





Outline

- Track Finding & Motivation
- Graph Neural Network (GNN) Algorithm Outline
 - Network Initialization
 - Gaussian Mixture Reduction
 - Neighbourhood Aggregation
 - State Extrapolation & Kalman Filter
 - Reweighting & Updating the Network
 - Track Splitting & Extraction
 - Community Detection & Kalman Filter
- Results
 - MC Toy Model
 - TrackML Model
- Ongoing & Next Steps
- Conclusions





Track Finding & Motivation

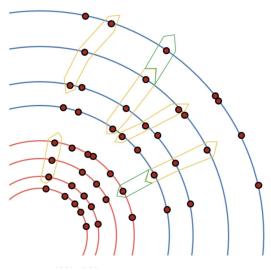
• Track finding as a Pattern Recognition Problem:

- Associate measurements ('hits') into sequences representing tracks
- Scale: O(10^5) hits per event, several 1000s tracks
- Current algorithms are based on combinatorial track following approaches
- Future upgrades → increased luminosity & pileup of particle detectors i.e. HL-LHC
- CPU time increase creates a huge demand for computing power
- Motivation for novel approaches in track finding & could lead to large savings in CPU
- Modern silicon detectors typically consist of several types of sensors:
 - Pixel (3D measurements)
 - Strips (2D measurements)

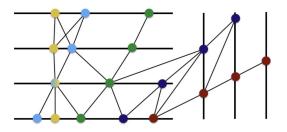
Aim: Explore track finding methods utilizing GNNs

- Clusters of hits are connected together into a graph network
- GNN algorithm will serve as a more sophisticated seeding for Pixel clusters
- Preliminary track seeds which can be refined & extended into Strips
- Such an approach could be very efficient for saving computation resources, if the GNN doesn't produce too many fake tracks

Example Combinatorial Seeded Approach



Example GNN illustration



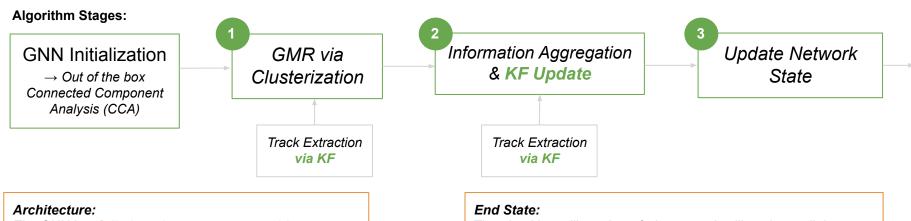


Track Finding on Graph Networks

- Algorithm Overview:
 - Iteratively resolve ambiguities & mask incompatible edge connections in order to improve track parameters
 - To efficiently exploit a priori knowledge about charged particle dynamics, the GNN-based algorithm uses simplified Kalman filters (KF) as mechanisms for information propagation & track extraction

How will this be achieved?

Utilizing pattern recognition techniques, we alternate between "edge outlier masking" via *Gaussian Mixture Reduction (GMR)* & message passing via *Neighbourhood Aggregation (NA)* to iteratively improve the precision of track state estimates. As the network evolves, the edge connections should stabilize.



The GNN is a **fully iterative pattern recognition** algorithm, at each iteration we discover new track candidates. **Application of KF** for 2 different uses.

The algorithm will continue & the network will evolve until there are no more candidates that fulfill the criteria for a good track. *Isolated nodes, track fragments & unresolved ambiguities will remain.*



Implementation of Kalman Filters

- KF is central to the tasks in this algorithm
- Kalman Filters implemented using Python package: Filterpy

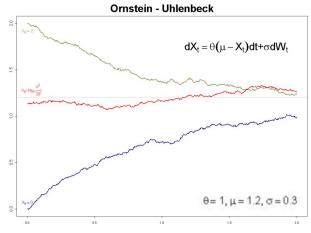
Two main applications:

1. Iterative Information Aggregation stage

- Connections/segments which we track as straight lines
- Process noise term due to multiple scattering
- Affects the track inclination variable

2. Track Extraction

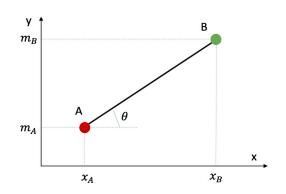
- Overall, the track bends due to the presence of the magnetic field
- Need a more sophisticated process noise model in the KF for extraction
- Ornstein-Uhlenbeck (OU) Process:
 - Used as a type of correlated noise
 - Represents the constant drift in the track azimuthal angle (ϕ) caused by presence of B-field
- KF model becomes 3-dimensional



Example of different OU-processes: Three sample paths showing correlated noise for varying hyperparameters [1]



Toy Model: Network Initialization



 y_A y_B -- unobservable track positions

 $m_A \ m_B$ -- measurements of track position

 t_A t_B -- unobservable $\cot \theta$

 σ_0^2 -- variance of the measurements

Track state vector: $X = \begin{pmatrix} y \\ t \end{pmatrix}$ $\hat{y}_{AB} = m_A$

State vector estimate: $\hat{X} = \begin{pmatrix} \hat{y} \\ \hat{t} \end{pmatrix}$ $\hat{t}_{AB} = \frac{m_A - m_B}{x_A - x_B}$

Given a node A, conditioned on its neighbourhood B;:

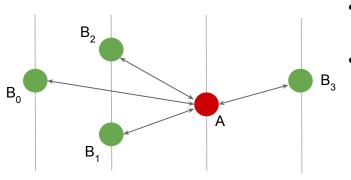
- Compute X_{ii} (track state estimate)
- Compute C_{ii} (edge covariance)
- This forms a **Gaussian component** φ_{ii}
- Store all components at node i
- Gaussian mixture g_i(X)

$$g_i(X) = \sum_{j} w_{ij} \varphi_{ij} (X, X_{ij}, C_{ij})$$

Definitions:

- e. Bidirectional edge weight {0, 1}
 - e = 0 inactive edge, e = 1 active edge
 - Arrow direction conventions: i → j transmission of messages from node i to node i
- w_{ij}
 Mixture weight for a Gaussian component transmitted from the neighbour node i to node i
- Prior probability of neighbourhood nodes j and central node i being on the same track, if a track can produce at most one hit per layer

Initialize all **bidirectional edges** e_{ij} as "active" = 1



Priors:

$$p_1 \& p_2 = 0.5, p_0 \& p_3 = 1.0$$

Mixture weight: For each track st

For each track state, initialize uniformly as 1/num nodes in neighbourhood of node A, $w_{ij} = 0.25$



Iteration 1: Gaussian Mixture Reduction

Aim: Identify & mask outlier edge connections

Why reduce the mixture?

- Recursively processing, no. of components & calculations can grow exponentially
- Solution: Given a node, model each edge as a Gaussian component, forms a Gaussian mixture with N components, find a reduced mixture with M < N components, such that some deviation measure is below a threshold

GMRC: Gaussian Mixture Reduction via Clustering

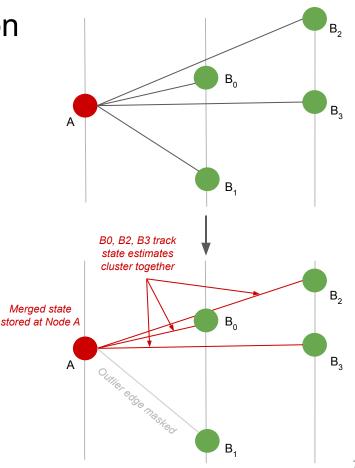
- Can be achieved in two ways:
 - Iteratively merging Gaussian components → forms a merged state
 - Pruning components by masking outliers

Pseudocode:

- Based on k means clustering, but with k=1
- Introduce a distance metric between all edge connections KL divergence
- Compute pairwise distances, start with the smallest:
- If metric < threshold → merge components
- Progressive convergence, check all edge pairs until no further merging possible
- Outliers identified & masked

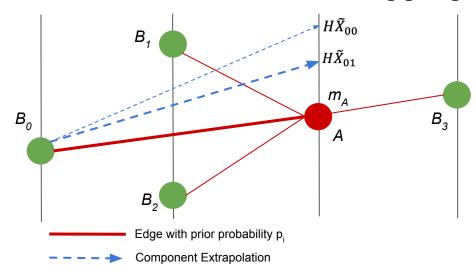
KL (Kullback–Leibler) divergence:

- Deviation measure, serves as a cost function
- Measure of the distance between 2 probability distributions
- Optimal KL threshold learned using a Support Vector Machine (SVM) classifier





Iteration 2: Information Aggregation & Kalman Filter



Extrapolation:

F_i is the jacobian from B_i to A

Q is the process noise matrix: encompasses all material effects modelled using "Ornstein-Uhlenbeck" (OU) process

$$\tilde{X}_{ij} = F_i X_{ij}$$

$$\tilde{C}_{ij} = F_i \left\{ \sum_{ij} C_{ij} + Q \right\} F_i^T$$



- The problem: given a neighbourhood $\mathcal{N}=\{B_i\}$, calculate the Gaussian mixture representing a possible track state at the node A conditioned upon a measurement $m_{\scriptscriptstyle A}$
- The model: at each neighbour node B_i the track state is represented by a Gaussian mixture, or a reduced mixture (merged state)

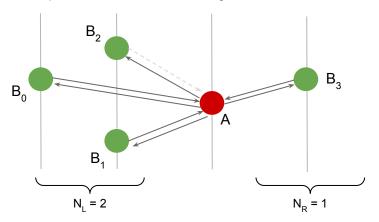
$$g_i(X) = \sum_{j} w_{ij} \varphi_{ij} (X, X_{ij}, C_{ij})$$

- Information aggregation: distribute messages to neighbourhood if edge connections are active
- State Extrapolation: merged state is extrapolated from neighbour node to node A using linear extrapolation equations
- Validation: compute the residual & chi2 distance between extrapolated state and the measurement at node A
- Perform KF update: If the chi2 distance is compatible
- Otherwise this edge connection is turned off



Updating Priors & Weights

- As the network evolves edge connections will become masked/remain active → graph structure will change
- Hence reweighting mixture components & recomputing priors will be needed
- If any weights < threshold, these edge connections are isolated
- Forms part of the mechanism for edge activation/deactivation



Consider the example above:

- Connection B_2 to A is deactivated ($e_{R2A} = 0$)
- Message passing/extrapolation from B₂ to A is incompatible
- From the perspective of node A the priors change: p_0 remains at 0.5 (its previous value), p_1 gets updated 1.0 and p_3 = 1.0
- B0, B1 and B3 components will get reweighted

 N_L = no. of layers on left N_R = no. of layers on right

Reweighting the mixture:

• Measurement likelihood (conditional on component) given by β_{ii}

$$\beta_{ij} = \left(2\pi \left|S_{ij}\right|\right)^{-1/2} e^{-\Delta \chi_{ij}^2/2}$$

• Updated weights for the mixture extrapolated from node B, are:

$$\widetilde{w}_{ij} = \frac{w_{ij}\beta_{ij}}{\sum_{k} w_{ik}\beta_{ik}} p_i$$

- Account for the no. of layers in the neighbourhood
 - Need the probability that a track passing through node A was detected at layer L
 - Hence \widetilde{w}_{ij} must be divided by the no. of layers N_S on the corresponding side of the neighbourhood
 - I.e. B₀, B₁, B₂ division by 2, B₃ division by 1
- Final Gaussian mixture with components:

$$\left|\varphi_{ij}\left(X,\tilde{X}_{ij},\tilde{C}_{ij}\right)\right| \left|\widetilde{w}_{ij}/N_{S}\right|$$



Track Splitting

Aim: Extract tracks iteratively as the network evolves after each iteration, good track candidates don't need to be processed again

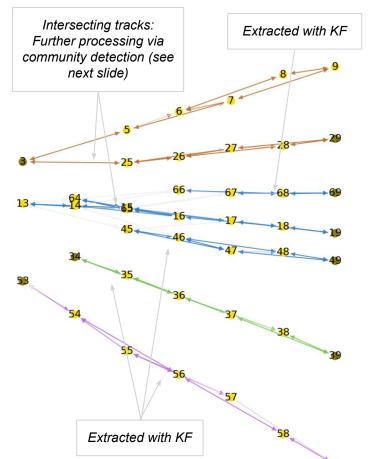
Some remaining networks/isolated nodes will remain as not 100% of ambiguities can be resolved

Criteria for a good candidate:

- >= 4 hits: no track fragments
- 1 hit per layer: no competing/intersecting tracks & no holes
- P-val acceptance threshold > 0.01 (chi2 distance with KF track fit)

Extracting good candidates:



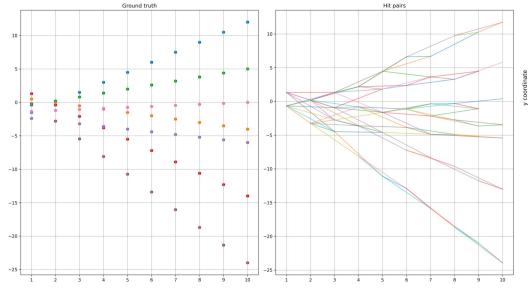


Results

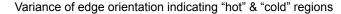


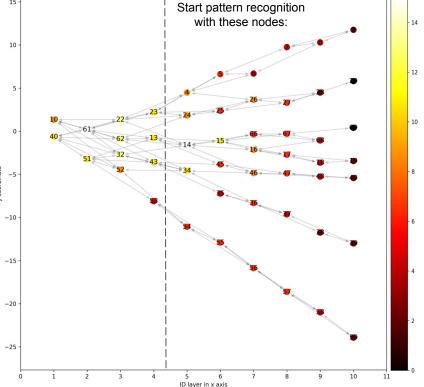
Toy Monte Carlo Model

- Initialize the graph network:
 - Simple 2D model (70 nodes) using the Python package: NetworkX
 - Kalman Filters implemented using Python package: Filterpy
 - Nodes as hits & predicted edges using a simple 'hit-pair-predictor'
 - Create a framework that automatically determines a suitable region for initiating pattern recognition
 - o Criteria: variance of edge orientation



- · Remove nodes with high variance
- Start the pattern recognition in "cold" regions





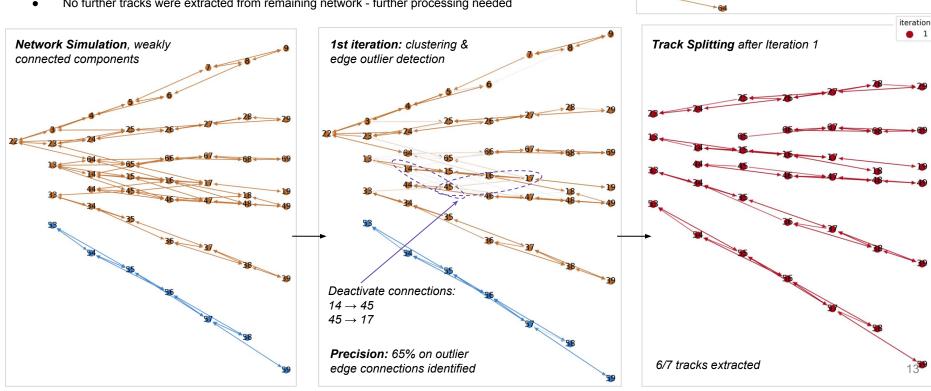


Remaining network after

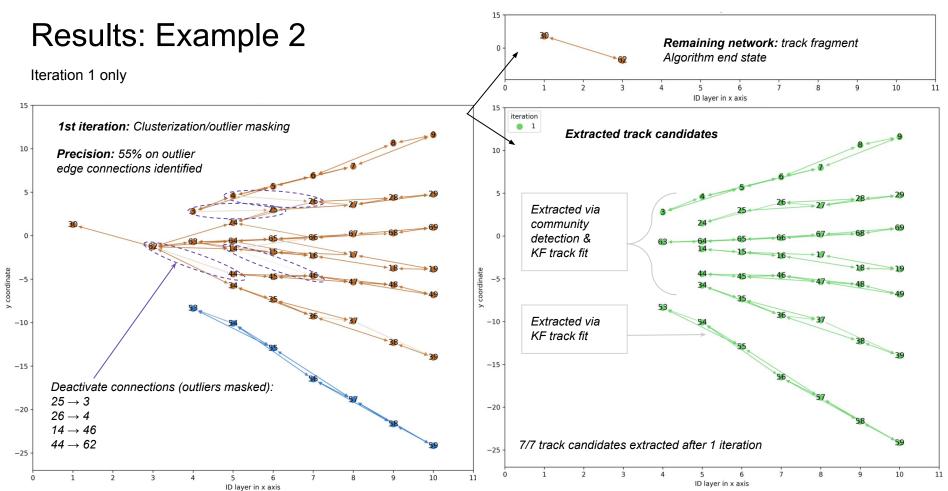
Iteration 1

Results: Example 1

- Iteration 1 only
 - 6/7 potential good track candidates are extracted fast convergence
 - Of which 100% precision with respect to MC
- No further tracks were extracted from remaining network further processing needed



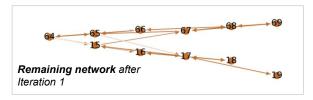




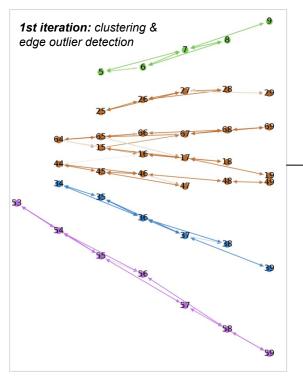


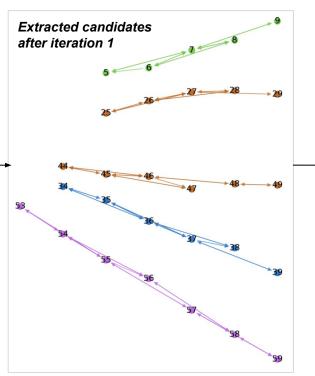
Results: Example 3

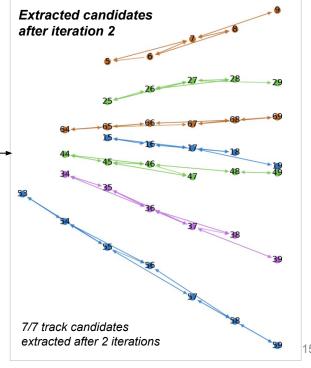
- Iteration 1 & 2
- This specific simulation was able to resolve all ambiguities within 2 iterations
- 100% purity wrt MC truth













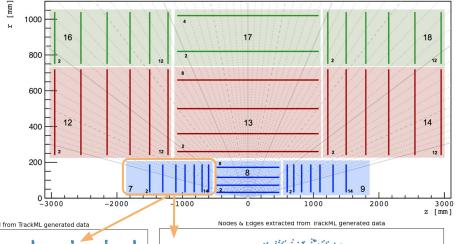
TrackML Model

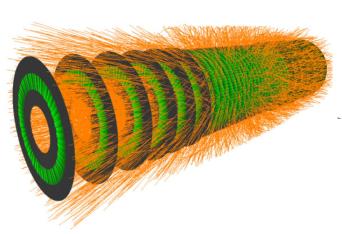
What is TrackML?

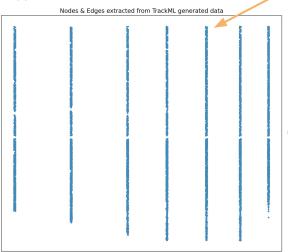
- More realistic detector model & generated data
- Open source (Kaggle) Data Science competition set out to improve the software needed to process & filter promising events

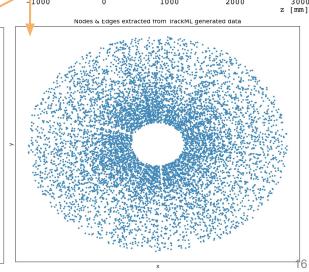
Using TrackML dataset:

- Here we focus on Pixel Endcap volume (region 7 only)
- An example of 1 event simulation
- Initialize network nodes & bidirectional edges
- Number of nodes: 8748, number of edges: 12852

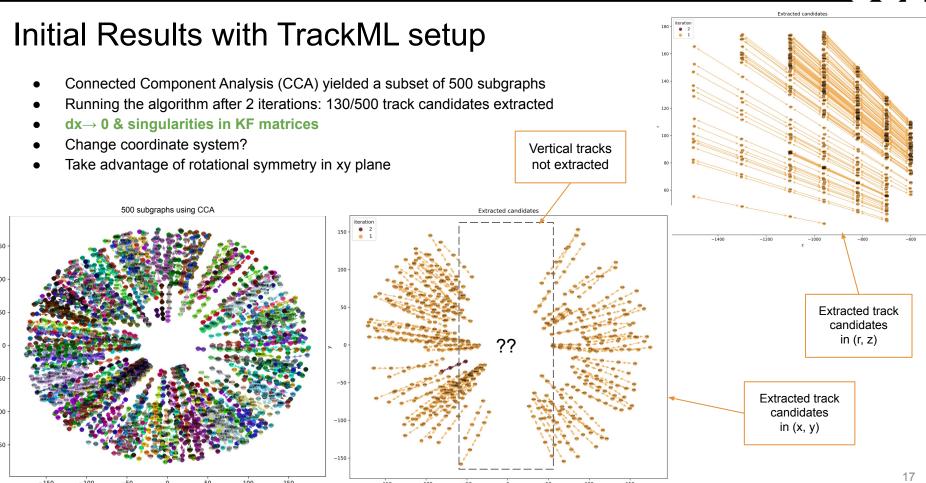




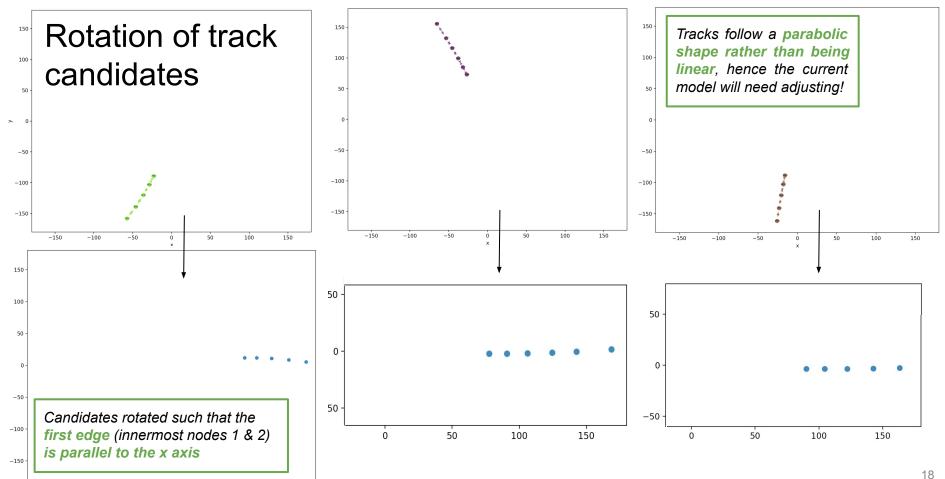














track purity

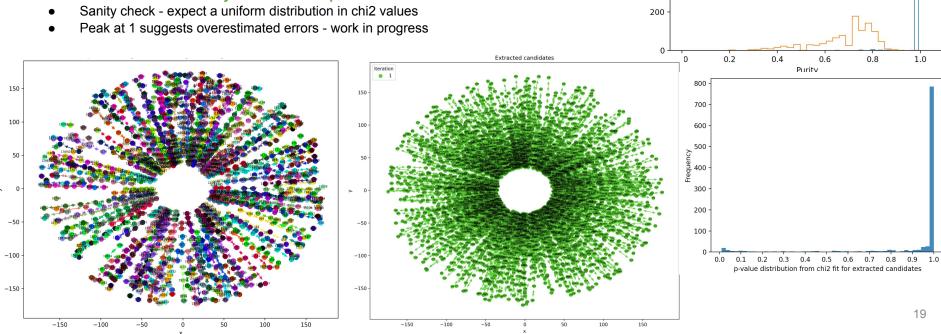
800

600

particle purity

Post-Rotation of Track Candidates

- Candidates extracted at all ϕ
- On a subset of 1683 subgraphs:
 - Without rotation: 35% extracted, with rotation: 62% extracted
- TrackML standard requirement: track purity & particle purity must be > 50%
- Track reconstruction efficiency:
 - > 90% efficiency for tracks with pT > 1GeV





Ongoing & Next Steps

• Handling of shared hits

- Intersecting tracks will contain shared hits
- Track extraction Leaving hits in the network which are shared
- o Identification of shared hits important addition to the algorithm

Community Detection

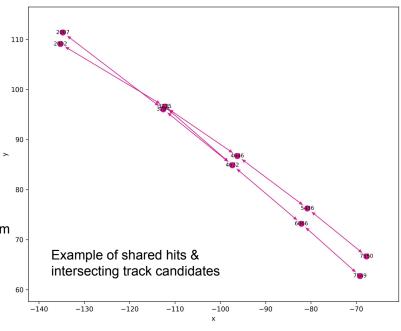
- Implementing a custom community detection
- Analysing node pairs & utilizing KL distance to identify communities

• Implement stopping criteria

• I.e. Quality of remaining networks < threshold, terminate the algorithm

Performance Studies/Testing

- Application of the Graph model to the entire TrackML dataset including the pixel barrel region
- Optimizations improve implementation i.e. parallelize code





Summary

- The approach developed here is a unique method, unlike the traditional approach whereby Multi-Layered Perceptrons (MLPs) are trained
- The graph network is allowed to learn local track parameters on its own by iteratively resolving ambiguities in order to discover new track candidates
- Preliminary result of > 90% track recon. efficiency for tracks with pT > 1GeV
- Main iterations of the algorithm include: Gaussian Mixture Reduction, Information Aggregation & Network Update
- The incorporation of KFs for both information aggregation & track extraction is a unique approach and has shown to give promising results on both a simple MC toy model & TrackML model
- Neighbourhood information aggregation via message passing is a powerful feature of GNNs which is leveraged here;
 the network has the ability to learn local track parameters
- Need to evaluate how well this approach works on denser hit environments where the number of potential track candidates is much greater, as well as the performance of this algorithm on both the Pixel Endcap & Pixel Barrel regions of the TrackML particle detector

Backup



Learning the Optimal KL Threshold

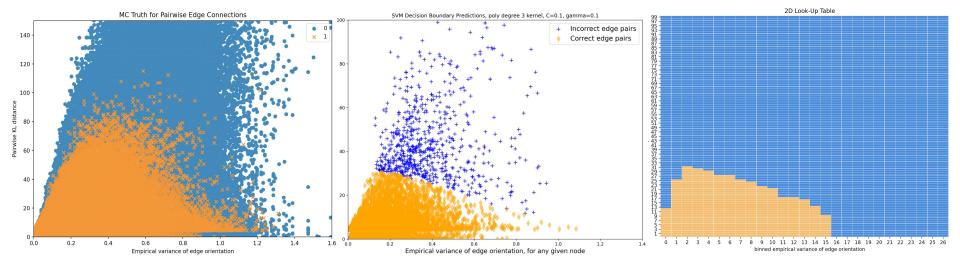
- Can we obtain a functional form?
 - Predict the optimal pairwise KL distance for correct edge pairs using MC truth
- Expectation:
 - if the variance is high, tighter cut on the KL distance is needed (& vice versa)
- Simulation:
 - o 10000 events, each with 10 tracks, Sigma0 = 0.5
 - Focused on nodes in 'cold' regions
 - Train: test split 70: 30
 - X feature vector: empirical variance of edge orientation, for any given node & pairwise KL distance

Training:

- SVM trained to maximise recall
- Optimum hyperparameters: Poly degree
 3, C=0.1, Y=0.1

Predictions:

- o Recall (TPR) 0.94, tuned to 0.95
- Decision boundary extracted & converted to 2D LUT for fast lookup





Iteration 2: Information Aggregation & Kalman Filter

Definitions:

Extrapolation:

- Extrapolation of the track state estimate X, where F is the Jacobian of for the extrapolation from node B to A
- Extrapolated covariance matrix C, with the addition of the process noise Q, and symmetrical product with Jacobian F
- Jacobian F and process noise Q both derived using Ornstein-Uhlenbeck (OU model)
- \circ α determines the dynamics, it is a correlation hyperparameter

Process Noise Q:

- O Q encompasses all material effects & is modelled by the OU process, which models the constant drift in ϕ due to the presence of the magnetic field
- OU process noise models this dynamic behaviour
- $\circ \qquad \sigma_{\text{ou}} \text{ is the uncertainty due to the OU process and } \sigma_{\text{ms}} \text{ is the uncertainty due to multiple scattering}$

Additional steps:

- Residual r_{ij} with measurement at node A & extrapolation, where H is the measurement matrix
- The covariance of the residual S
- The chi-squared distance Δχ_{ii}²

$$F = \begin{pmatrix} 1 & dx & g1 \\ 0 & 1 & f1 \\ 0 & 0 & e1 \end{pmatrix}$$

$$e_1 = e^{(-|dx|\alpha)}$$

$$f_1 = \frac{(1 - e_1)}{\alpha}$$

$$g_1 = \frac{|dx| - f_1}{\alpha}$$

$$Q = \begin{pmatrix} dx^{2}(\sigma_{ms}^{2} + \frac{dx^{2}\sigma_{ou}^{2}}{4}) & dx(\sigma_{ms}^{2} + \frac{dx^{2}\sigma_{ou}^{2}}{2}) & \frac{dx^{2}\sigma_{ou}^{2}}{2} \\ dx(\sigma_{ms}^{2} + \frac{dx^{2}\sigma_{ou}^{2}}{2}) & \sigma_{ms}^{2} + dx^{2}\sigma_{ou}^{2} & dx\sigma_{ou}^{2} \\ \frac{dx^{2}\sigma_{ou}^{2}}{2} & dx\sigma_{ou}^{2} & \sigma_{ou}^{2} \end{pmatrix}$$

$$H = \begin{bmatrix} 1 & 0 & 0 \end{bmatrix} \quad dx = x_B - x_A$$

$$r_{ij} = m_A - H\tilde{X}_{ij} S_{ij} = H\tilde{C}_{ij}H^T + \sigma_0^2 \Delta \chi_{ij}^2 = r_{ij}^T S_{ij}^{-1} r_{ij}$$



Gaussian Components & Reweighting

Matrix definitions:

- At each node, all edge connections form a weighted Gaussian mixture
- Weights are given by w_ij and each edge connection is comprised of its track state vector X_ij and the edge covariance C_ij derived from the associated measurement errors

The edge weights are defined as a ratio, together with the prior probability p_i and the measurement likelihood B_ij defined as the normalized Gaussian measurement likelihood, as a function of the chi-squared distance between the extrapolated state and the measurement at the node

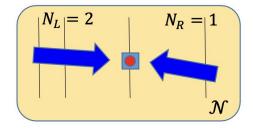
 The final weights are then divided through by the number of layers on each respective side of the MC toy model, i.e. N_L = no. of layers on left and N_R = no. of layers on right, as the track direction needs to be taken into account

$$g_i(X) = \sum_{j} w_{ij} \varphi_{ij} (X, X_{ij}, C_{ij})$$

$$\widetilde{w}_{ij} = \frac{w_{ij}\beta_{ij}}{\sum_k w_{ik}\beta_{ik}} p_i$$

$$\beta_{ij} = (2\pi |S_{ij}|)^{-1/2} e^{-\Delta \chi_{ij}^2/2}$$

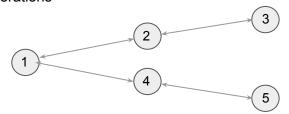
$$\widetilde{w}_{ij}/N_S$$

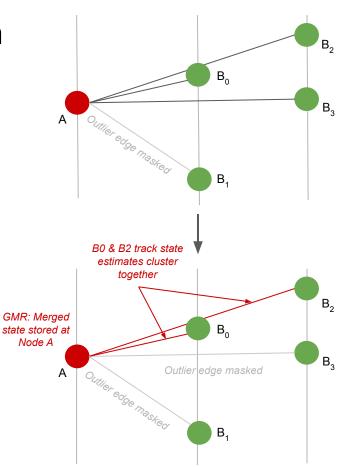




Iteration 3: Gaussian Mixture Reduction

- Gaussian mixture reduction is executed again on any remaining networks to further resolve ambiguities
- Perform clusterization & merging on updated track states outputted from the previous iteration
- Propagation of higher precision estimates
- Outliers are masked, priors & weights are updated
- Scenario where merging is forbidden:
 - A node has only 2 competing edge connections & components come from 2 different nodes in the same layer (i.e. nodes 2 & 4)
 - More precise extrapolated tracks from 2 & 4 will give sharper discrimination in later iterations







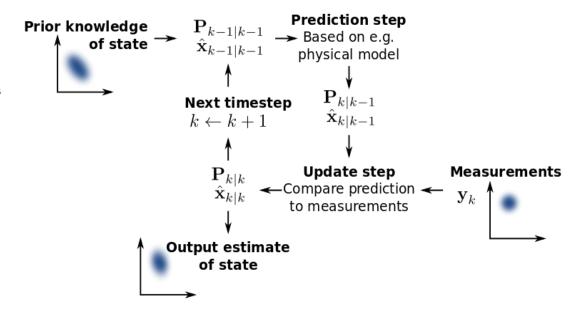
The KF Algorithm

Kalman filtering, also known as **linear quadratic estimation** (**LQE**), is an algorithm that uses a series of measurements observed over time, including statistical noise and other inaccuracies, and produces estimates of unknown variables that tend to be more accurate than those based on a single measurement alone, by estimating a joint probability distribution over the variables for each timeframe.

Very powerful technique used in track fitting/trajectory optimization.

The algorithm works by a two-phase process. For the prediction phase, the Kalman filter produces estimates of the current state variables, along with their uncertainties. Once the outcome of the next measurement (necessarily corrupted with some error, including random noise) is observed, these estimates are updated using a weighted average, with more weight being given to estimates with greater certainty.

The algorithm is recursive. It can operate in real time, using only the present input measurements and the state calculated previously and its uncertainty matrix; no additional past information is required.





Community Detection

- Community structure of a network = division of its node set
- Partition the network s.t. nodes in the same subgraph are closely connected & nodes in different subgraphs are sparsely connected
- Each subgraph is called a community

Aim:

- Resolve ambiguities earlier & aim for faster convergence.
- Extract communities within intersecting track candidates or >1 hit per layer

Modularity Maximization:

- Modularity: benefit function that measures the quality of a division of a network into communities, measures the relative density of edges inside communities w.r.t edges outside communities; high values correspond to good division
- Popular modularity maximization approach is the Louvain method (LM), iteratively optimizes local communities until global modularity can no longer be improved given perturbations to the current community state
- LM for directed networks: Integrates greedy strategy and hierarchical clustering, O(nlogn) where n is the number of nodes in the network

For a weighted, directed graph the functional form of modularity is given below:

$$Q_{d} = \frac{1}{m} \sum_{v,w} \left[\left(a_{vw} - \frac{k_{v}^{out} \cdot k_{w}^{in}}{m} \right) \cdot \delta_{C_{v},C_{w}} \right]$$

Algorithm:

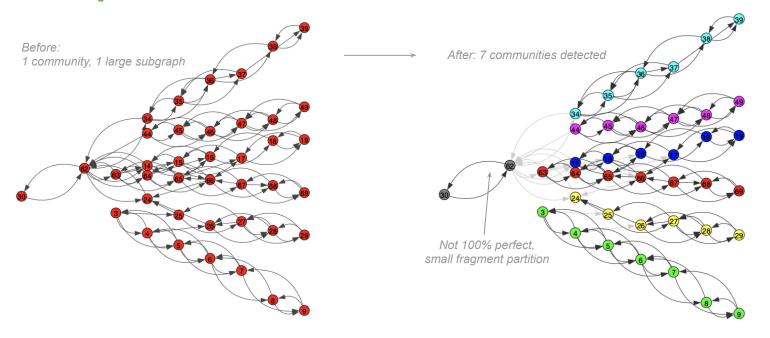
- Starting from singletons partition of vertices, the algorithm tries to increase the modularity by moving vertices from their community to any other neighbor one.
- Compute the gain obtained by removing vertex i from its own community Ci
- Repeat as long as it exists a move that improves the value of modularity



Community Detection

- Community structure of a network = division of its node set
- Partition the network s.t. nodes in the same subgraph are "closely connected"
- Distance metric: directed modularity
- Each subgraph/colour represents a different community
- Greater proportion of good track candidates established at an earlier iteration
- Faster convergence

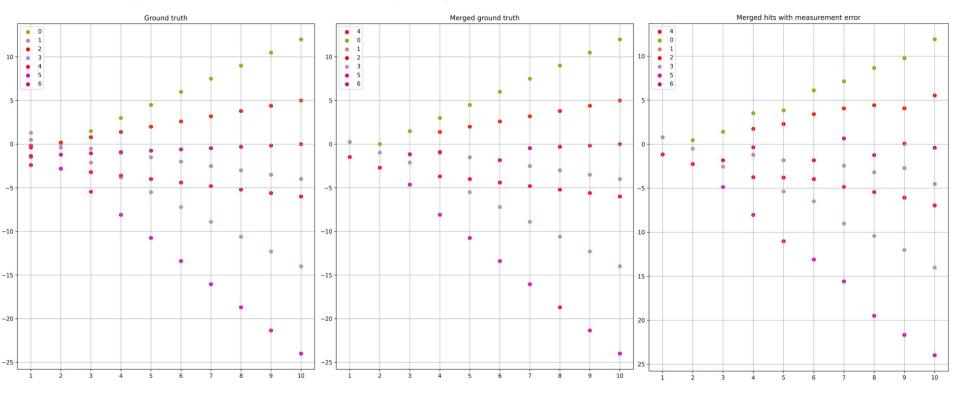
1. Connected Component Analysis 2. Kalman Filter Track Fit Detection 3. Community Detection





Toy MC Model - Network initialization & Hit Merging

- Hits which are in close proximity to each other generated by the simulation need to be merged together, in order to reflect the behaviour of the detector and cluster hit merging.
- Record of ground truth tracks/hits need to be kept particularly for merged hits



Sigma0 = 0.3

distance



Chi2 Acceptance Threshold for Extrapolated Merged State

- Varying sigma0 and recording the chi2 distance for extrapolated states
- Plotted chi2 distance for states where the node and neighbour node has truth 1
- Distance is independent of sigma0
- Chi2 acceptance threshold set to 2

60

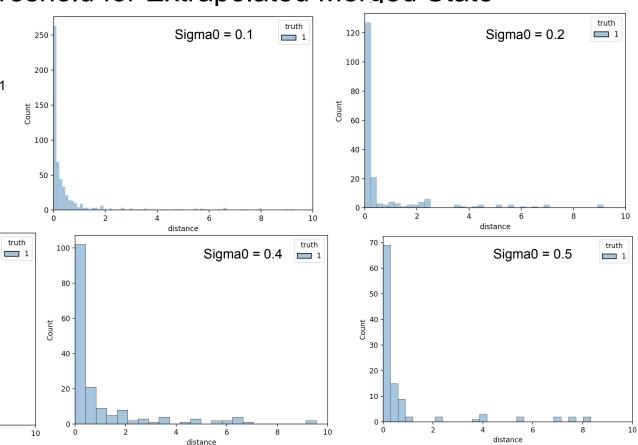
50

40

Count 00

20

10

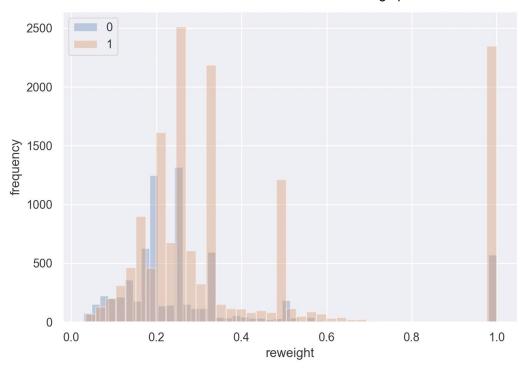




Tuning the Reweight Threshold

- If the weights of components < threshold → deactivate these edge connections
- Plot: Edge connections reweight distributions:
- Tuning the reweight threshold parameter
- Look at remaining networks after the first reweighting calculation has been executed
- Edge MC truth (1 or 0) & edge reweight
- Both distributions overlap considerably, there is not a lot of difference separating the two distributions
- Therefore, as we do not want to turn off a large proportion of "good" edge connections, then reweight threshold of 0.1 is fine.

Reweight distribution after iteration 2 of edge connections for MC truth correct and incorrect edge pairs





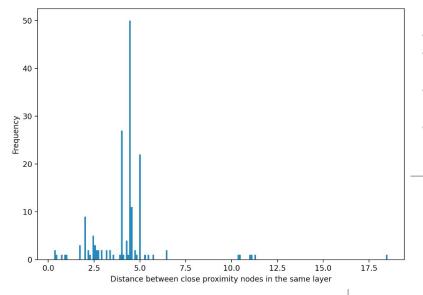
TrackML Model Hit-Pair Predictor

Edge prediction for network nodes:

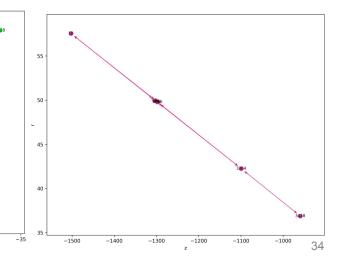
- We use the algorithm (FastTrack) submitted to the TrackML competition
- Github repo: https://github.com/demelian/fastrack
- Edge predictor algorithm:
 - In the Pixel detector there is a strong correlation between the lengths of pixel clusters and track inclination angle, found within data exploration
 - Train a binary classifier to identify hit-pairs which correctly belong to the same track
 - Discriminate between hit pairs that have correct hit association & hence belong to the same track, vs hit pairs that do not belong to the same track
 - Predicted results are converted into a to fast Look-Up-Table



TrackML - Node Merging



- Tuning of 3d separation distance first considered module_id
- However not easy to calculate how close each hits are to each other due to arrangement of modules
- Calculation of 3d separation of the 2 nodes → threshold from distribution
- Small improvement stats on the endcap: $515/1683 \rightarrow 583/1683$ subgraphs extracted on entire endcap region in iteration 1
- Will be useful for first iteration as these track candidates have been extracted first, and will make further iterations much faster
- Flexible in the sense that at the moment I am only looking for a specific type of subgraph (Any number of layers containing 2 nodes → apply distance cut)





Track Purity, Particle Purity, Track Reconstruction Efficiency

- Only particles with four hits or more are considered, and only proposed tracks with four hits or more are considered
- Each track is matched with the ground truth *majority particle* sharing with it the greatest hit number
- Track purity:
 - The ratio of this intersection to the number of hits of the reconstructed track
- Particle purity:
 - The ratio of this intersection to the number of hits of the underlying particle
- Both ratios > 50% to define a good track so that a one-to-one relationship between particle and track can be defined
- Same definition as what is used in the TrackML study

Track Reconstruction efficiency:

 We consider reference particles which are fully contained in the volume we are currently working on (endcap volume 7), this defines our reference tracks

$$Reconstruction\ efficiency = \frac{\textit{No.of}\ \textit{successfully}\ \textit{reconstructed}\ \textit{tracks}}{\textit{No.of}\ \textit{reference}\ \textit{tracks}\ \textit{in}\ \textit{volume}\ \textit{of}\ \textit{interest}}$$



Parabolic Approach

- 1) Local (node specific) coordinate-system
- 2) Track states at node A: Parabolas
- 3) Equations for parabola parameters at node A:

$$m_O = a(x_O)^2 + bx_0 + c$$

$$m_A = c$$

$$m_B = a(x_B)^2 + bx_B + c$$

$$m_O=0, m_A=0$$

- 4) We assume:
- 5) Measurement error matrix, where σ_0 represents the boundary states $S = diag[\sigma_0^2, \sigma_A^2, \sigma_B^2]$ etc:

Pseudocode:

- Given a node & its neighbourhood
- Transform coordinate axis
- Obtain the measurement vector [m0, mA, mB]
- Obtain the track state parameters [a, b, c] using H⁻¹
- Store track state vector & covariance
- Clusterization

