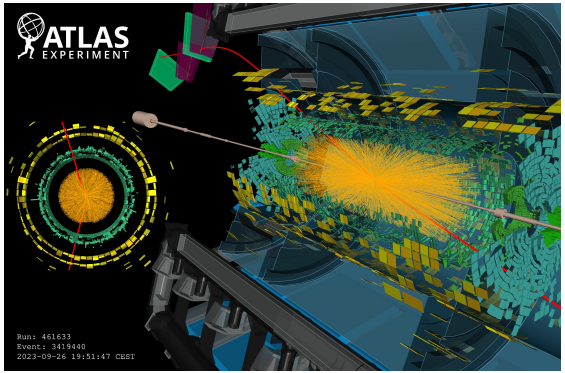


Vertexing in high luminosity environment

- The primary challenge: Pile-Up
  - ➢ Increased vertex density along the beamline.
  - ➢ Distinguishing hard scatter vertex from pile-up.

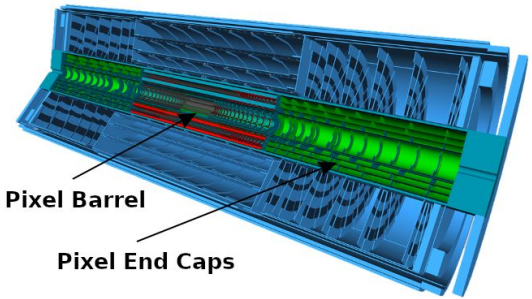
  } PV
  - ➢ Track-vertex association becomes highly complex.
  - ➢ Merged and split vertex errors.
- Impact of Increased Track Density
  - ➢ Makes any kind of pattern recognition challenging.
  - ➢ Increased combinatorial complexity of vertex finding.
  - ➢ Potential for ghost tracks and fake vertices.



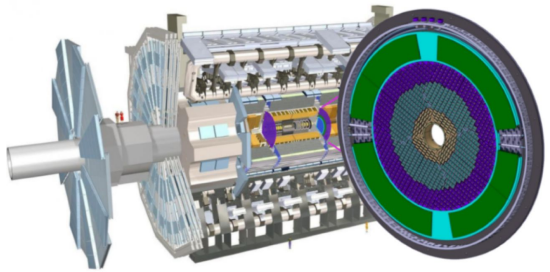


Maintaining and enhancing vertexing precision

- Importance of impact parameter and spatial resolution.
  - ➢ ATLAS Inner Tracker (ITk): increased granularity.
- Leveraging time information (4D-vertexing).
  - ➢ ATLAS HGTD and CMS MTD: precise timing information.



ATLAS ITk



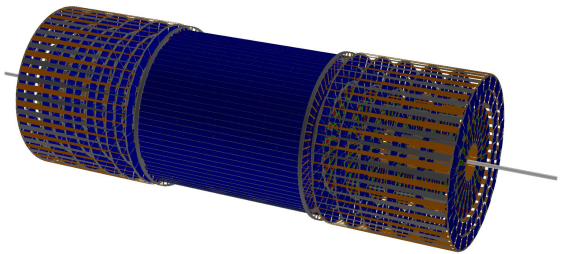
ATLAS HGTD

ACTS: *A Common Tracking Software*

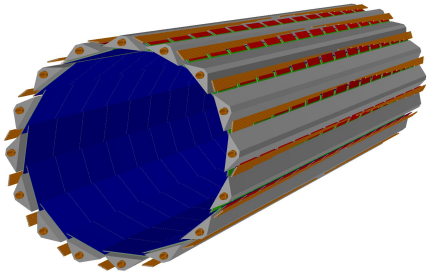
- Evolved from *ATLAS Common Tracking Software*
- Key Features:
  - ➢ Flexible tracking geometry description.
  - ➢ Simple and efficient event data model.
  - ➢ Algorithms for seed finding, track propagation, track fitting and primary vertexing.
- Designed in modern C++ (C++17/20): emphasis on parallel execution.
- Existing primary vertexing algorithms in ACTS:
  - ➢ Iterative Vertex Finder (IVF)
  - ➢ Adaptive Multi-Vertex Finder (AMVF)

ODD: Open Data Detector

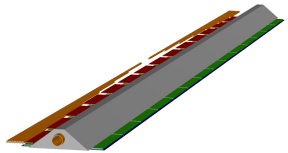
- Designed for algorithm research and development.
  - ➢ Based on the detector used in the TrackML challenge.
  - ➢ Provides a template for an HL-LHC detector, inspired by ATLAS Inner Tracker (ITk) upgrade.
- ODD serves as a crucial platform for testing and benchmarking ACTS track reconstruction algorithms. It provides a full reconstruction chain.
  - ➢ We extend the ACTS+ODD ecosystem for our secondary vertexing research for HL-LHC.



The full Open Data Detector



Innermost layer (r = 36 mm)



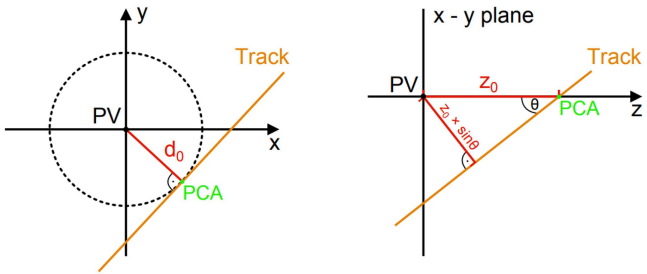
A single stave

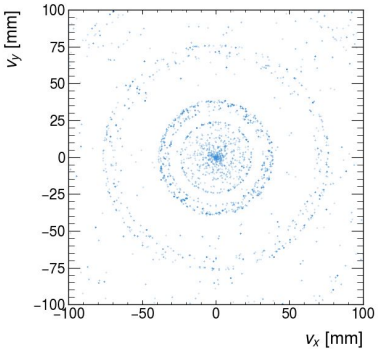
Preparation of synthetic dataset

- Inside the ACTS toolkit, the $pp \rightarrow t\bar{t}$ process is generated using Pythia 8.
- Full Geant4 simulation of the OpenDataDetector geometry.
- The value of **pile-up** is chosen to be **200**.
- Built-in track and vertex reconstruction is performed after simulation.
- Each event takes around ~ 5 minutes, for gen+sim+reco.

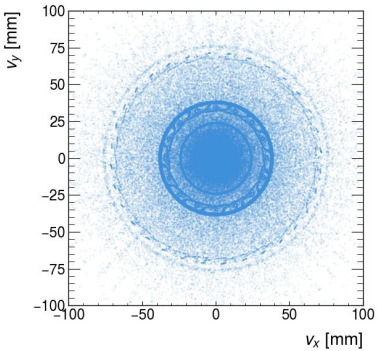
Hadronic interactions in ODD

- Secondary vertex finding should work in the presence of material interaction between hadrons and detector layers.
- To enhance the number of tracks originating from such interactions, the ODD sim+reco chain has been modified:
  - ➢ `SeedFinderConfig`
    - d_0 : 5 mm→20 mm
  - ➢ `ParticleSelectorConfig`
    - ρ : 24 mm→1000 mm





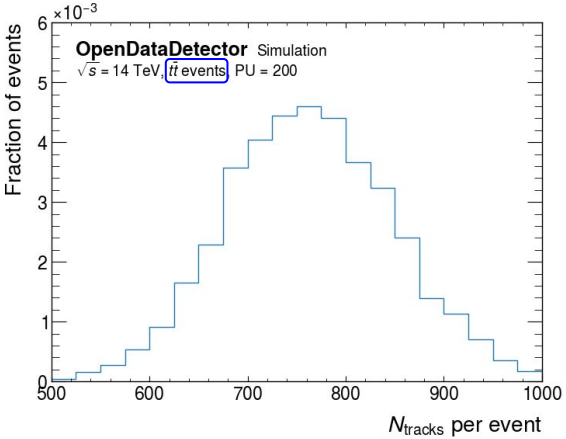
From simulated particles

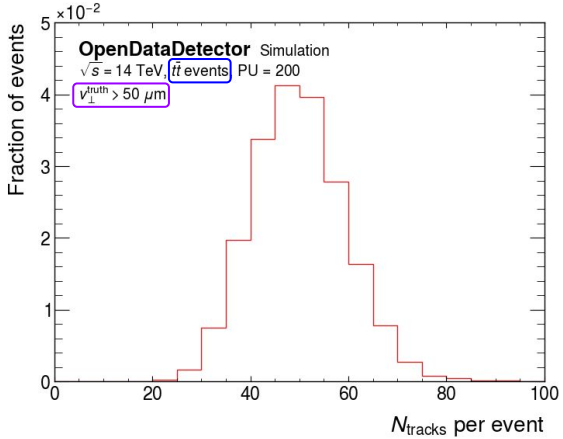


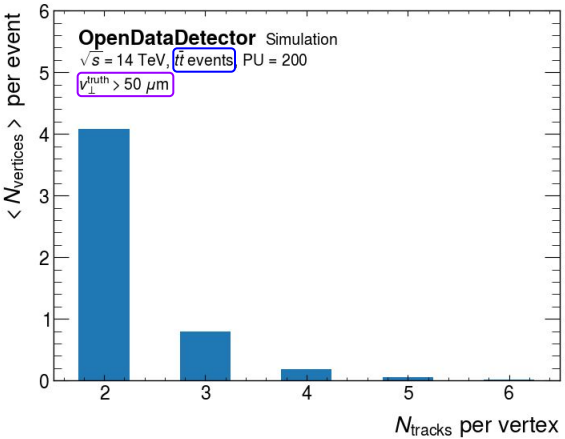
From reconstructed particles

ρ refers to the maximum radial distance in the cylindrical coordinate system.

Understanding the ODD dataset





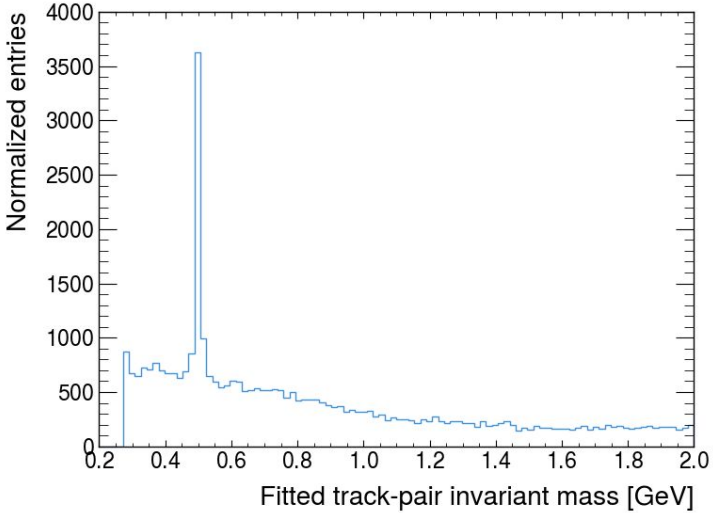


- Average number per event:
  - ➢ Total tracks: ~750
    - For the training dataset, only events with ≤ 1000 tracks have been selected.
  - ➢ Non-prompt tracks: ~50
  - ➢ ~4 two-track vertices and 1-2 multi-track vertices.

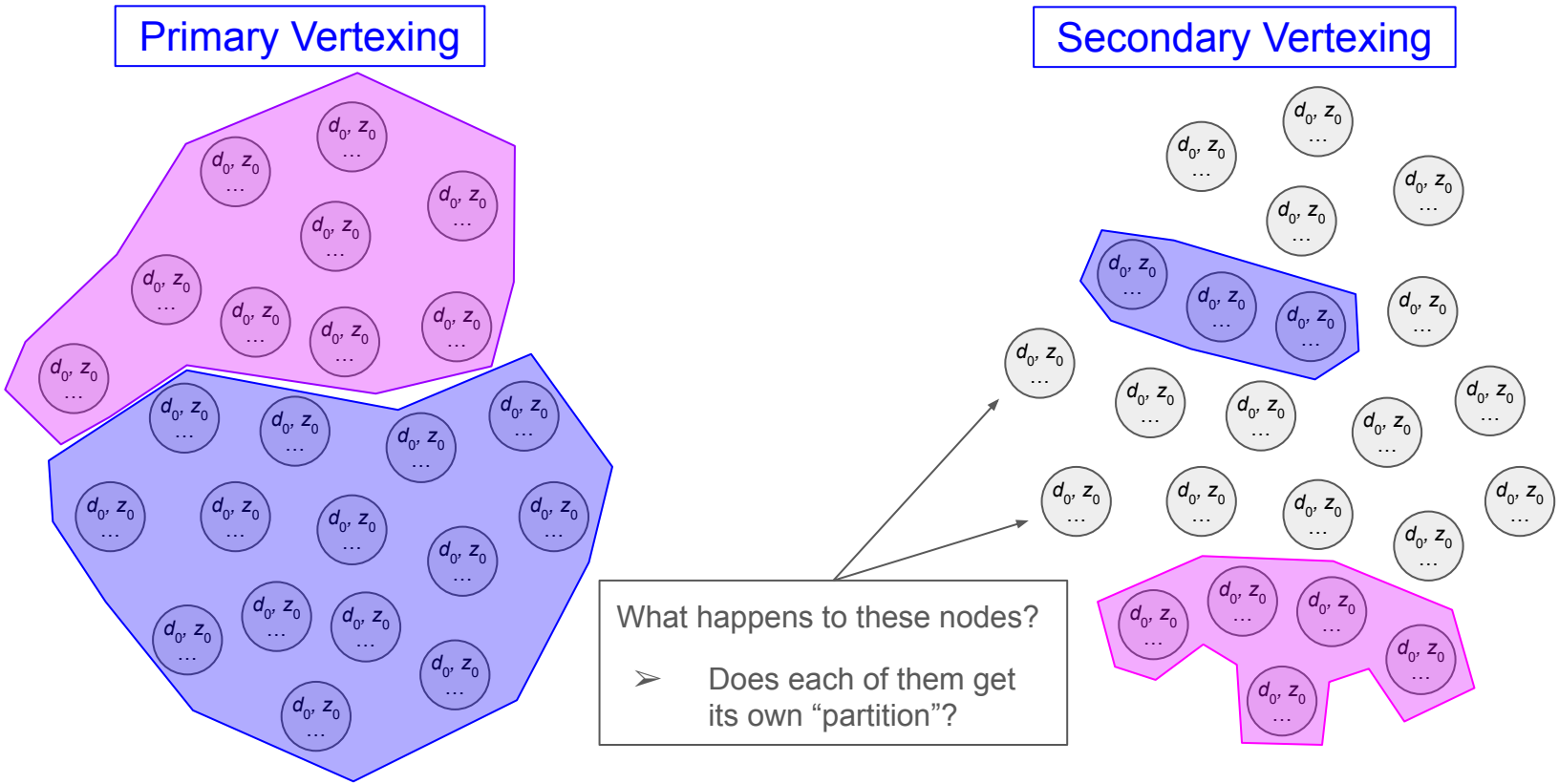
Calculating track-pair compatibility matrix

Billoir fit can be performed between each pair of tracks:

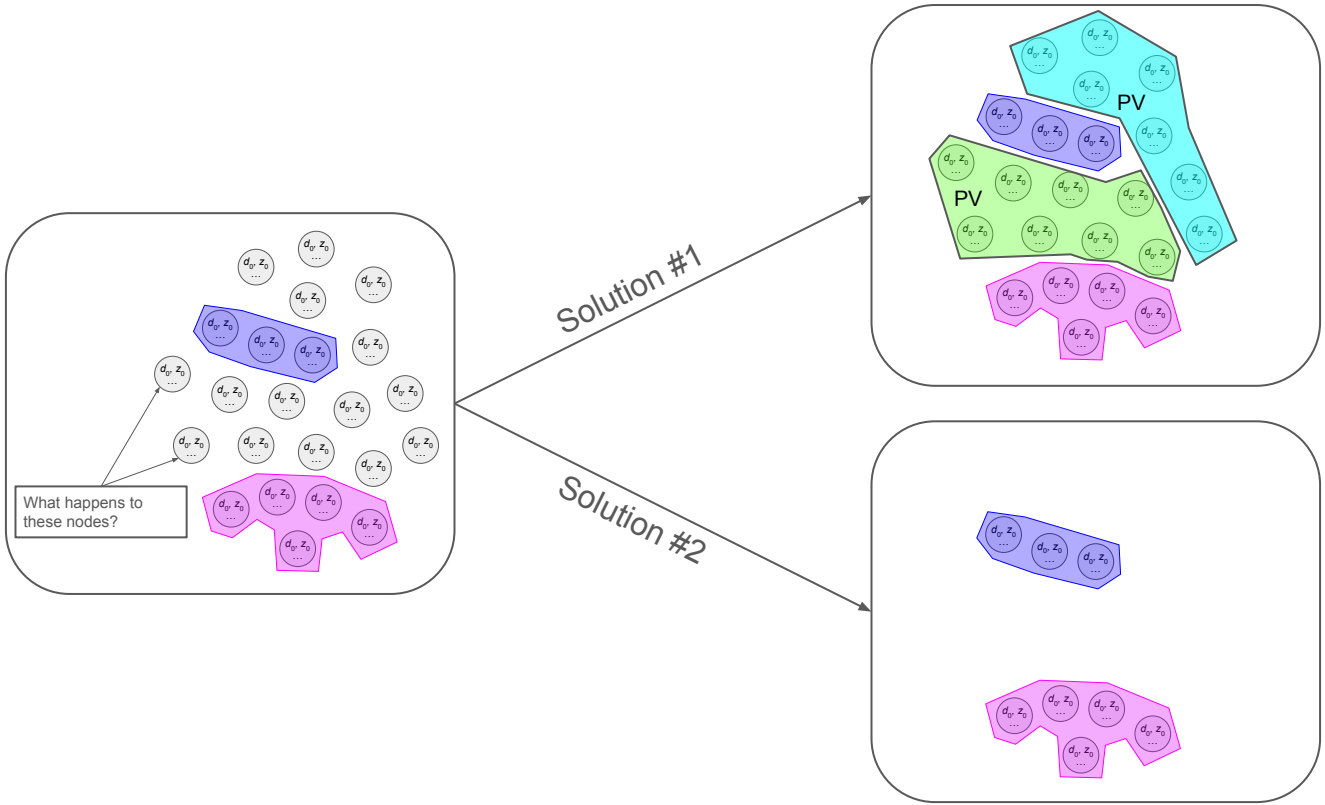
- 5 parameters from each fitted track, along with their (co)-variances, are used: d_0, z_0, ϕ, θ, q/p.
- The primary vertex has been chosen at (0,0,0), with a very large uncertainty in its z-coordinate.
- The fit returns the vertex position, mass, and χ^2 as a measure of the goodness of fit.



Framing Vertex finding as a graph partitioning problem



SV finding is not really a graph partitioning problem



Perform PV and SV finding simultaneously

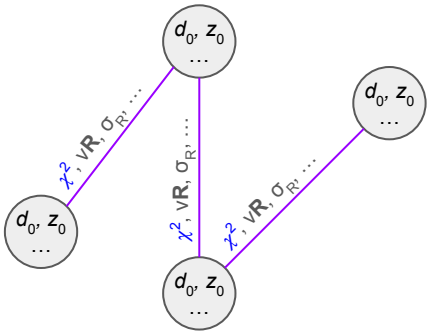
Get rid of the isolated nodes, *possibly in a soft way*

Framing vertex finding as a clustering problem

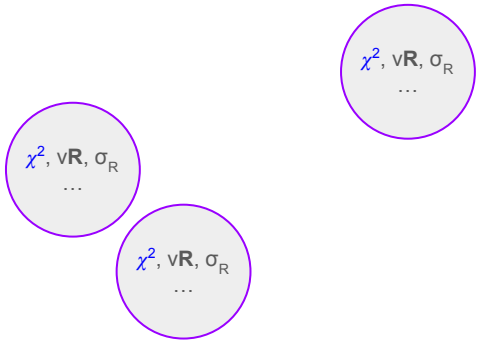
- Most obvious approach: A vertex is a cluster of **tracks**.
  - ➢ Consider the tracks as nodes.
    - Track params are node features.
    - Different quantities from track-pair Billoir fit can be taken as edge features.
  - ➢ This is the chosen strategy for MaskFormer as well as the previous primary-vertexing work.
- Alternate approach: A vertex is a cluster of one or more **two-track vertices**.
  - ➢ Each track-pair satisfying **Billoir fit** is a node (in a Point Cloud).
    - Different quantities from track-pair Billoir fit are node features.
    - No edge feature. The Euclidean distance might be taken as one.
  - ➢ Immediately offers us a bounding box heuristic.
  - ➢ For two-track vertices, the performance is guaranteed to be at least as good as Billoir fit.
  - ➢ Trivial to implement using `sklearn.cluster.DBSCAN` to establish a baseline.
    - Useable with better clustering techniques (e.g. lifted multicut* graph partitioning)

* Margret Keuper, Evgeny Levinkov, Nicolas Bonneel, Guillaume Lavoue, Thomas Brox, Bjorn Andres; *Efficient Decomposition of Image and Mesh Graphs by Lifted Multicuts*; Proceedings of the IEEE International Conference on Computer Vision (ICCV), 2015, pp. 1751-1759

Framing vertex finding as a clustering problem

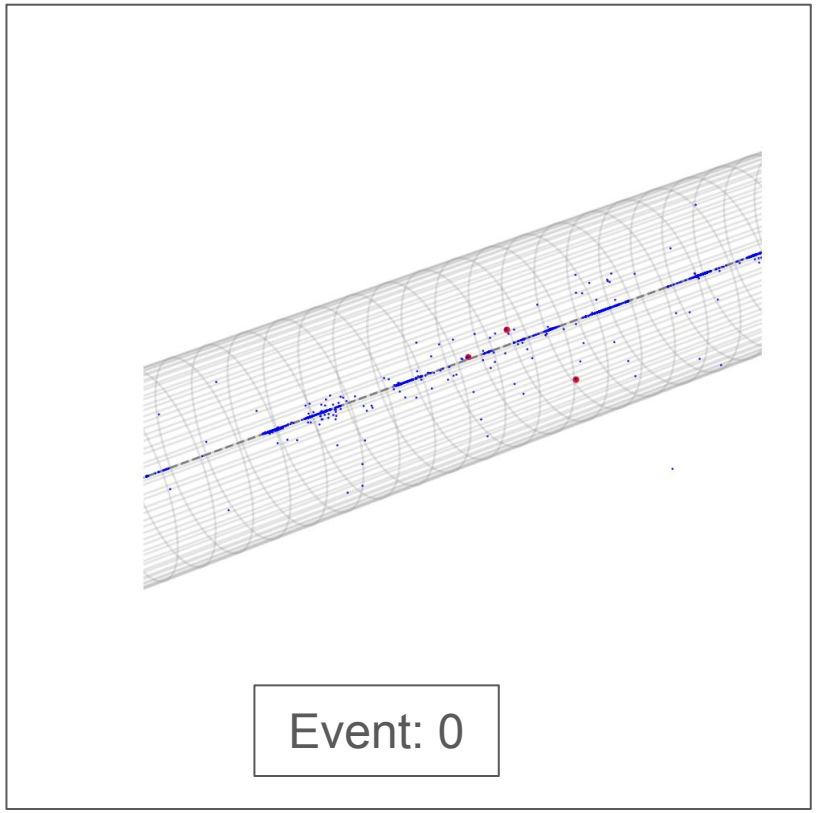


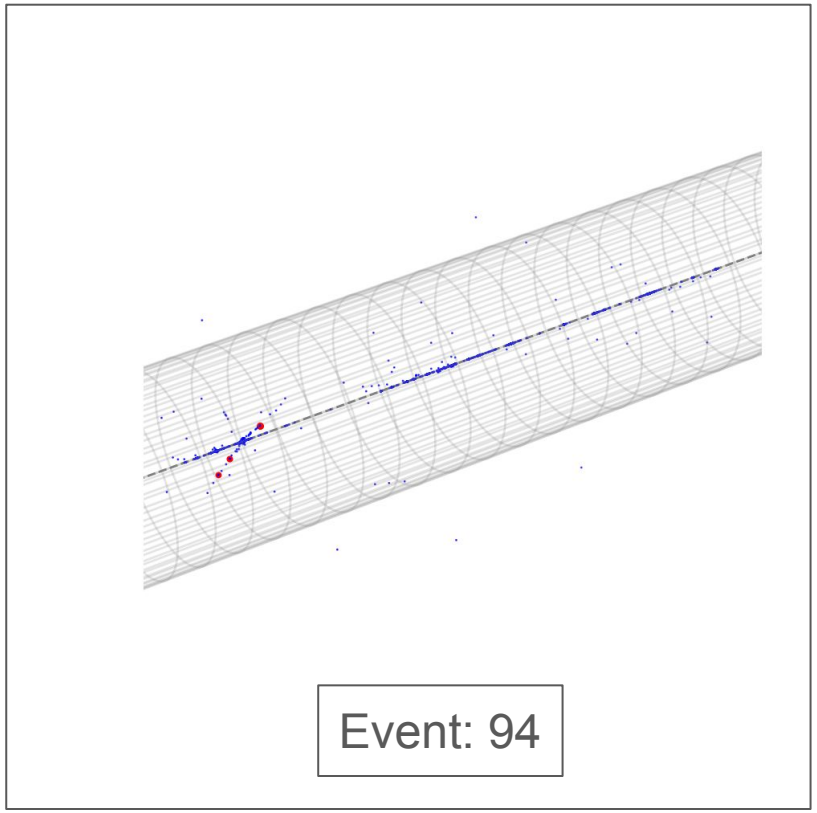
- Each track is a node.
- Each edge is a two-track vertex from Billoir fit.



- Each node is a two-track vertex from Billoir fit.
- Point Cloud based on v**R**.

Visualizing vertices clusters in ODD

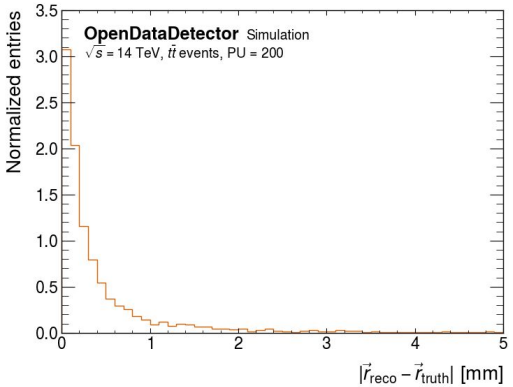


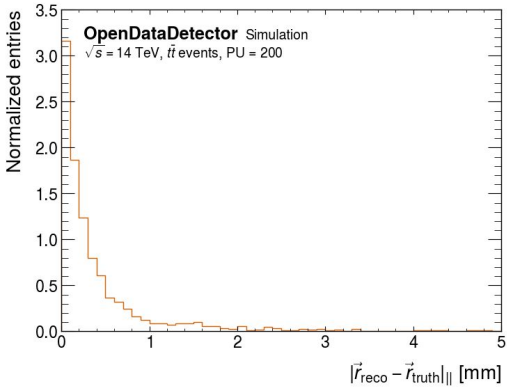


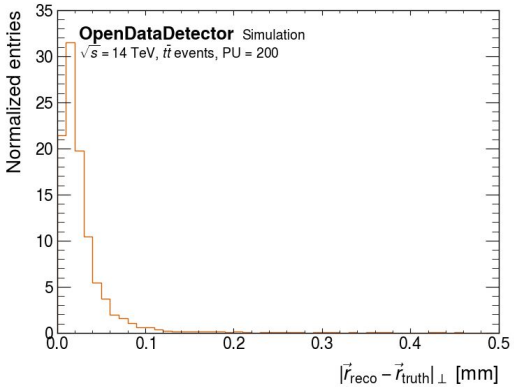
Performance metric for vertex finding

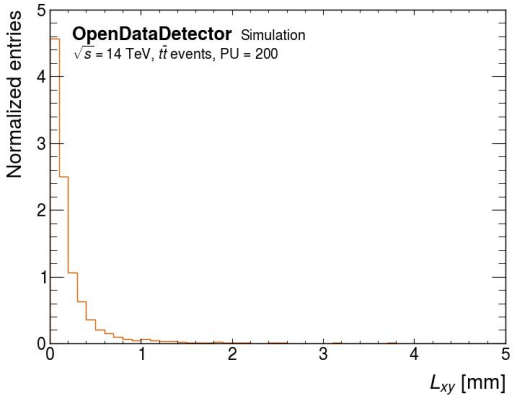
- Strategy for truth-matching:
  - ➢ At least 50% of the tracks from a truth vertex need to be associated with the reco vertex.
  - ➢ If multiple truth vertices match with a single reco vertex, the one with higher number of *common* tracks is chosen.
    - ■ If ambiguity still persists, the one closest to the cluster-centre is chosen.
- For measuring the performance of the clustering method:
  - ➢ Only the truth vertices with 3 or more tracks have been considered.
    - ■ The fraction of such vertices matched with a reco one is a metric for clustering.
- For measuring the performance of “Billoir fast vertex fit” itself:
  - ➢ Only the two-track truth vertices have been considered.
    - ■ For truth matching, **both** tracks are required to be associated with the reco one.

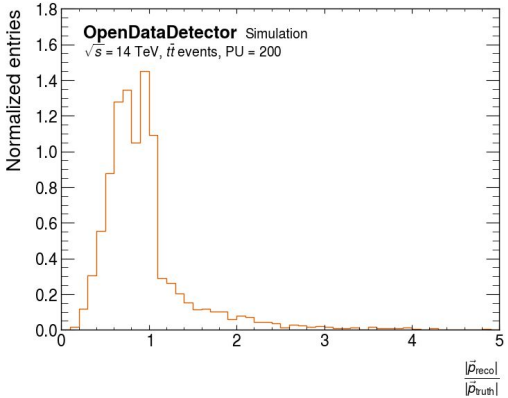
Performance of Point Cloud clustering







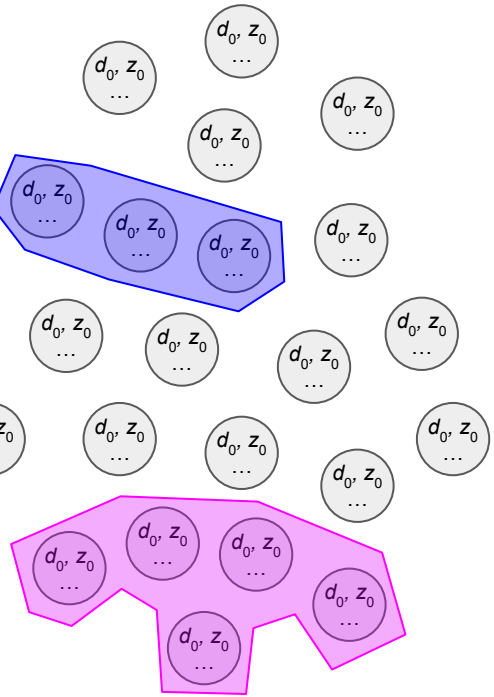




From Point Cloud to HyperGraph

- Point Clouds (of two-track vertices) are nice for Physical intuition, providing a simple bounding-box heuristic enabling us to use any clustering method.
- But they have a significant caveat: Individual track features are lost!
  - ➢ No way to improve upon Billoir fit for estimating track-pair compatibility.
    - Theoretically one can append the features of the two tracks to the vertex-level features.
      - But this looks like more like a hack (might work nevertheless).
- Let's try to find some alternative way to represent the problem.
  - ➢ Hypergraph: Generalization of graph, but with hyperedges.
    - Hyperedge: Generalization of edge, connecting two or more nodes.
      - Secondary vertices can be represented as hyperedges.

From Graph (of tracks) to HyperGraph



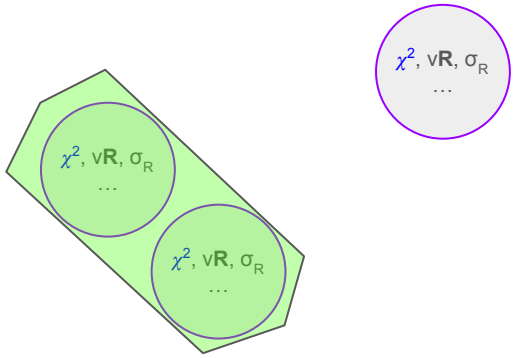
What happens to these nodes?

- Does each of them get its own “partition”?

This issue disappears as soon as we frame it as a **HyperEdge prediction** problem:

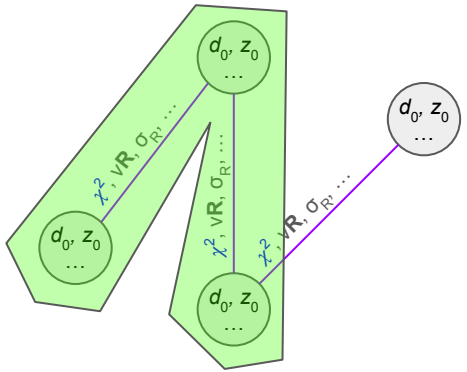
- A hyperedge can connect any number of nodes.
- A node can belong to multiple hyperedges.
- There can be isolated nodes.

From Point Cloud to HyperGraph



Combine two nodes to form a “cluster”.

➢ Using some node feature(s), e.g. v**R**.

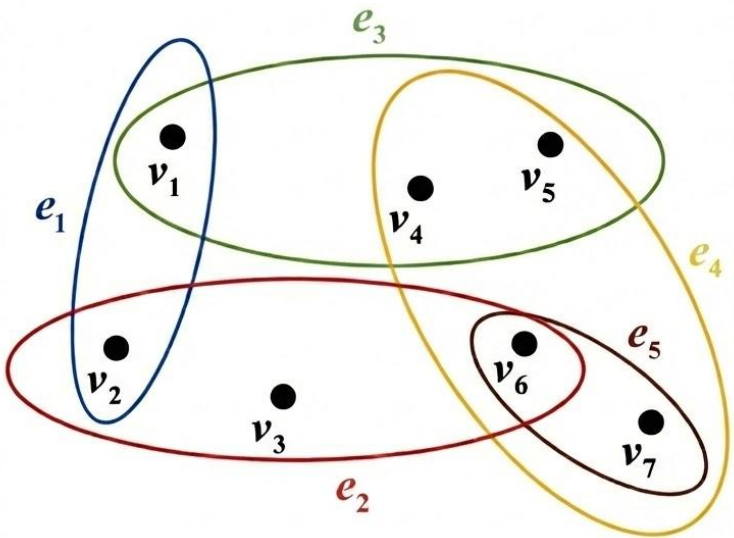


Combine two edges to form a HyperEdge.

➢ Using some edge feature(s), e.g. v**R**.

v**R** refers to the position of the fitted two-track vertex in the 3D space.

HyperGraph representation: Incidence matrix



	e_1	e_2	e_3	e_5
v_1	1	0	1	0
v_2	1	1	0	0
v_3	0	1	0	0
v_4	0	0	1	0
v_5	0	0	1	0
v_6	0	1	0	1
v_7	0	0	0	1

H

Incidence matrix

	d_0	z_0	θ	ϕ	q/p
v_1					
v_2					
v_3					
v_4					
v_5					
v_6					
v_7					

X

Features matrix

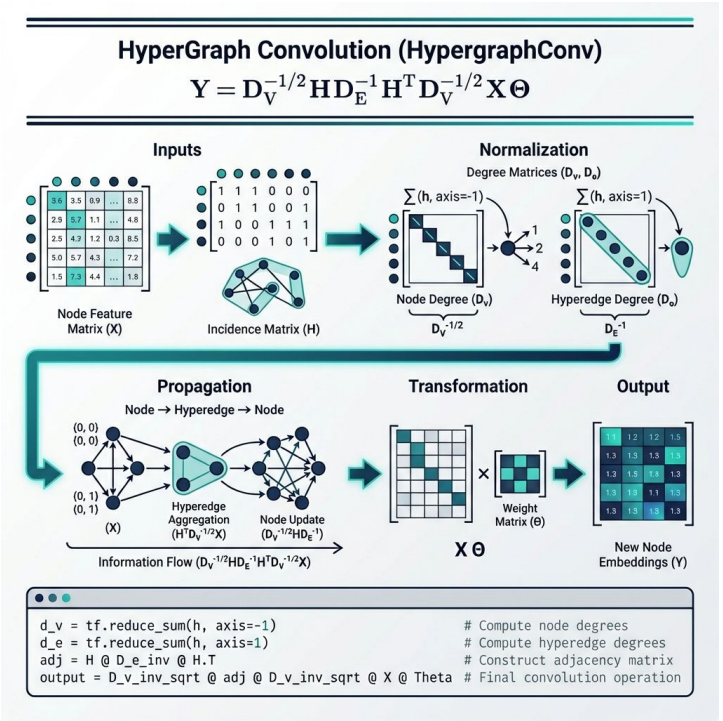
$$H_{ij} = \begin{cases} 1, & \text{if } v_i \in e_j \\ 0, & \text{otherwise.} \end{cases}$$

Message passing on HyperGraph: generalization of GCN

$$\mathbf{X}^{(l+1)} = \sigma\left(\mathbf{D}_V^{-1/2}\mathbf{H}\mathbf{W}\mathbf{D}_E^{-1}\mathbf{H}^T\mathbf{D}_V^{-1/2}\mathbf{X}^{(l)}\Theta\right)$$

Where:

- $\mathbf{X}^{(l)}$ is the input node features.
- $\mathbf{H}$ is the **Incidence Matrix** (defining the hypergraph structure).
- $\mathbf{D}_V$ and $\mathbf{D}_E$ are degree matrices for vertices and hyperedges.
- $\mathbf{W}$ is the hyperedge weight matrix (assumed to be Identity $\mathbf{I}$ in this specific code implementation).
- Θ is the learnable weight matrix (the filter).



Message passing on HyperGraph: The Clique Expansion

$$\mathbf{A} = \mathbf{H}\mathbf{D}_E^{-1}\mathbf{H}^T$$

Intuition:

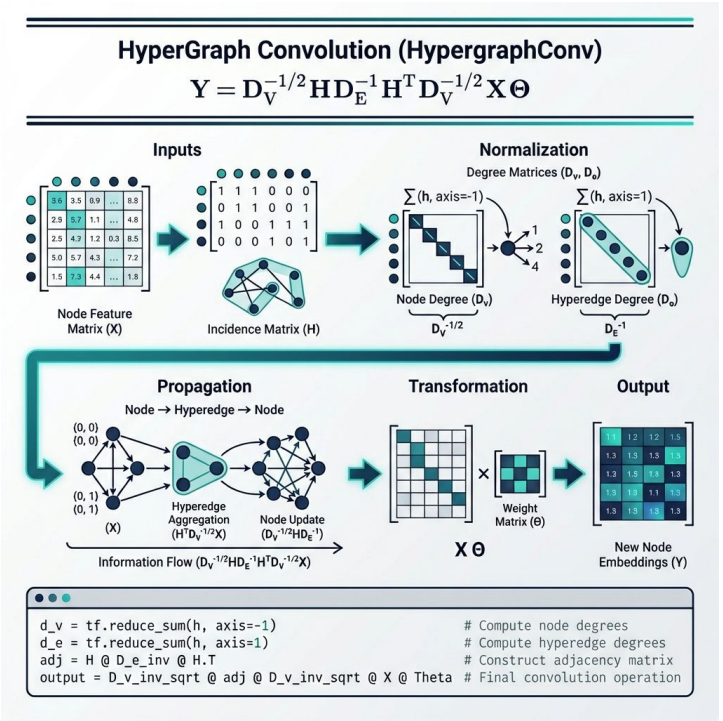
1. $\mathbf{H}^T\mathbf{X}$: Aggregates information from Nodes $\rightarrow$ Hyperedges.
2. $\mathbf{D}_E^{-1}$: Normalizes this information by the size of the hyperedge (averaging).
3. $\mathbf{H}(\dots)$: Distributes information from Hyperedges $\rightarrow$ Nodes.

This effectively converts the hypergraph into a weighted graph where two nodes are connected if they share a hyperedge, weighted by the size of that hyperedge.

Symmetric normalization: $\hat{\mathbf{A}} = \mathbf{D}_V^{-1/2}(\mathbf{H}\mathbf{D}_E^{-1}\mathbf{H}^T)\mathbf{D}_V^{-1/2}$

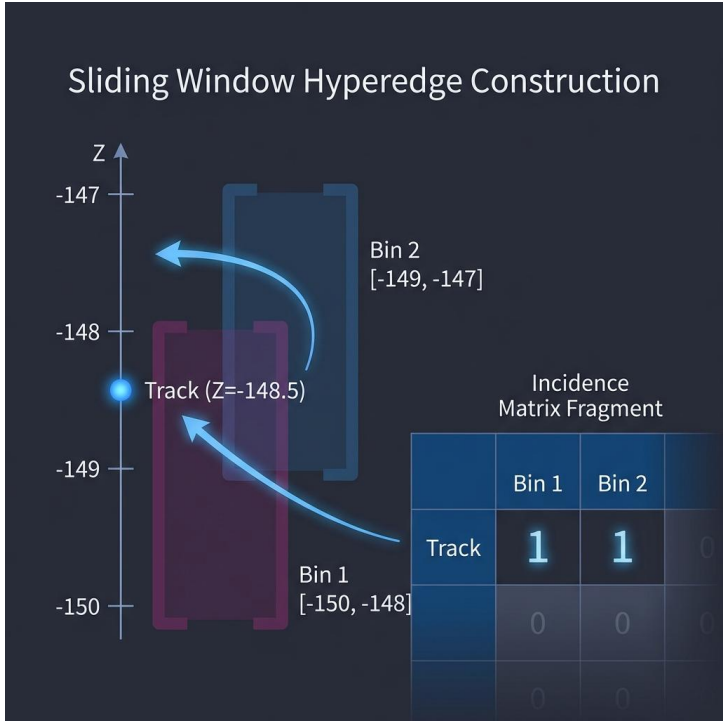
$\mathbf{Y} = \hat{\mathbf{A}}\mathbf{X}\Theta + \mathbf{b}$ ($\mathbf{X}\Theta$ can be replaced with a DNN)

$\mathbf{X}' = \sigma(\mathbf{Y})$



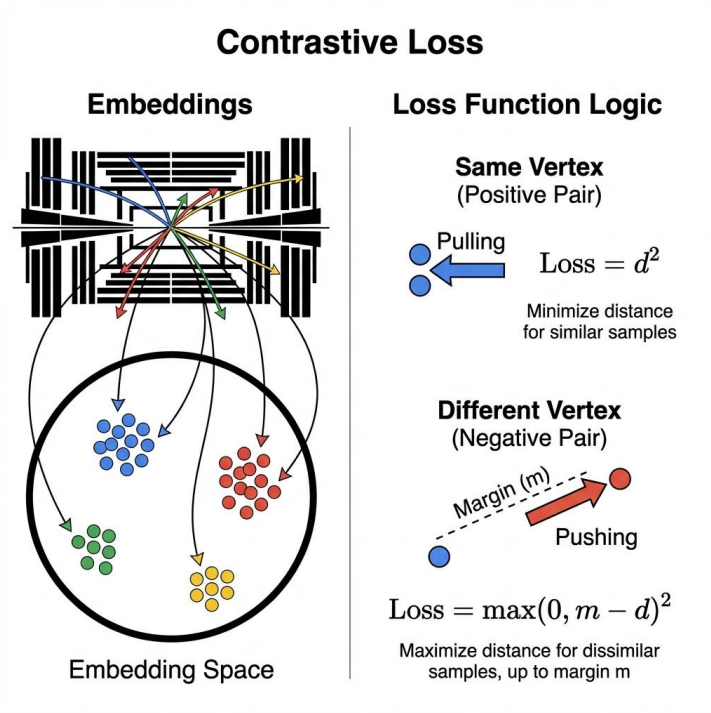
The SV finding algorithm using HyperGraph convolution

- Start with a HyperGraph of tracks as nodes.
  - ➢ Initial incidence matrix is formed by z_0 binning.
  - ➢ Message passing through the hyperedges:
    - Updates the node features.
    - Updates the incidence matrix.
- Final output: Two possibilities
  1. The model outputs the final incidence matrix.
     - Can be immediately used to get the SVs.
     - Constructing the loss function is a bit tricky.
  2. The model transforms the node features to an abstract vector space where clustering is possible.
     - Contrastive loss can be used to train this.



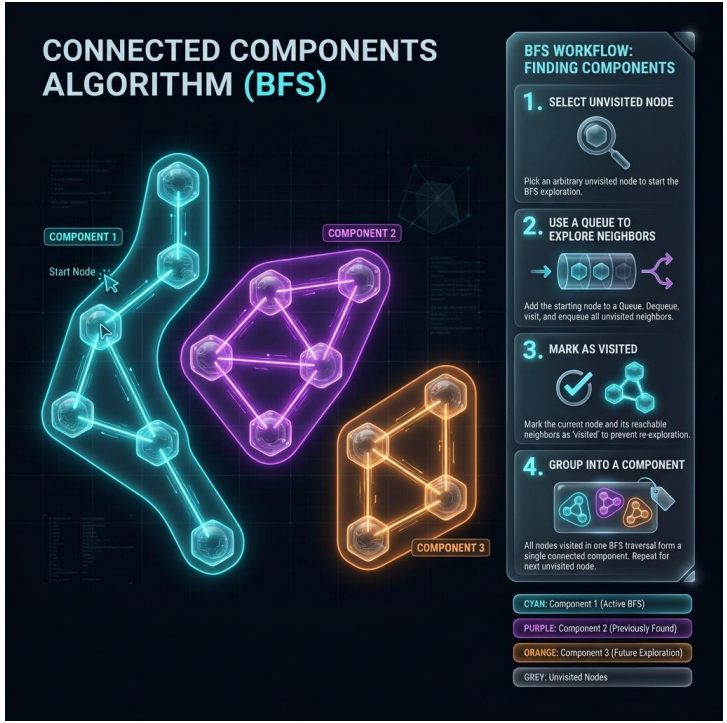
Clustering tracks using *contrastive loss*

- The HyperGraph model transforms the node features into 16-dim vectors.
- The model learns a *transformation*, which:
  - ➢ Minimizes the (Euclidean) distance among the nodes (tracks) from the same cluster (vertex).
  - ➢ Maximizes the distance between two nodes from different clusters, upto a margin m (here, m=1.0).
- Any standard clustering algorithm can be used to find the clusters.
  - ➢ A simple *connected components* algorithm, implemented as a BFS, has been used for this.



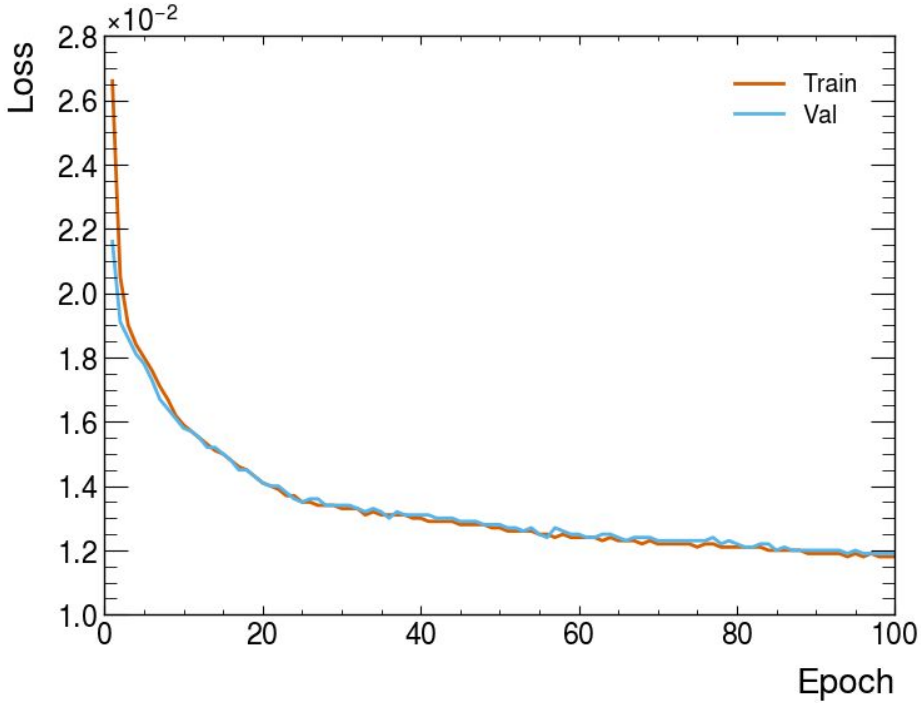
Finding the clusters

- The following simple steps has been used to find the clusters:
  1. The model outputs a 16-dim vector for each node.
  2. Calculate pairwise distances in that 16-dim space.
  3. Put a threshold (0.5, as m=1.0) on those distances to calculate the (boolean) adjacency matrix.
  4. Apply the *connected components* algorithm.
- DBSCAN could also be used for this.
  - ➢ Although it would likely be an overkill.



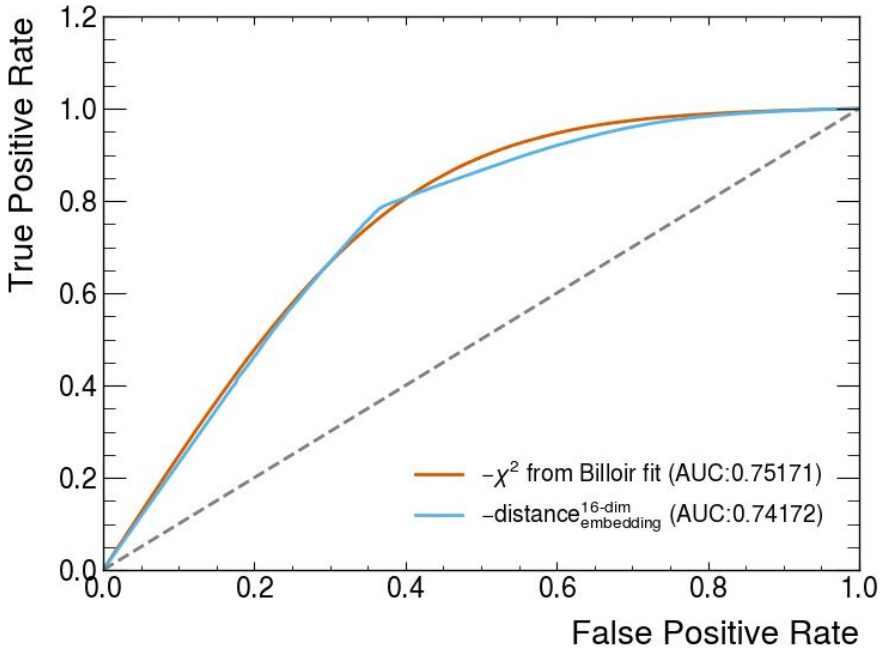
Training setup

- Using a dataset of 6381 events.
  - ➢ Simulated ttbar events using Pythia8 and Geant4 (for ODD with ACTS).
  - ➢ 80:20 train/val split.
- Sequential model:
  - ➢ Layers:
    - HypergraphConv(64, "relu")
    - HypergraphConv(32, "relu")
    - Dense(16, activation=None)
  - ➢ Input padding:
    - MAX_TRACKS = 1000
    - MAX_VERTICES = 200



Performance

- For initial performance estimate:
  - ➢ The model is compared with Billoir fit for track-pair compatibility task.
    - A binary classification task.
  - ➢ Performance of this HyperGraph model is already similar to Billoir fit.
- Points to note:
  - ➢ The HyperGraph model doesn't use any information from Billoir fit.
  - ➢ Uses only 5 track features: d_0, z_0, θ, ϕ and q/p.



Summary and outlook

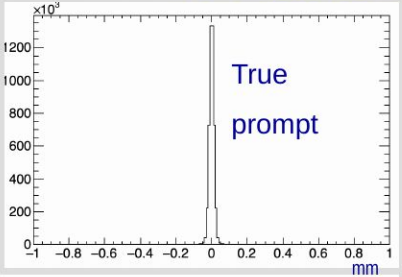
- Secondary vertexing at HL-LHC can be formulated in two different ways:
  1. Simultaneous primary and secondary vertex finding.
     - Computationally expensive, but can be readily framed as a graph-partitioning problem.
     - Might be susceptible to fake or impure (mixed) vertices.
  2. Standalone secondary vertex finding.
     - Significantly less computational complexity, but needs a way to treat isolated nodes.
     - Might suffer from less efficiency to find SVs close to the beam line.
- A preliminary convolution-based HyperGraph model has been developed.
  - ➢ Currently uses *contrastive loss* to map the tracks to a low-dim space.
    - … where the SVs can be found as clusters.
  - ➢ Can be modified to directly predict the vertices (hyperedges) as incidence matrix.
  - ➢ Alternate methods of message passing (e.g. attention based) will be investigated.

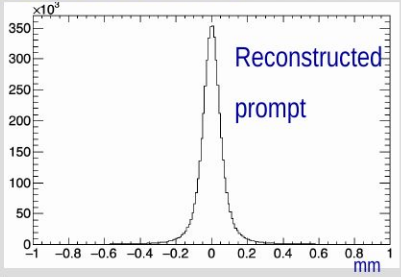
Backup

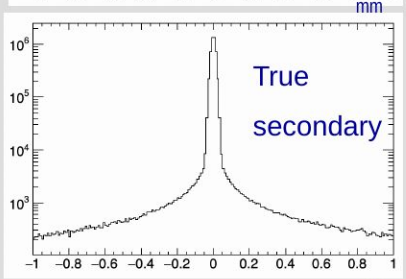
SV challenge

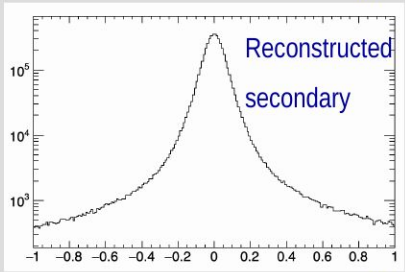
Universität Siegen

Track impact parameters wrt the beamline

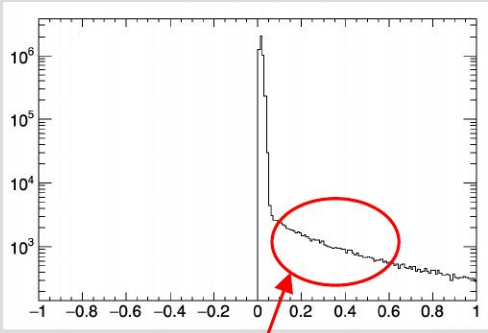






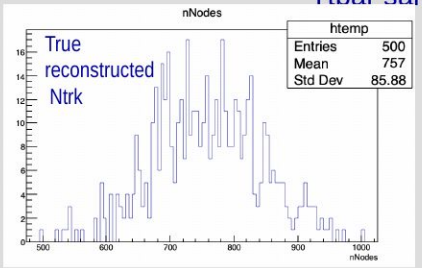


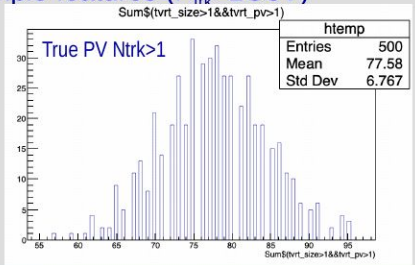
True R of vertices

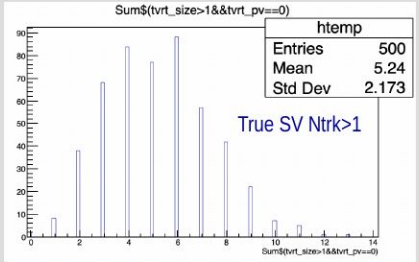


Problematic region for PV/SV reconstruction due to resolution (~equivalent to image blurring?). Hoped to resolve using ML.

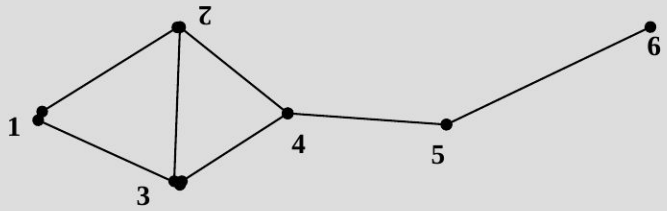
Ttbar sample features (P_{trk}>1GeV)







Edge weights with DGL



Example:
6 tracks (nodes)
7 possible 2-track vertices (edges)

Node vector of features(track parameters): td0, tZ, tPhi, tEta, tQoP, tTheta, tChi2, tNDoF, tCovD0, tCovZ,tCovD0Z, tSignif

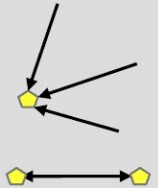
Edge vector of features(2-track vertex): vChi2, vX, vY, vZ, vcovXX, vcovXY, vcovYY, vcovXZ, vcovYZ, vcovZZ, vsumPt, vEta, vPhi, vDZ, massPiPi, vtrue, vCharge, isGamma, isKs, isLambda + truth_label

Edge weights estimation is implemented in DGL

1) Node_hidden_state = NN{Concat(Node_features, Mean(Edge_features)}

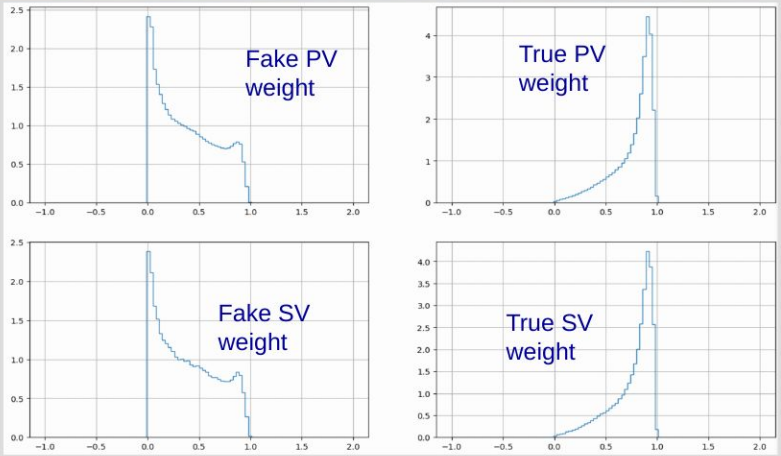
2) Edge_weight = NN{ Concat(Node_hidden_state_i, Edge_features, Node_hidden_state_j)}

3) Node_hidden_state = NN{Concat(Node_features, Weighted_Mean(Edge_features)}
4) Upd_Edge_weight = NN{ Concat(Node_hidden_state_i, Edge_features, Node_hidden_state_j)}



Loss – binary cross-entropy (classification)
NN activations – Mish + Sigmoid to get probability

DGL results (ttbar 1000ev)



AUC PV= 0.8472 AUC SV= 0.8403

For comparison - XGBoost classification of edges based on the same edge features: AUC ~ 0.746

Exploit Minimum Cost Multi-Cut algorithm to cluster track compatibility graphs with GNN-weighted edges

LMP weight	Ncl 1-track	Ncl N-track	effic. SV	purity SV	mixed 2trk clst	Lost sec.track	VI PV	ARI PV	VI SV	ARI SV
GNN wgt	190	54	9%	60%	2.1	49%	2.33	0.443	0.76	0.112
Ideal	65	83	100%	100%	0	0	0	1	0	1

Statistical metrics: Variation of Information(VI), Adjusted Rand index (ARI) are calculated separately on prompt track (PV) and secondary track (SV) collections