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# Graph Networks for Track Reconstruction

Mini Workshop on Machine Learning, ICNFP 2021

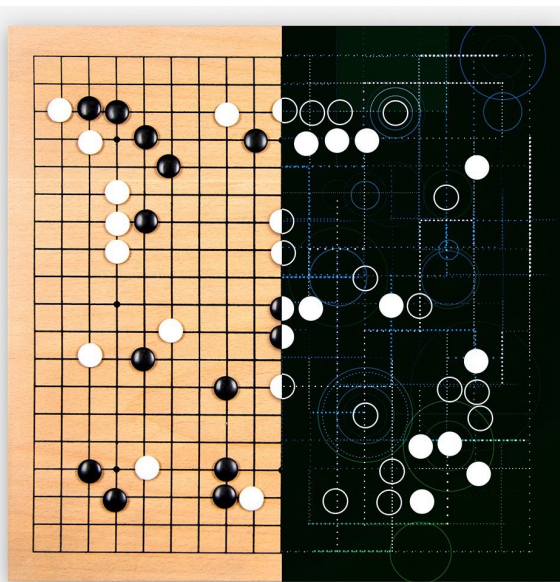
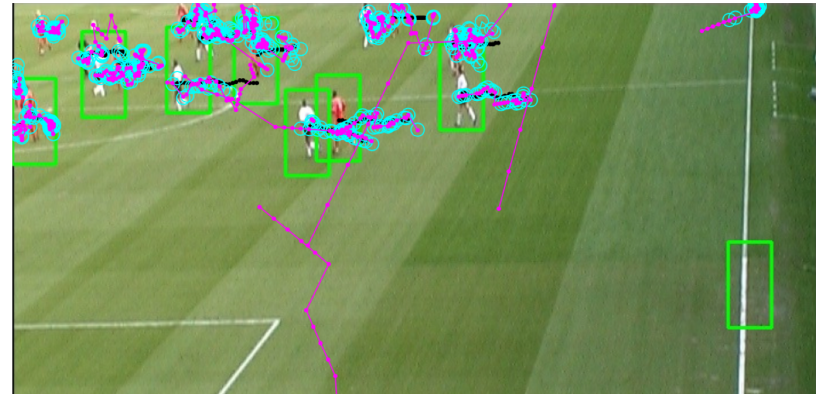
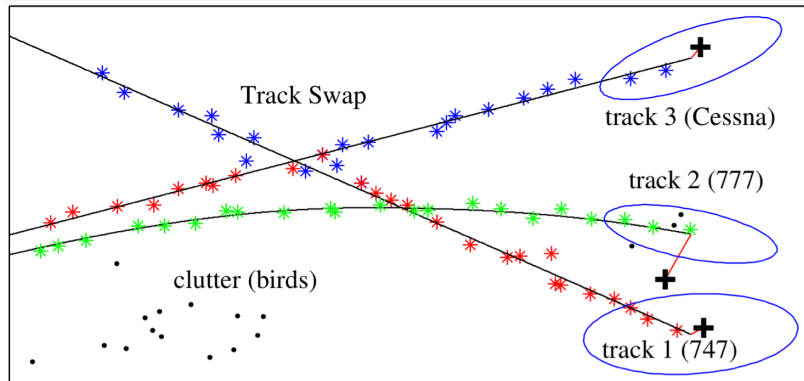
**Marcel Kunze, Heidelberg University**



# Pattern Recognition/Tracking



Pattern recognition/tracking is a very old, very hot topic in Artificial Intelligence, but very varied  
Note that these are real-time applications, with CPU constraints

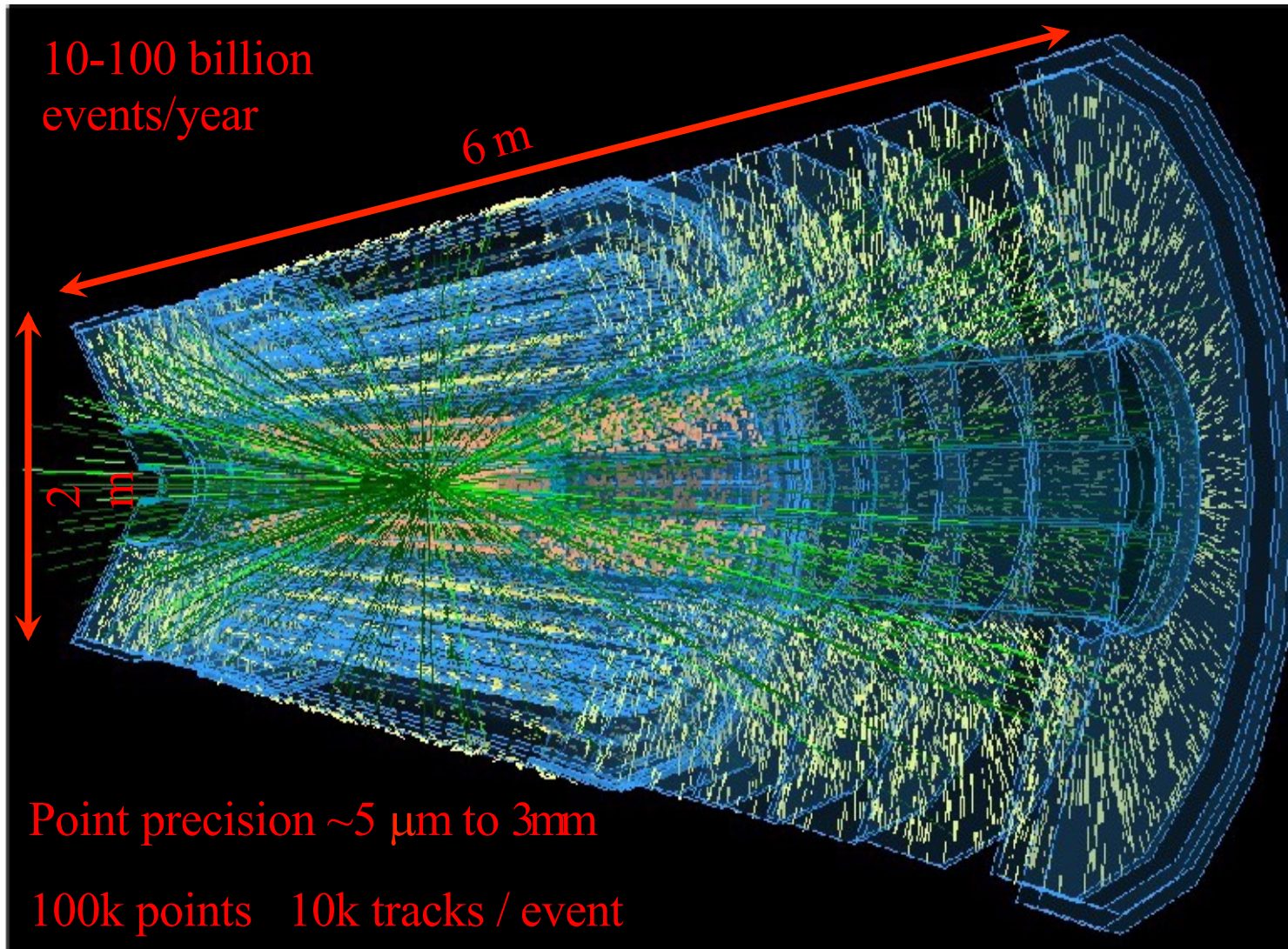




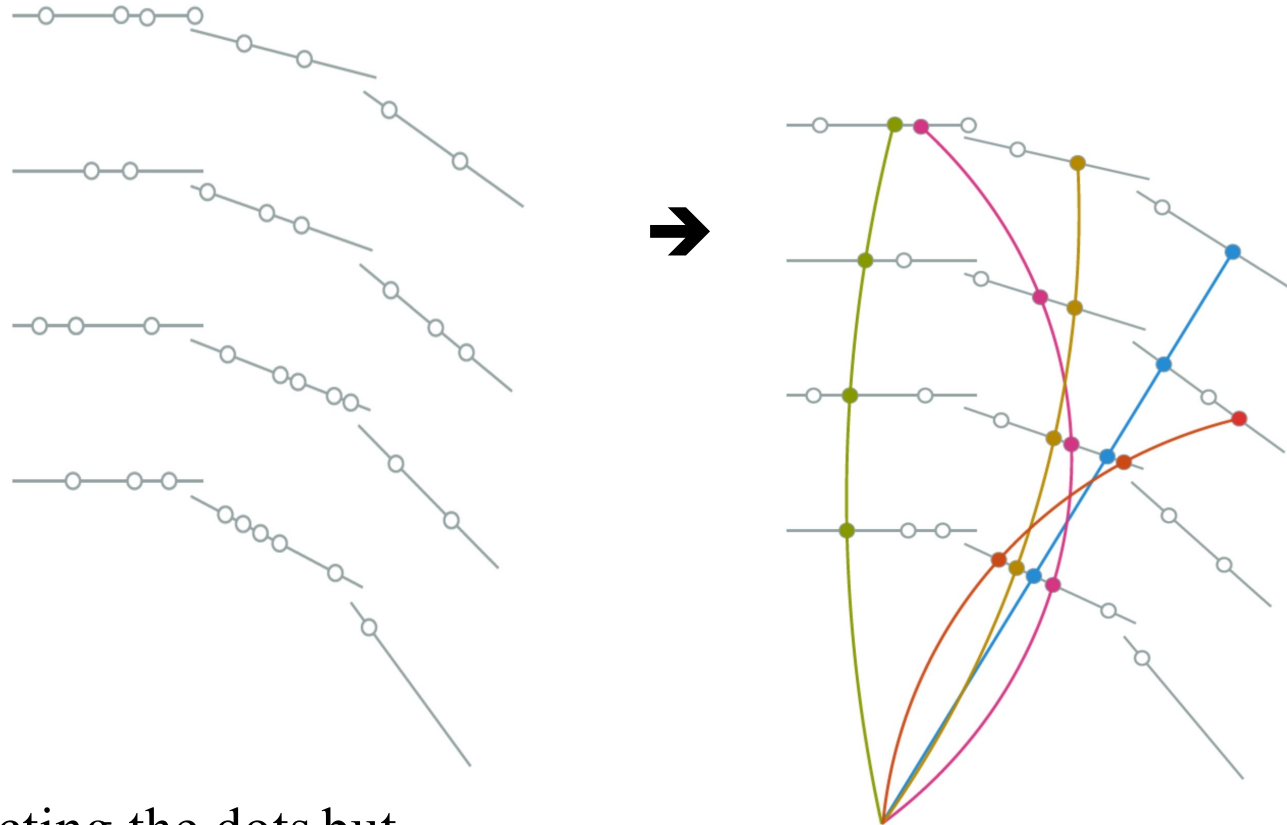
# HL-LHC All Silicon Tracker (Simulation)



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# Problem Definition

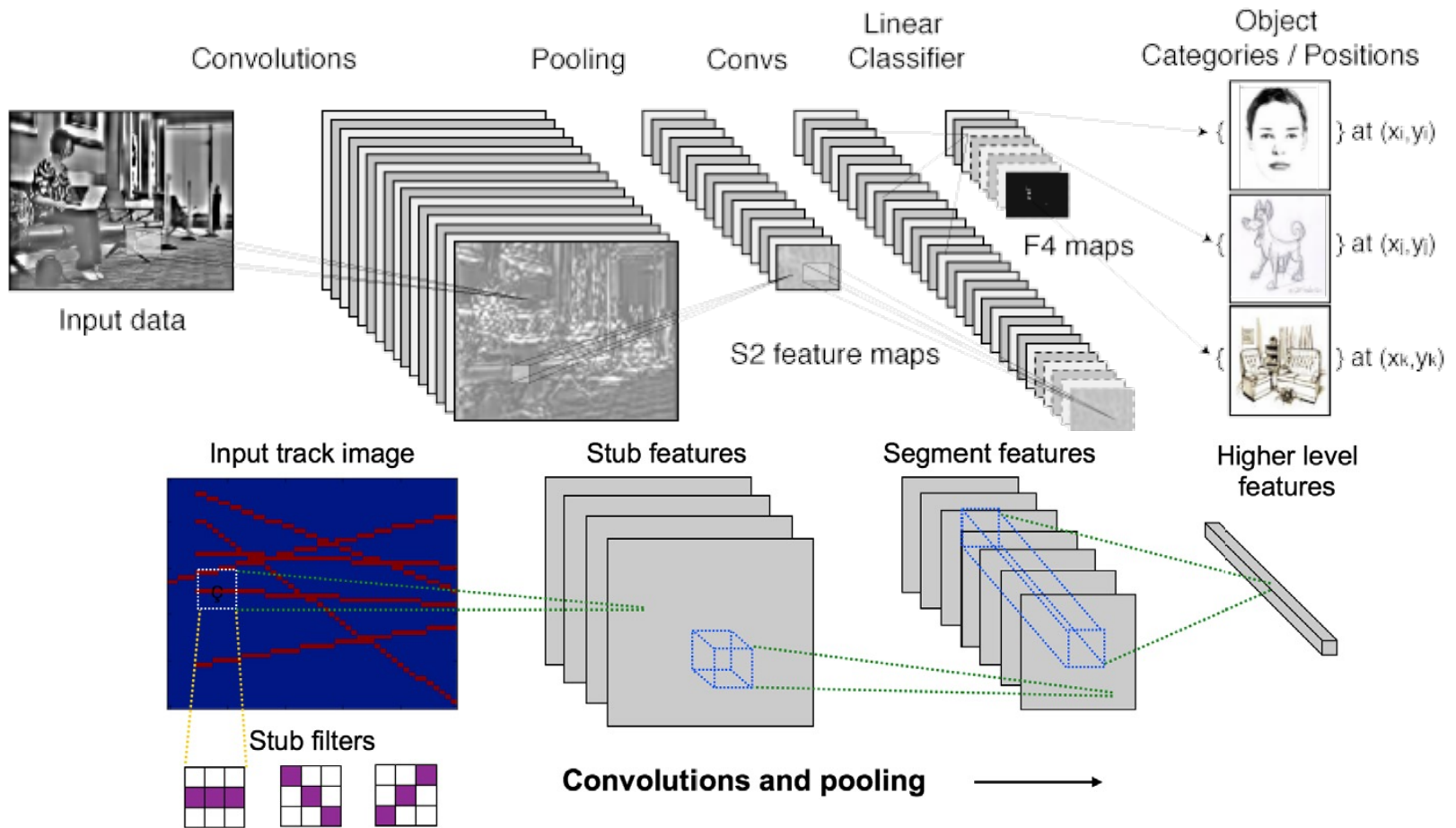


Connecting the dots but

- 3 dimensions
- 100'000 points into 10'000 tracks

# Convolution NN ?

## Image based Approach

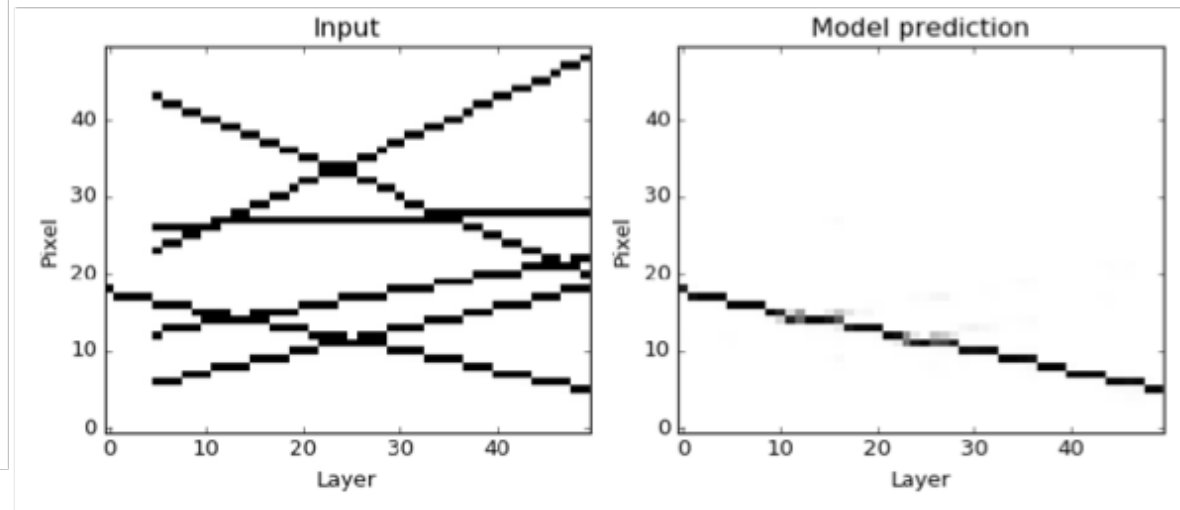
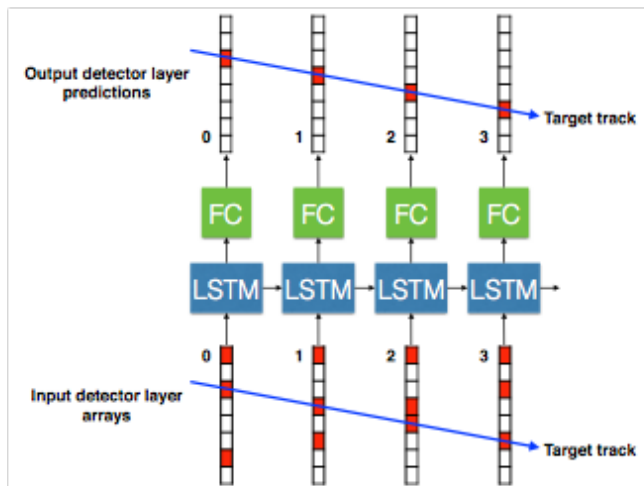


# Recurrent Neural Networks (RNN) ?

## Point based Approach



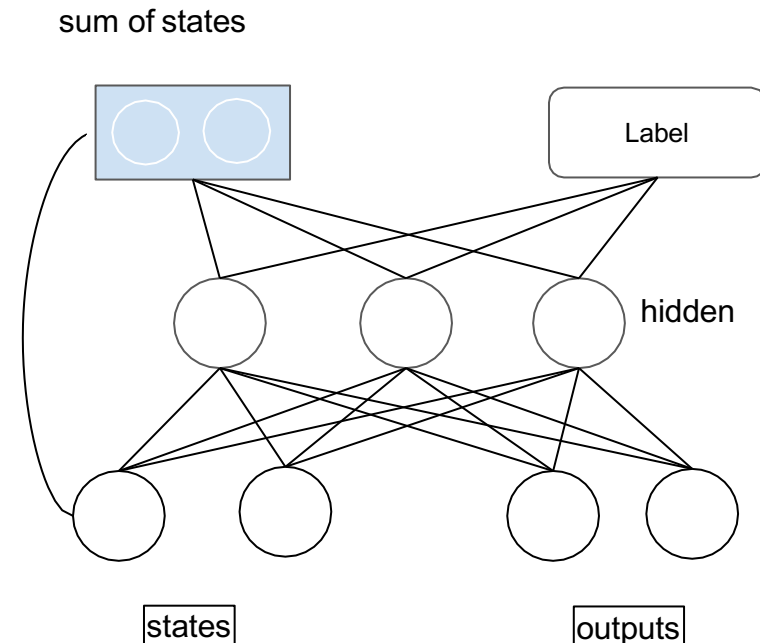
## Long Short Term Memory (LSTM)



# Graph Neural Network



- A graph is processed node by node in a random order
- For a node in graph, the sum of the state vectors of neighboring nodes are computed and concatenated to its own label vector
- The algorithm guarantees a convergence of the state nodes to a stable and unique solution

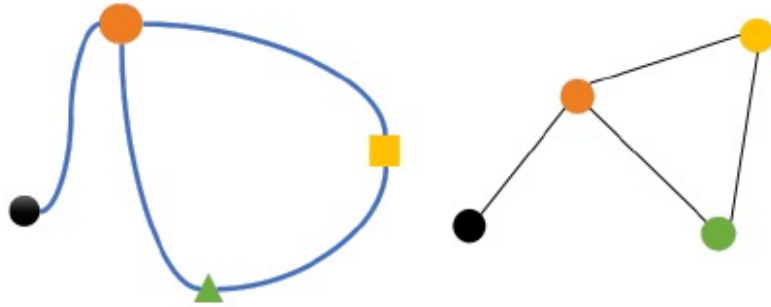




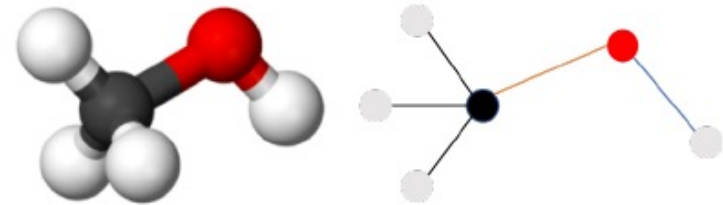
# Application Domains



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Computer Science:  
Routing + tracking algorithms



Chemistry:  
Molecular engineering



# TrackML Throughput phase 3rd place



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Phase 2 cloudkitchen



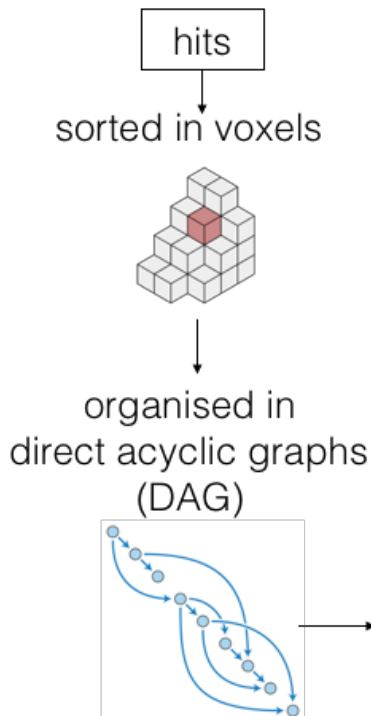
Accuracy: 0.93  
Time/event: ~7 sec  
Memory: 0.7 Gb

Author: Marcel Kunze

partly based on top quarks Phase 1 solution

1 - Top Quarks 0.92182 10 2mo

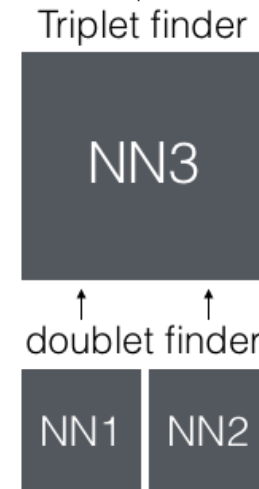
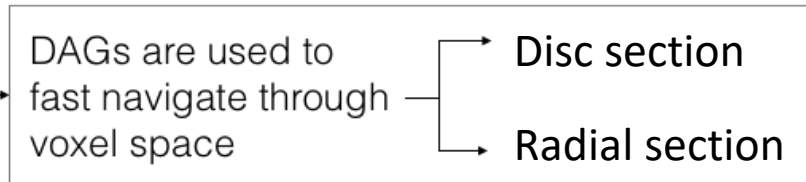
Algorithm outline



Main steps

- Select promising pairs  
• 7 million / 0.99
- Extend pairs to triples  
• 12 million / 0.97
- Extend triples to tracks  
• 12 million / 0.95
- Add duplicate hits to tracks  
• 12 million / 0.96
- Assign hits to tracks  
• 90% of hits / 0.92

DAGs are pre-trained on ~25 events ground truth



# Graph Network Training



## Define spatial elements in $\phi*\theta$ (voxel)

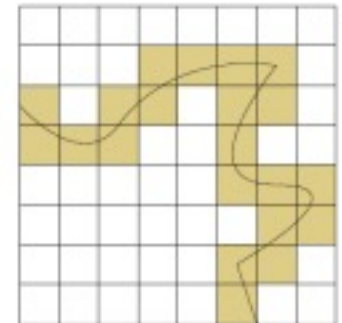
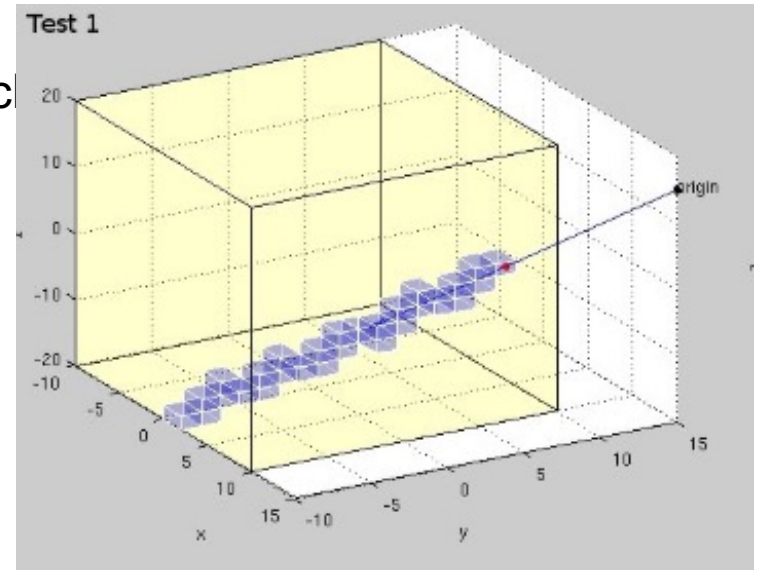
- Organize the voxels in DAGs according to track evolution in radial direction
- Flexible to model even arbitrary paths (kinks, missing hits, outliers, random walk, ..)
- Training is done with MC tracks of typically 15-25 events

## Multiscale resolution

- Multiple networks for doublet finding ( $\theta$ )
- Multiple networks for triplet finding ( $\phi, \theta$ )

## Path finding

- Sort event hits into the trained networks
- Seed and follow the path strategy
- Which is the right direction to go?
- Classify doublet and triplet patterns of points





## Intuition

- Model free estimator
- Start with basic quantities
- Coordinates, simple derived values
- Only very basic detector specific information

## Feature space

- Polar coordinates ( $R_t, \phi, z$ )
  - Directional cosines wrt. points
  - Simple helix calculation (score)
- } In principle not needed, but speeds the things up !

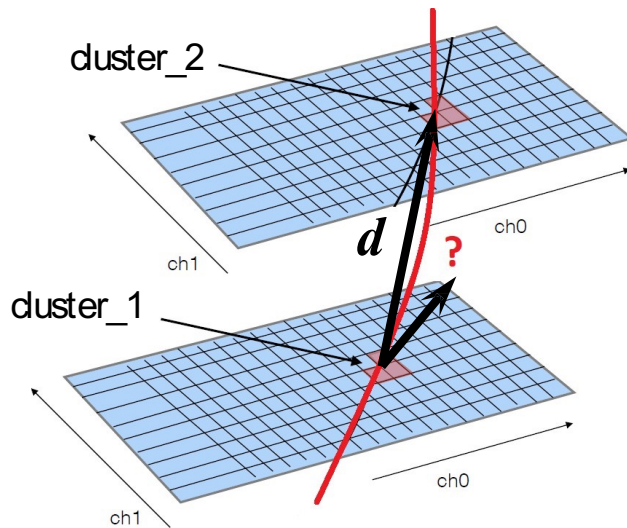
## Training

- Supervised: presenting MC ground truth

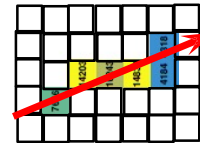
# Feature Space



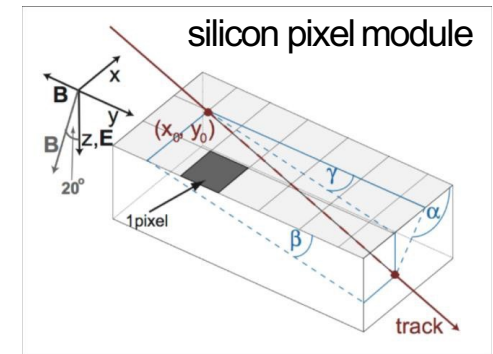
Given two hits (clusters of silicon cells): predict if they belong to the same track



- Estimate track direction from the cluster shape:



eigenvector of covariance matrix of the silicon cells



## Features for the training

- Polar coordinates of the hit doublet:  $(r_1, \phi_1, z_1), (r_2, \phi_2, z_2)$
- Triplet finder works the same with a hit triplet
- Simple helix score
- Angle/length deviations of the vector  $d$  projection from the values predicted by the shape of cluster 1
- Angle/length deviations of the vector  $d$  projection from the values predicted by the shape of cluster 2



# Feature Folding



## The tracking problem is symmetric wrt. polar coordinates

- Fold the input parameter space into an octagon slice using “abs” function
- Considerable improvement of the separation strength of the parameters
- Need less statistics / yield better results

```
-----  
: Rank : Variable   : Separation  
-----  
: 1 : log(score) : 5.039e-01  
: 2 : rz3         : 5.491e-04  
: 3 : phi3        : 7.552e-05  
: 4 : z3          : 4.986e-05  
: 5 : rz2         : 1.519e-05  
: 6 : rz1         : 9.568e-06  
: 7 : phi2        : 4.101e-06  
: 8 : z1          : 1.967e-06  
: 9 : z2          : 1.965e-06  
: 10 : phi1       : 1.503e-06  
-----
```



```
-----  
: Rank : Variable                                     : Separation  
-----  
: 1 : log(score)                                     : 5.978e-01  
: 2 : rz3                                             : 6.329e-04  
: 3 : abs(abs(phi3)-1.57079632679)                 : 1.317e-04  
: 4 : abs(z3)                                         : 5.522e-05  
: 5 : rz2                                             : 2.067e-05  
: 6 : rz1                                             : 1.675e-05  
: 7 : abs(abs(phi2)-1.57079632679)                 : 4.335e-06  
: 8 : abs(z1)                                         : 3.592e-06  
: 9 : abs(abs(phi1)-1.57079632679)                 : 3.038e-06  
: 10 : abs(z2)                                       : 2.963e-06  
-----
```

# Hit Doublet / Triplet Classification: MLP

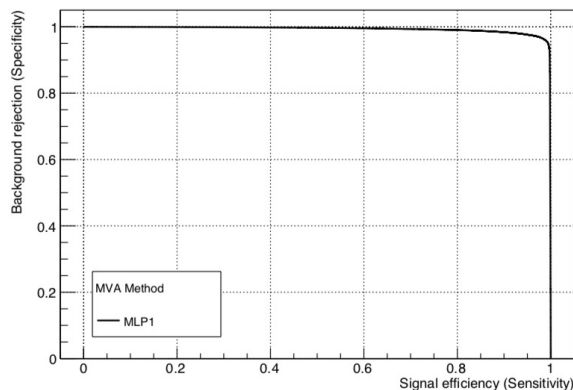
“Shallow learning” ;)



- **Classify the doublets and triplets with neural networks**
  - Multi Layer Perceptron: MLP1 8-15-5-1 / MLP2 9-15-5-1 / MLP3 10-15-5-1
  - Input: hit coordinates, directional cosines towards the clusters, helicity score wrt. origin
  - Output: doublet/triplet quality, supervised training with Monte-Carlo ground truth
  - Training: Typically 10 events, O(Mio) patterns, 500 epochs, one hour on standard PC
  - “Receiver Operation Characteristics” (ROC) curves indicate good quality

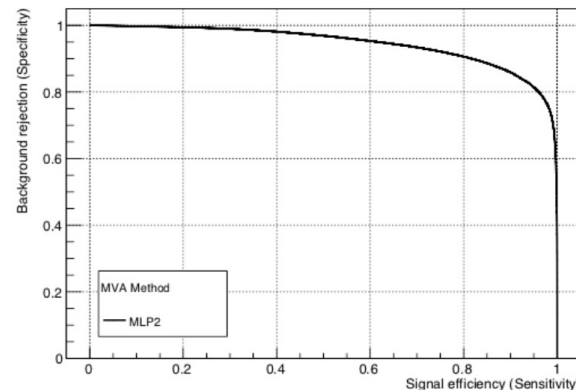
Doublet finder (disc)

Signal efficiency vs. Background rejection



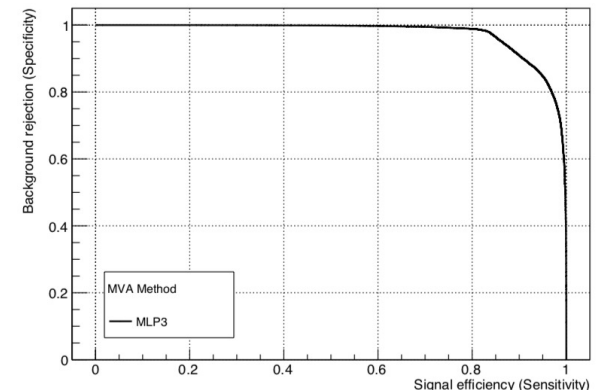
Doublet finder (tube)

Signal efficiency vs. Background rejection



Triplet finder

Signal efficiency vs. Background rejection



Worse due to vertex shift !



# Takeaway Messages



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## Graph Networks

- Very natural data representation for a lot of scientific problems.
- Promising performance in pattern recognition tasks.

Work has been published:

Amrouche, S. et al. *The Tracking Machine Learning challenge: Throughput phase* (2021). [2105.01160](#).



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