Fermilab U.S. DEPARTMENT OF ENERGY Office of Science

Using Next-Generation Detectors with Graph Neural Networks

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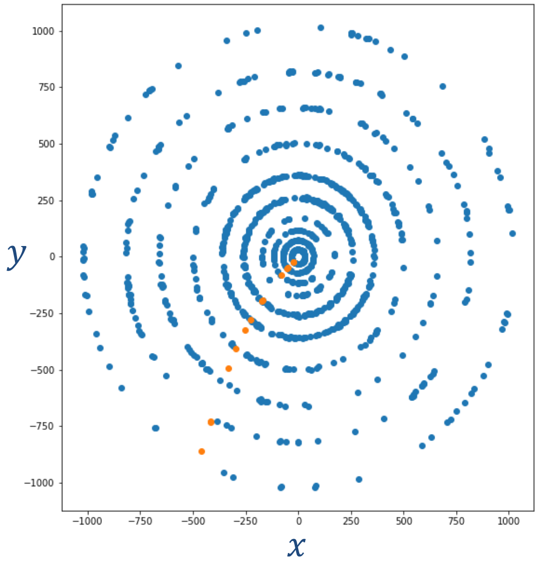
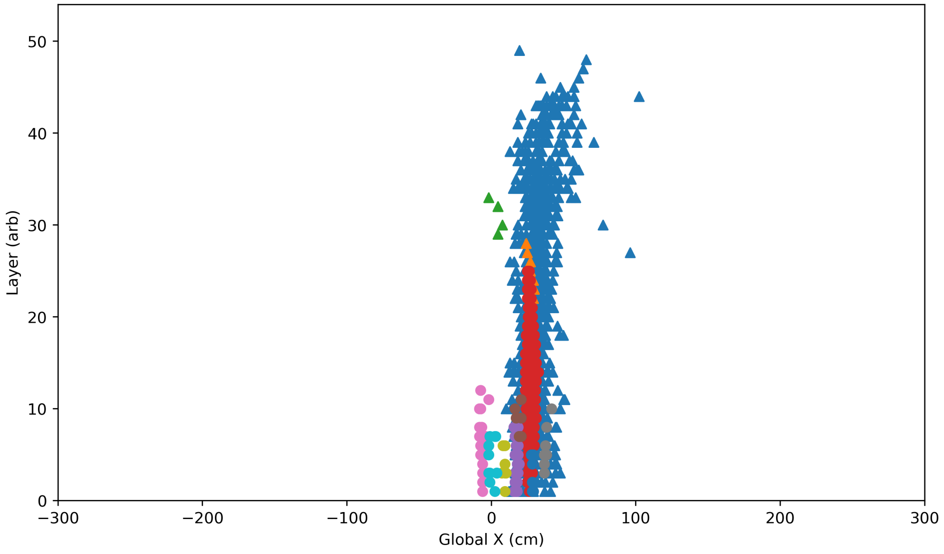
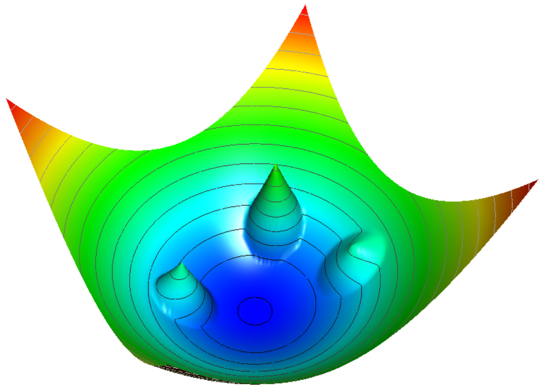
SLAC FPD Seminar
4 August 2020



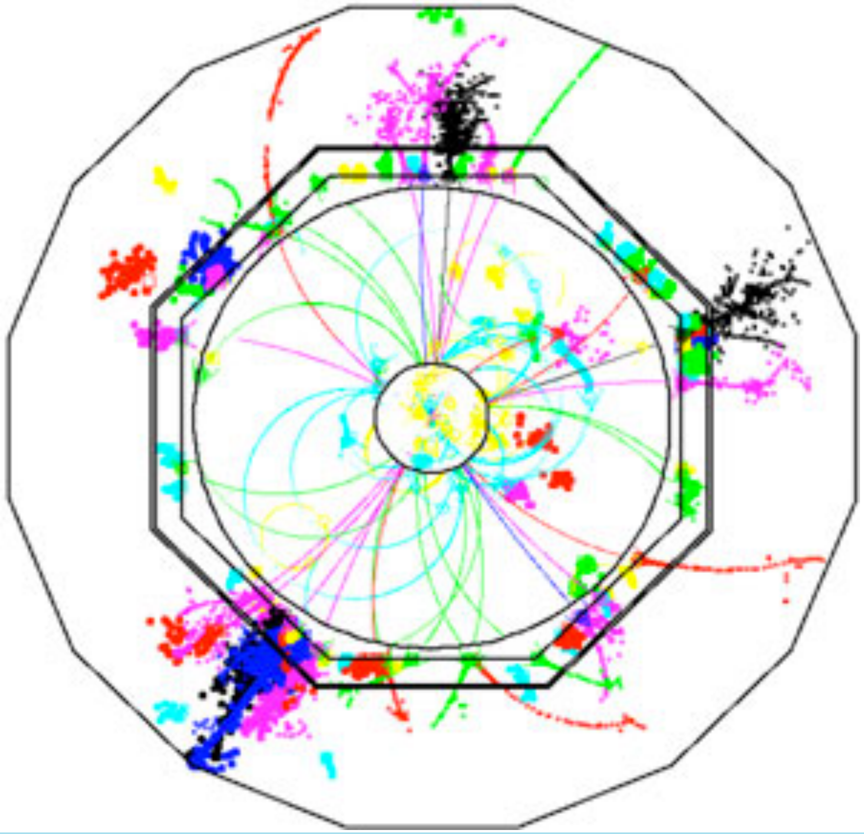




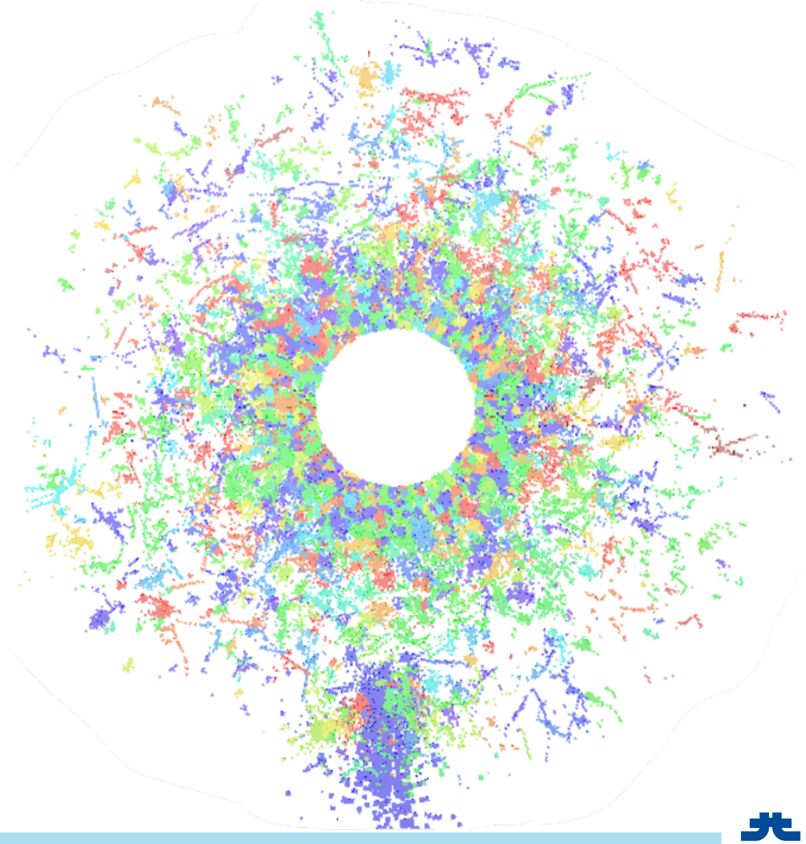
Modern detectors are significantly more complex

- Detectors are changing, they’re becoming more larger, more granular
  - DUNE, the CMS High Granularity Calorimeter (HGCAL)
  - HL-LHC Trackers + Timing Detectors
- They’re aiming for high performance in strenuous environments
  - ILD aiming for electron positron collider, HGCAL for HL-LHC
  - Readouts include precision timing information, but have to correlate x,y,z,t & E
  - Detector performance depends much more on algorithmic physics performance

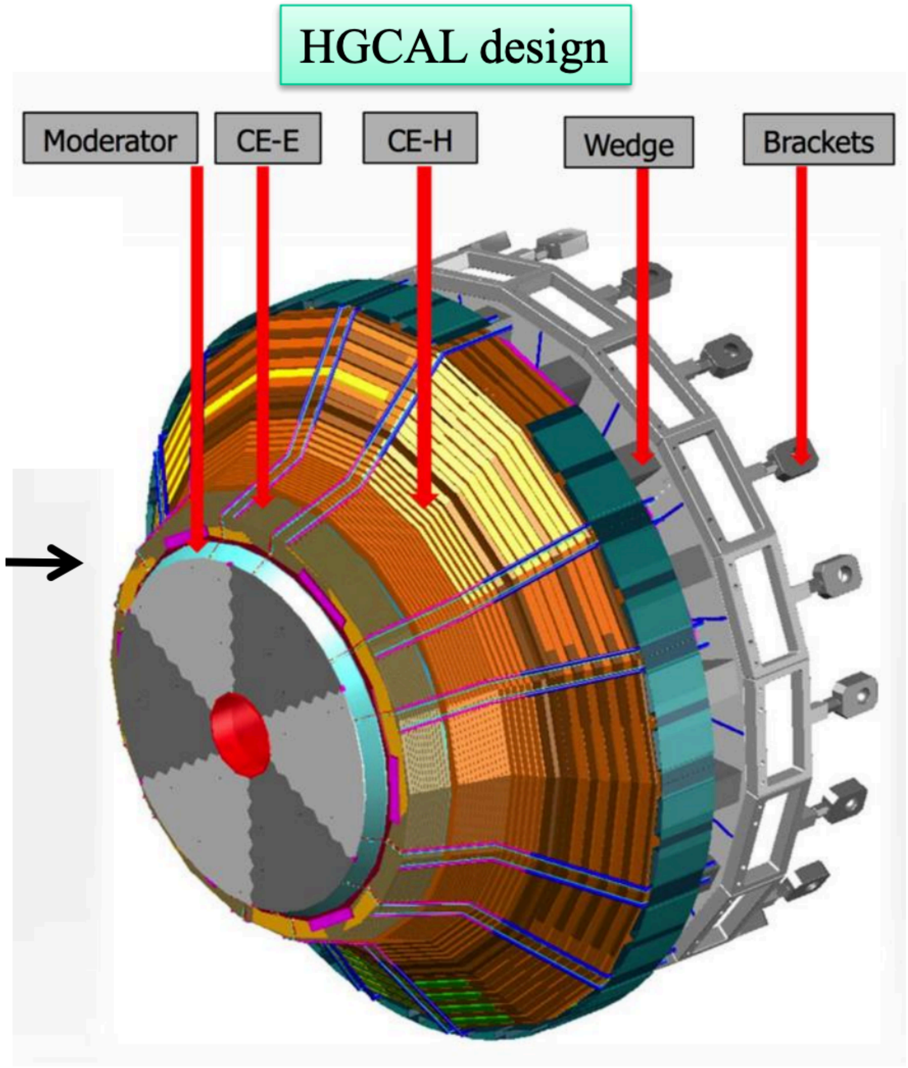
ILD Event Display (whole detector)

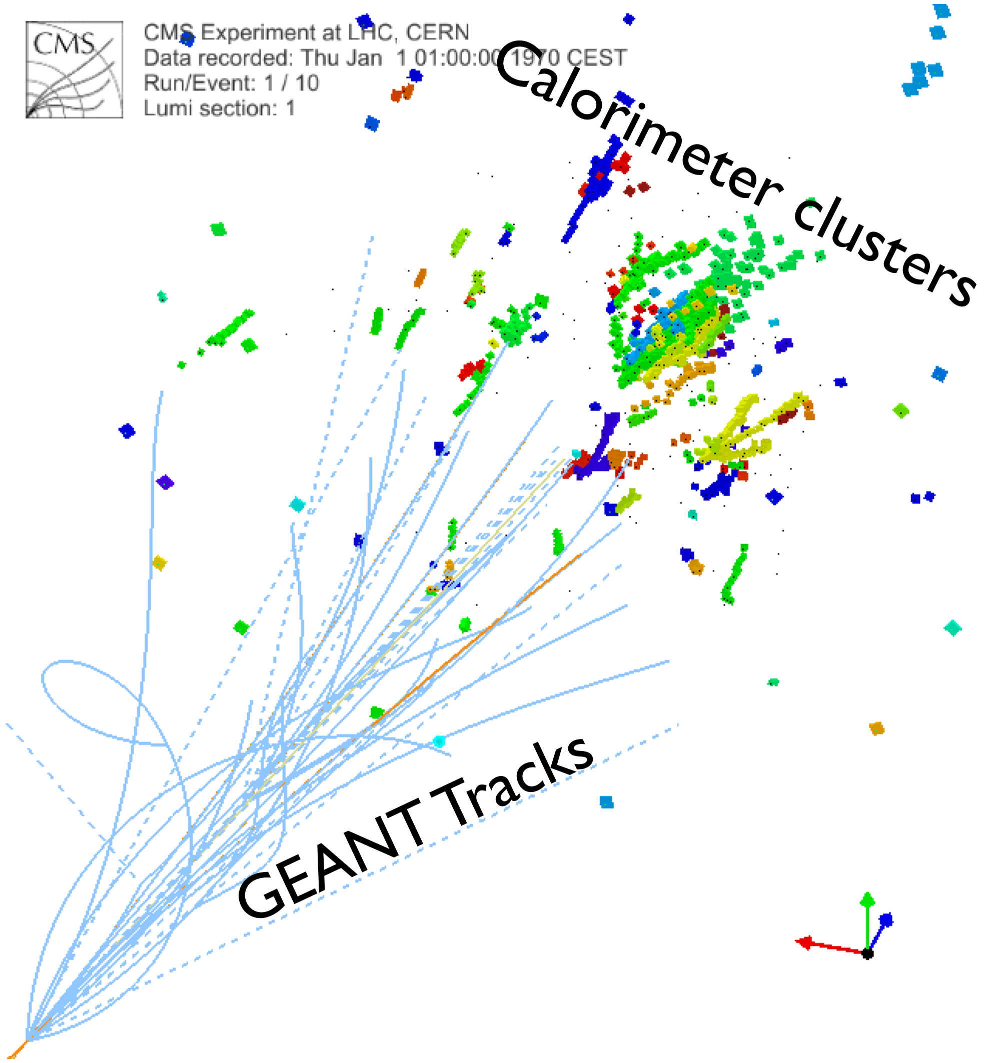


HGCAL Event Display (one endcap)



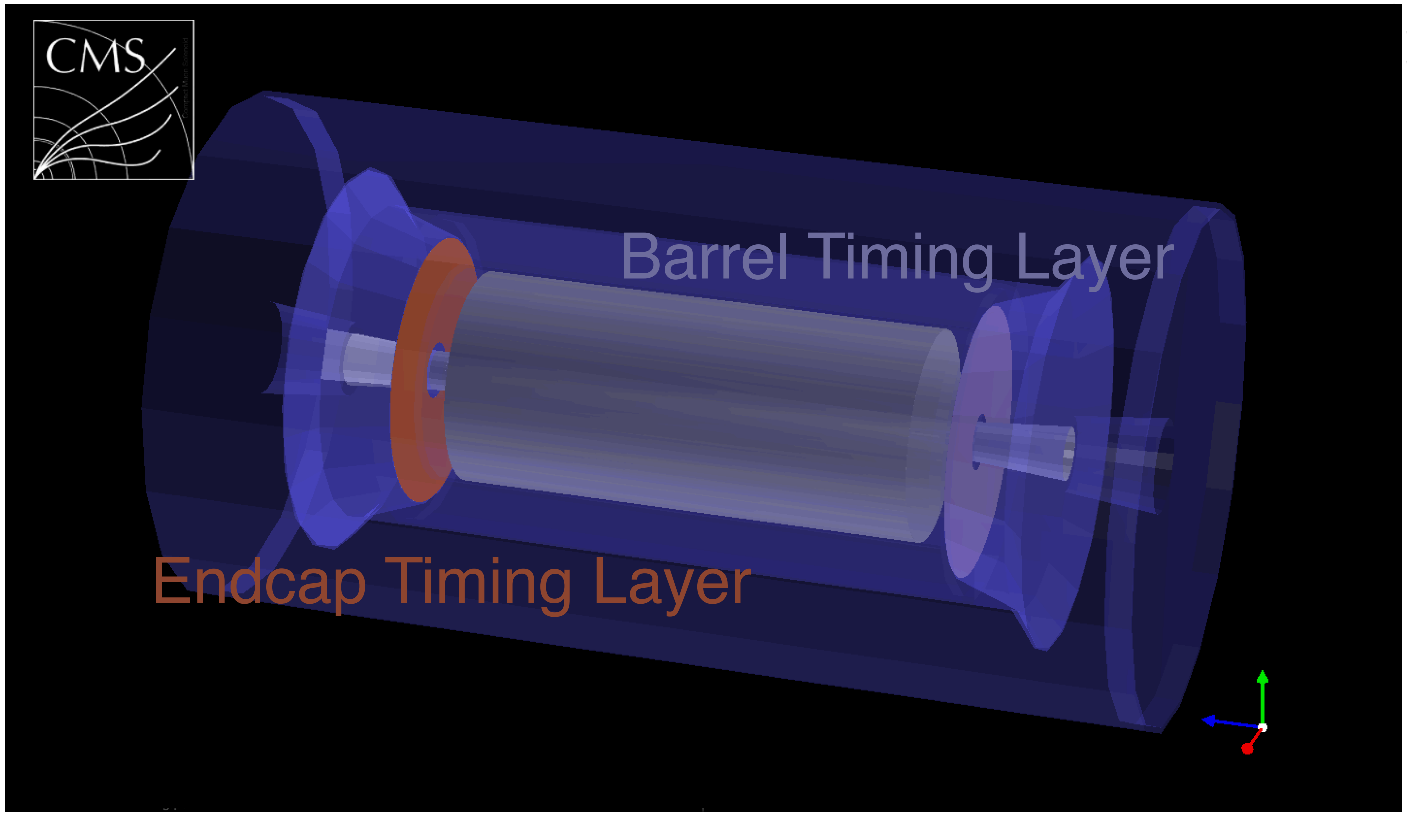
Imaging Calorimetry With HGCal

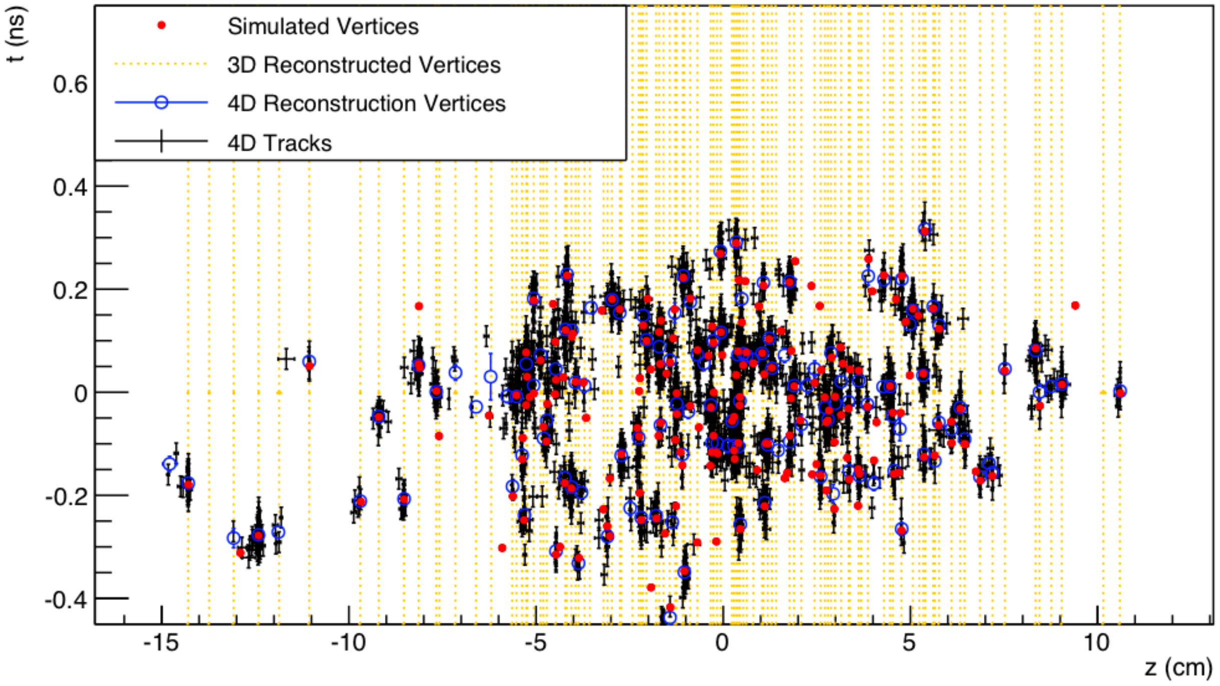




- Rough 6 million channels individually read out
  - Provides sampling calorimetry with 50 instrumented readout planes
  - Can capture the evolution of EM and hadron showers in space as well as time
    - Dedicated timing readout with excellent precision for large energy deposits
  - Higher-dimensional data leads to more easily discernible patterns
- Multiple reconstruction algorithms efforts ongoing to use this device

Timing in Tracking for HL-LHC





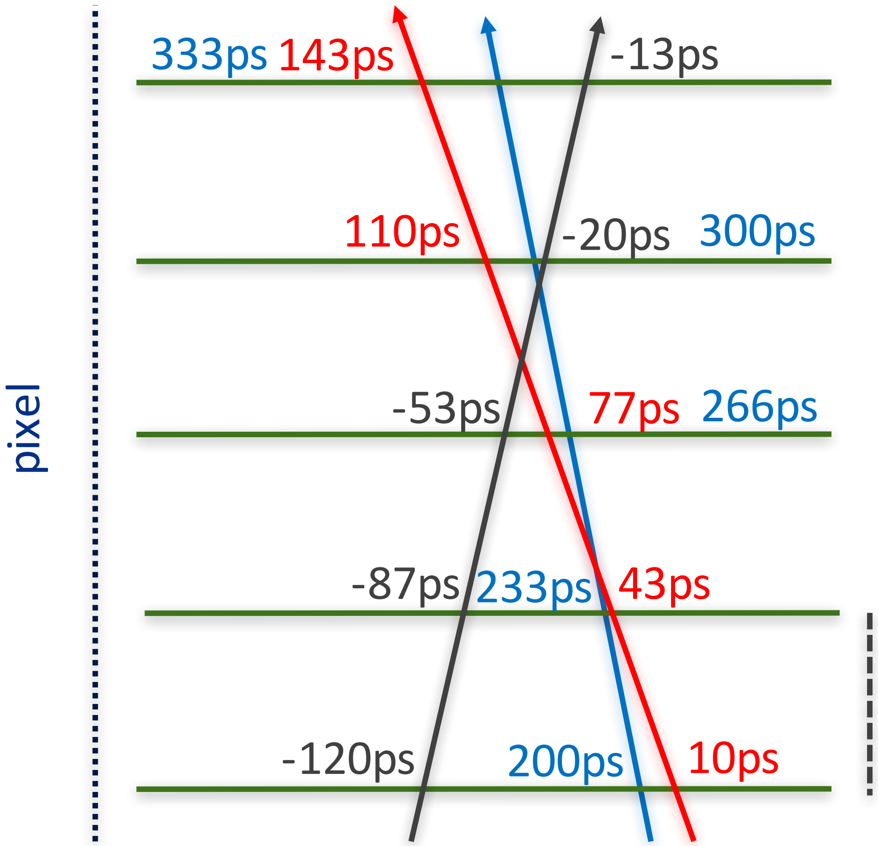
MTD TDR CMS-TDR-020

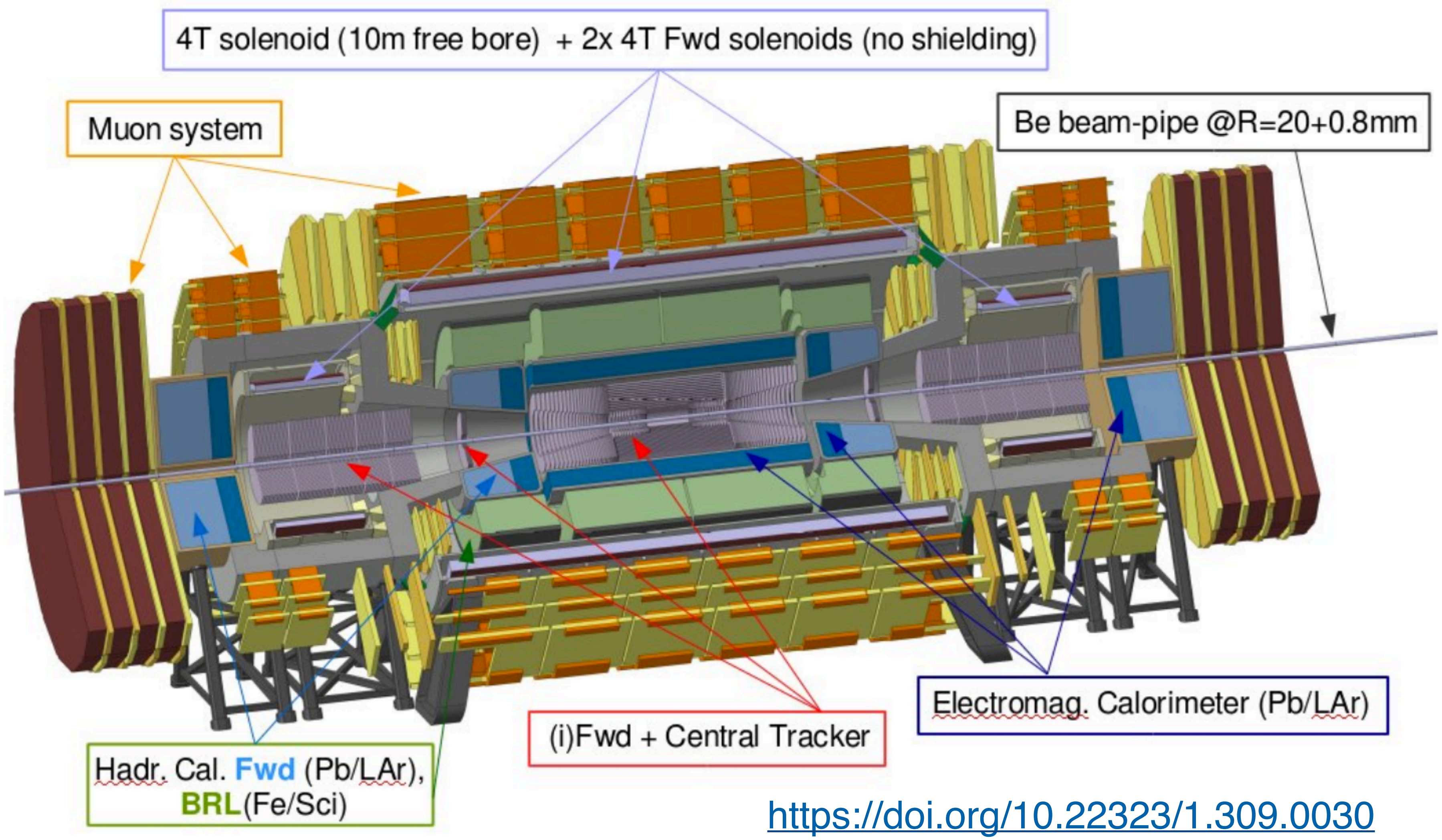
- CMS - MIP Timing detector
  - Strategy is to match precision timing hits to inner-detector tracks, back propagate time to vertices with ~30ps precision at beginning of life
  - Results in pileup removal in isolation cones, particle ID capabilities, excellent sensitivity to a variety of long-lived particles
  - Being integrated into general CMS tracking algorithms to make most informed choices
  - Higher-dimensional data leads to more easily discernible patterns
- Forward-only detector in ATLAS - HGTD to bolster forward tracking

Where granularity and timing in detectors is going:

- FCC-hh concept designs include timing in most or all layers of trackers extending to $|\eta| < 6$
  - Precision timing capabilities anticipated in all calorimetry as well, necessary to make sense of neutral particles in 1000 pileup, many billions of channels
- Timing pixel research ongoing, possible LHCb VELO upgrade

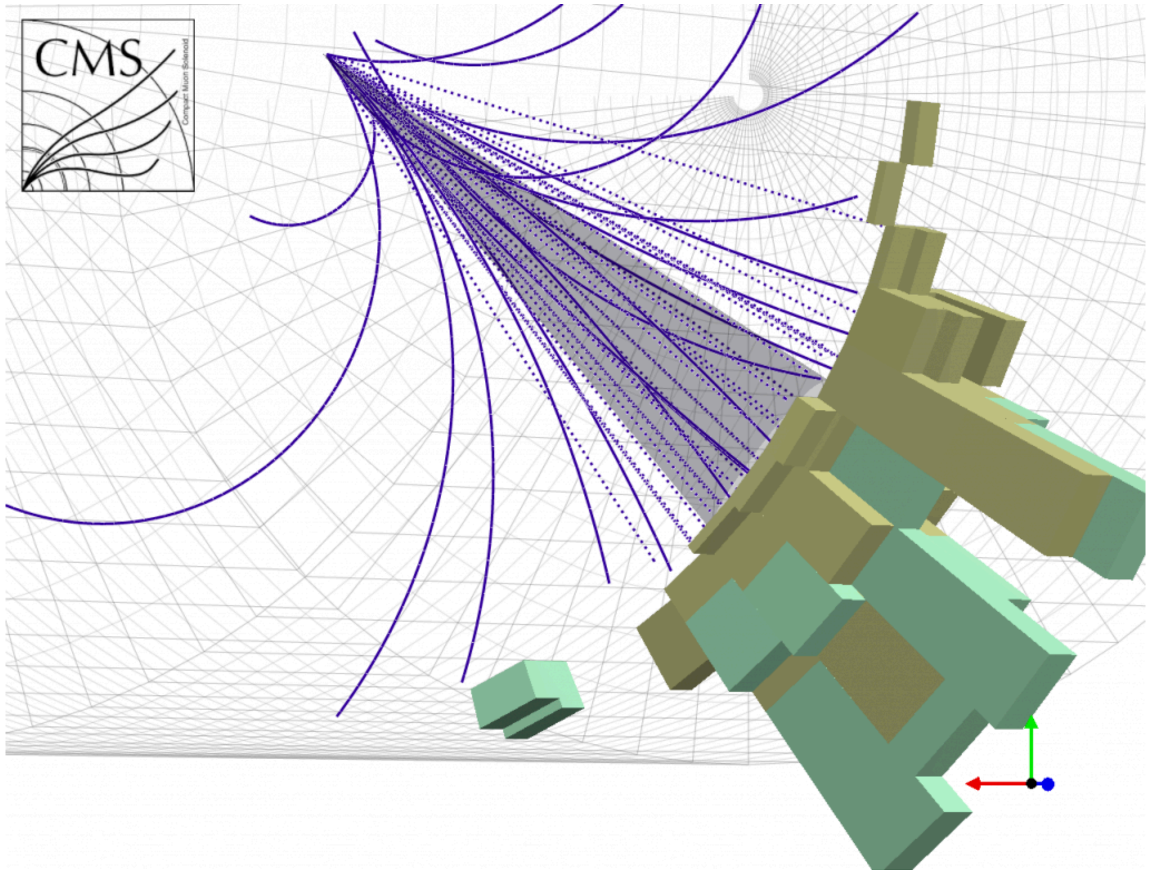
Assume σ_t = 30 ps per layer

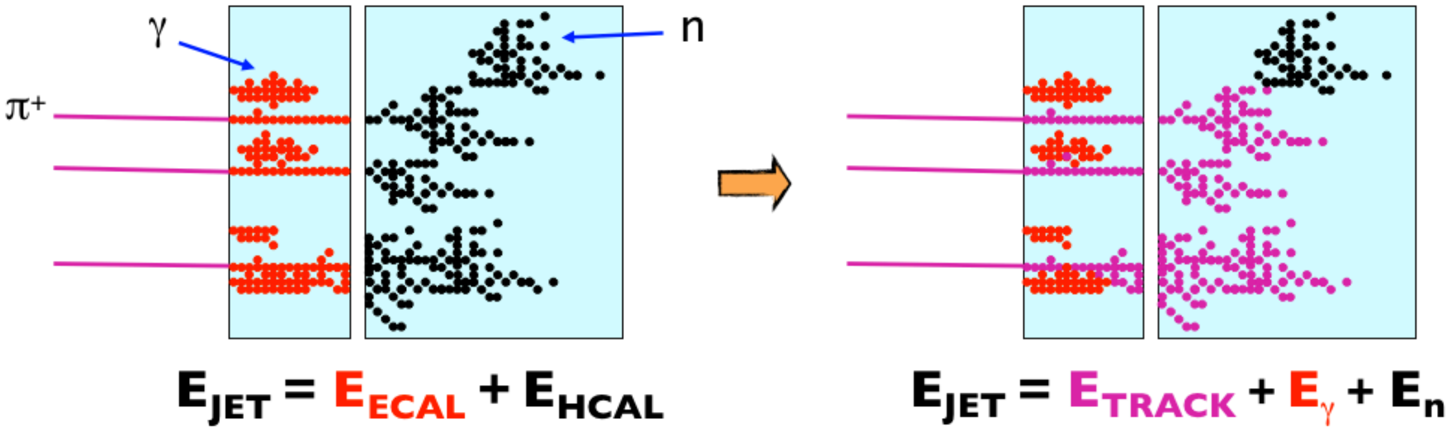




https://doi.org/10.22323/1.309.0030

Algorithms govern detector performance more and more

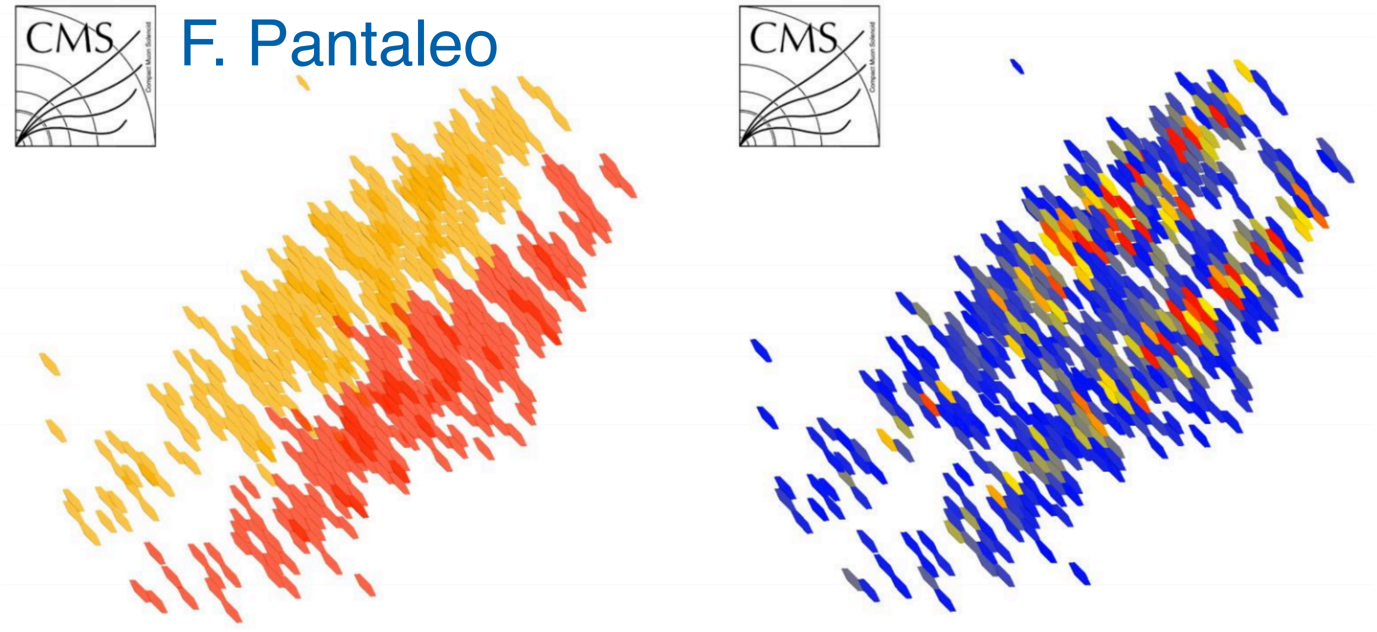




- Finer granularity yields more precise shower identification
  - At the cost of easily conceptualized energy summing rules (e.g. summing towers top left)
  - Now need algorithms to define bounding volumes, etc…
- Particle Flow algorithms help by associating tracking with calorimetry
  - Can use tracking information to bring additional topological information to clustering
  - Further identification of particles allows precise calibrations to be applied (top right)

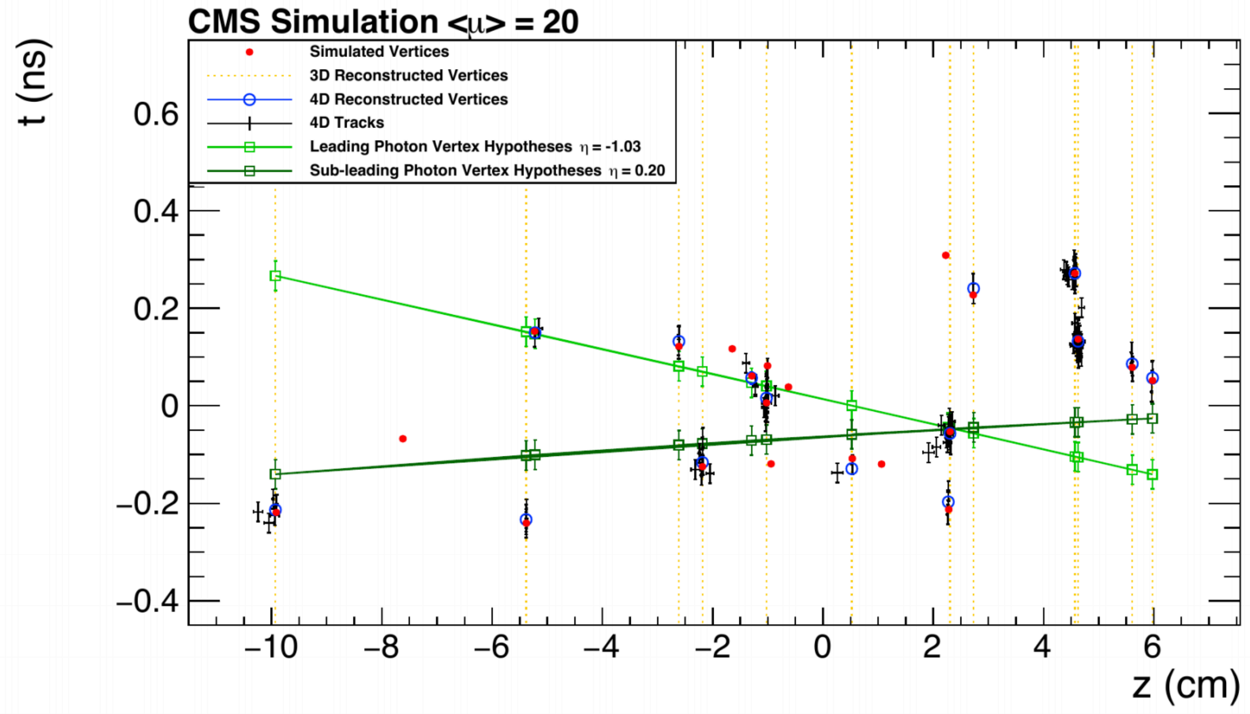
The cost of having more information:

Overlapping photons in HGCal



F. Pantaleo

Cross-references neutral and charged precision timing information

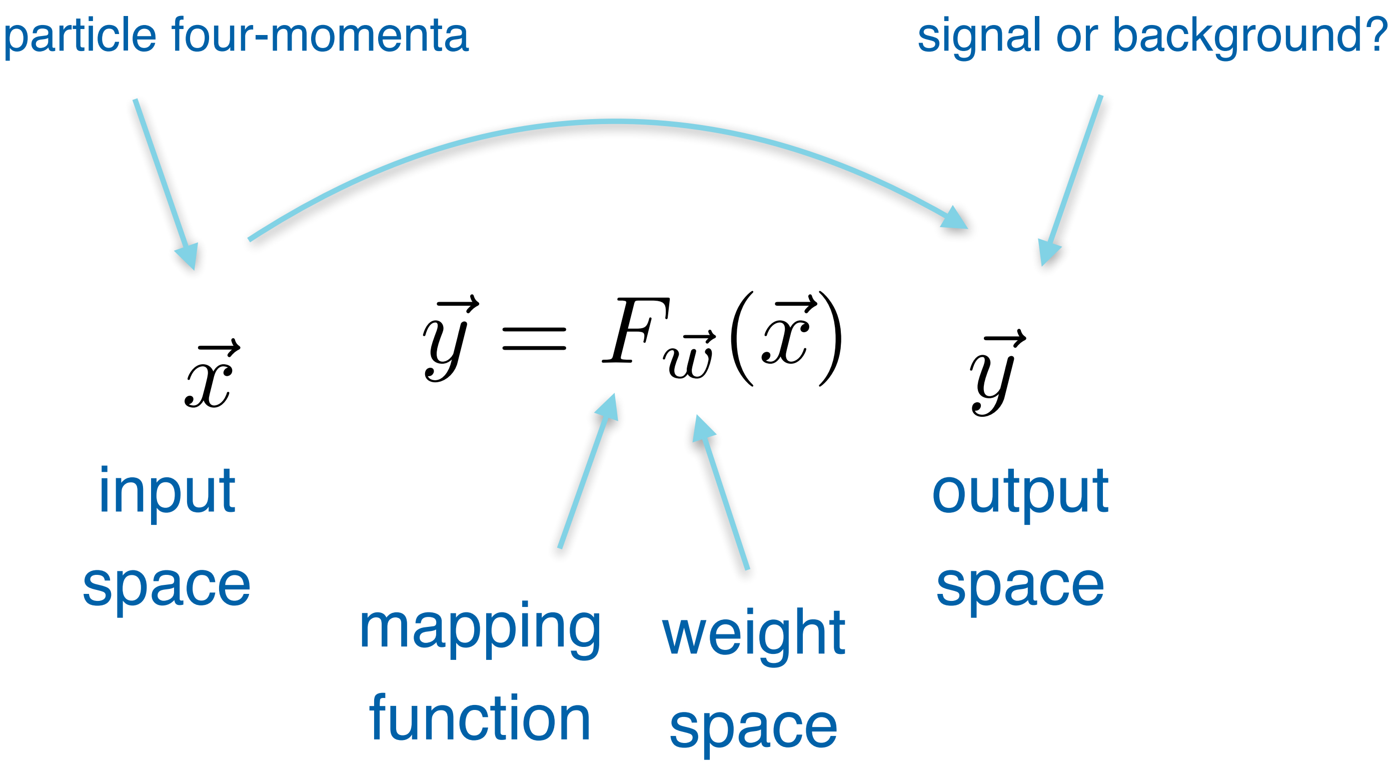


- While the computing costs of more data are clear, it takes significant human time to engineer algorithms that take advantage of more data
  - High dimensionality, while more sparse is far more difficult to reason with effectively
  - For instance: thinking in projections often leads to designing algorithms that mischaracterize some behavior
- The best approach by far, is to try to handle the detector information in its full dimensionality, but humans are not well equipped to do that above 3D
  - Moreover, each detector has its own unique geometry which has to be specifically accounted for

ML and Neural Networks in a Nutshell

- Goal: find the parameters w of a function F that best maps x onto y
  - Do this by minimizing a chosen “loss function”
  - ML is the set of numerical algorithms that solve this problem

- Neural Networks are a subset of these algorithms that are defined recursively from inputs to outputs
  - Any mapping function F can be approximated by a sufficiently large NN
- For detector data, this means that adding timing information or more samples is turned into a problem of scale



particle four-momenta

signal or background?

$\vec{x}$

$$\vec{y} = F_{\vec{w}}(\vec{x})$$

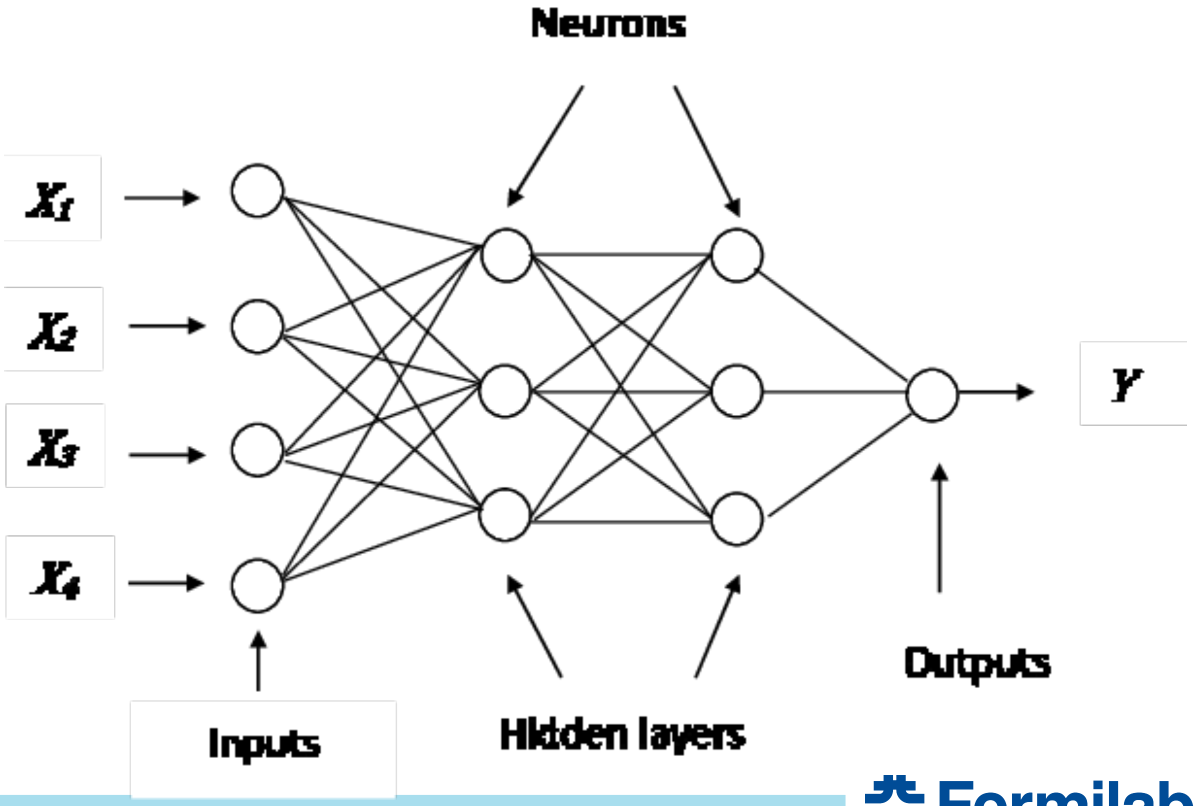
$\vec{y}$

input space

mapping function

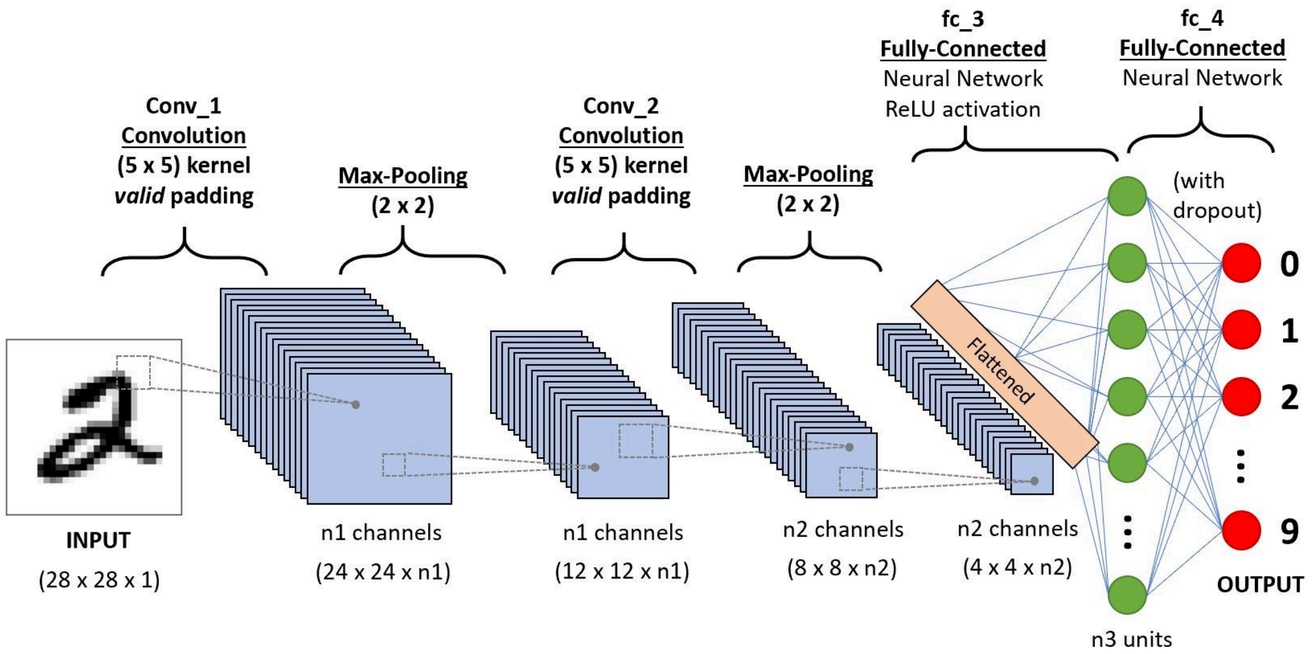
weight space

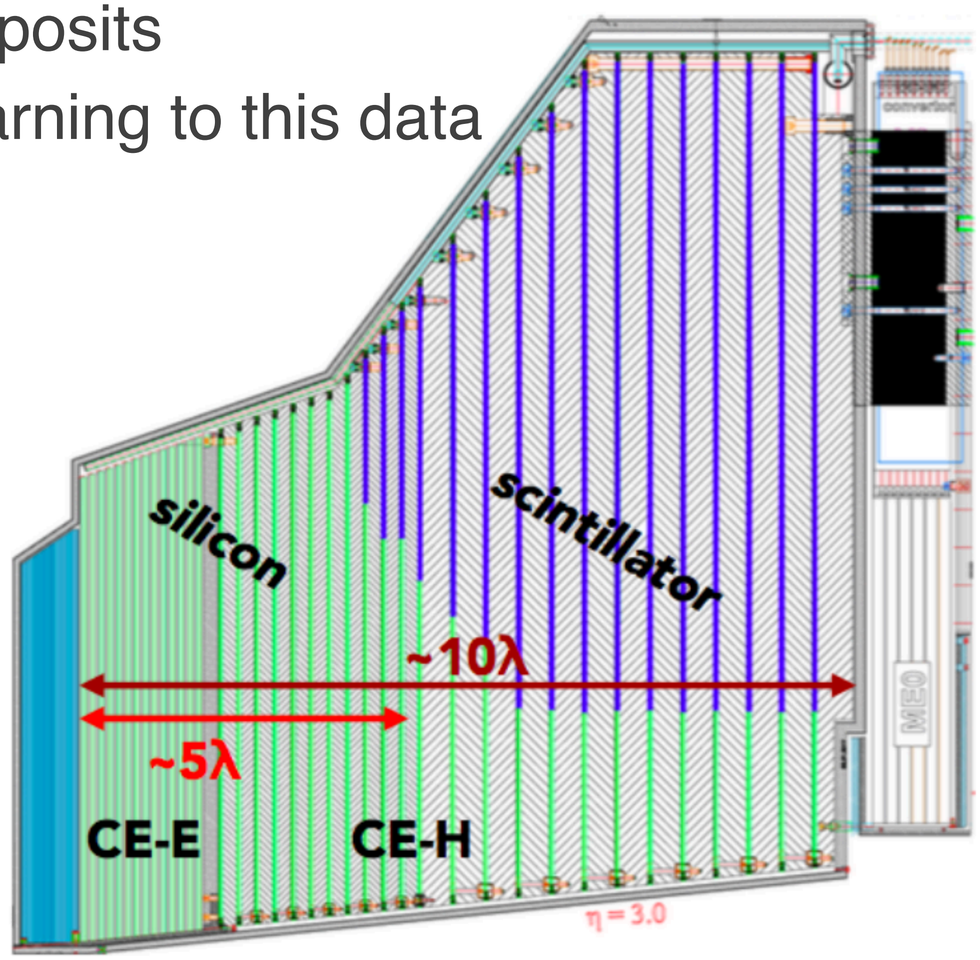
output space



Exploiting granular information with machine learning

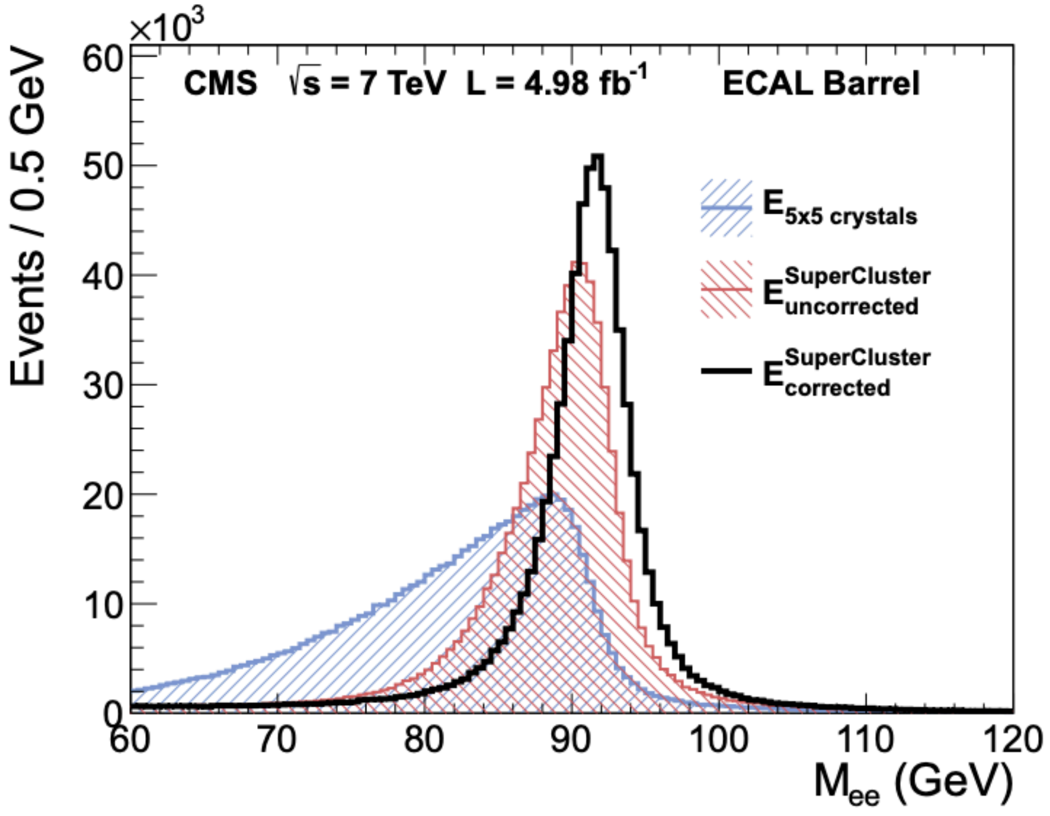
- Modern machine learning can determine important discriminating information in the course of training if the input 'shape' is fixed
  - Using convolutional neural networks for example, images are given as-is for training examples, discriminating features encoded in filters and high-dimensional 'latent spaces'
- However, many next generation particle physics detectors have irregular geometries with zero-suppressed outputs
  - Varying material with sparse sampling of energy deposits
  - Requires different approaches to apply machine learning to this data

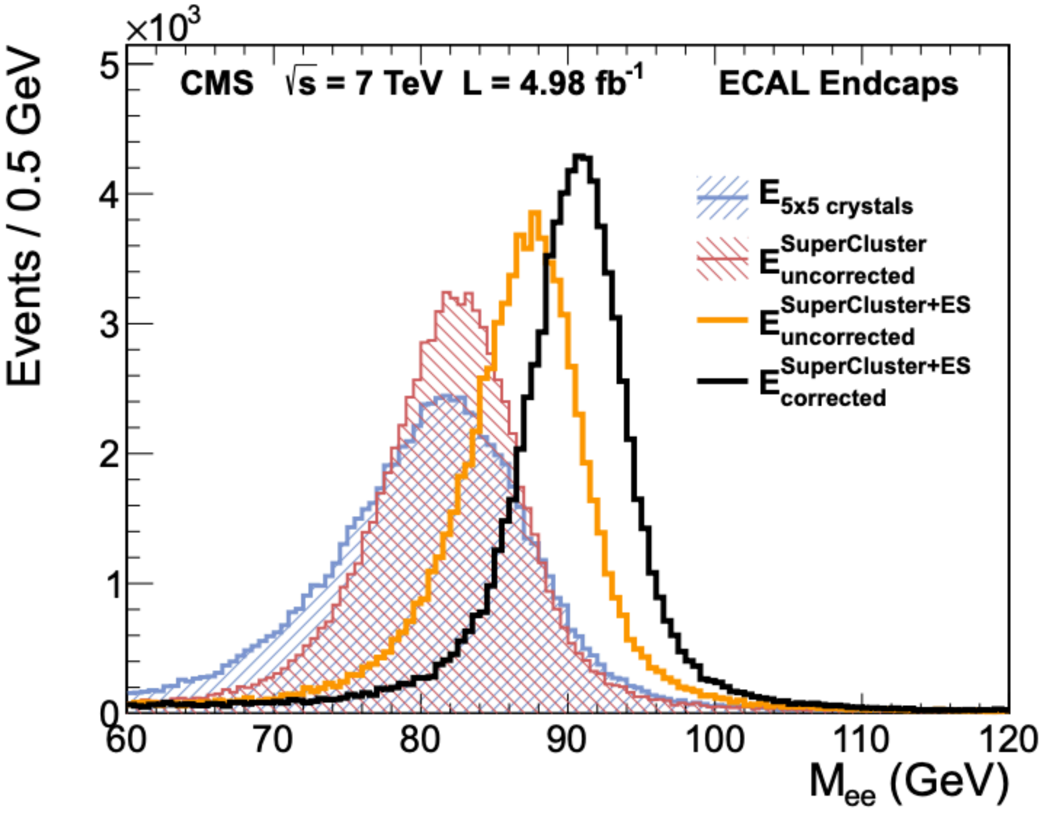




Electromagnetic calorimeter energy corrections

- Boosted Decision Trees (BDTs) have had a long history of use within the CMS Collaboration
  - Relatively fast inference and training times before 2012
  - Functions by making progressively finer cuts in the input space
- Use average over numerous binary-cut based selections to generate a classifier
  - This can be used to discriminate categories or to regress quantities
  - Can handle position dependent corrections as in CMS ECAL, with enough data



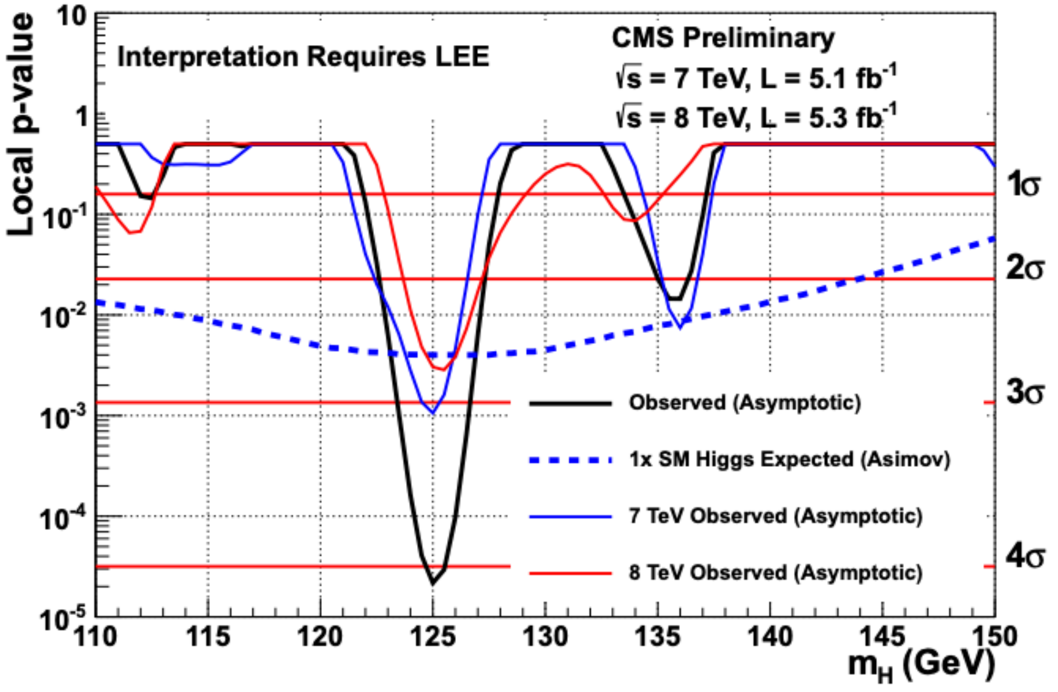


Higgs to γγ Discovery

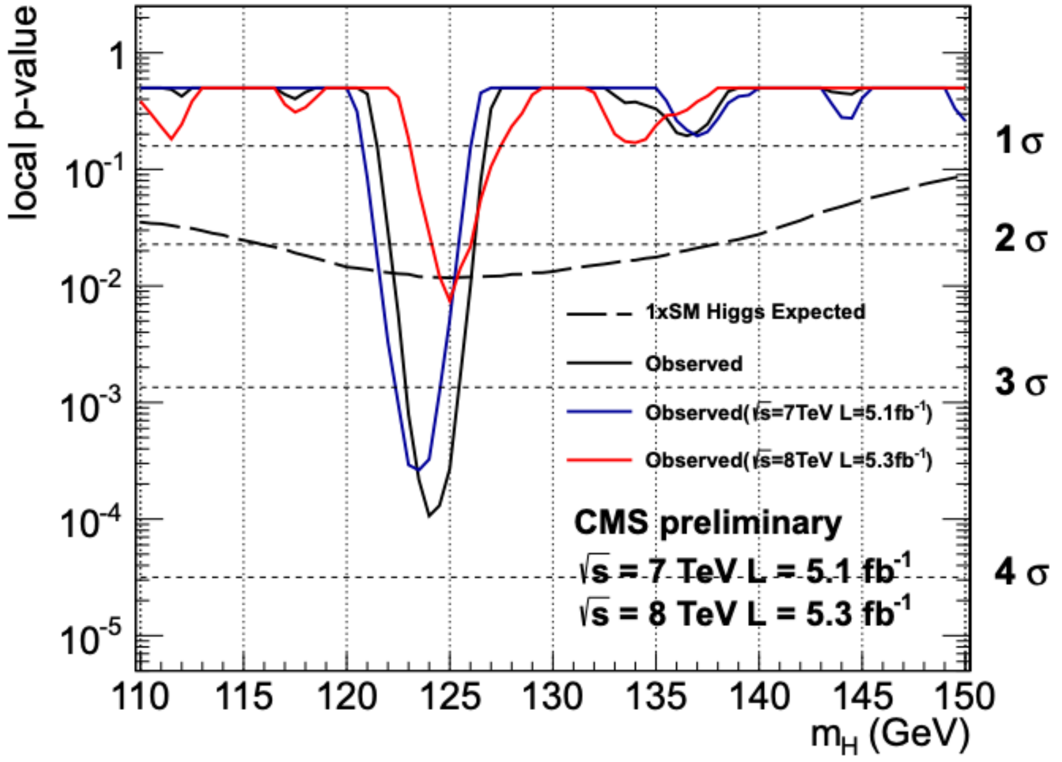
- Usage of ML techniques led to an analysis workflow that is easier to describe and maintain
  - Training based workflow instead of re-optimizing cuts by hand
  - Trade some abstraction for ease of use

- Improved sensitivity
  - At the cost of a lot of jokes about “BDTs all the way down”

- Demonstrable control of systematics related to multivariate modeling of the input data
  - This is now the status quo



(a) mass-fit MVA.



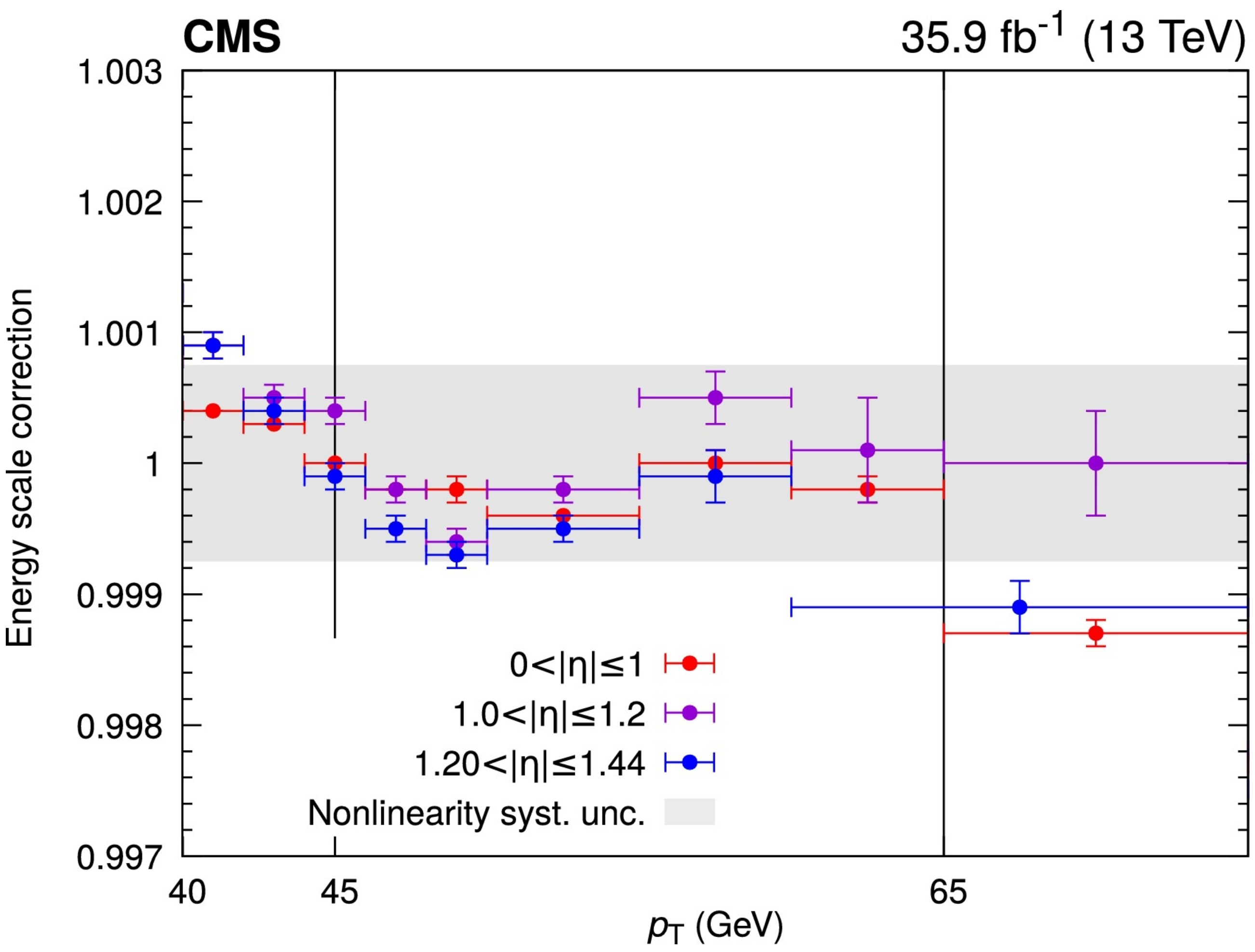
(b) Cut-based analysis.

http://cds.cern.ch/record/1460419

Current usage and performance of ML regression in CMS

- Coming to modern times: the ML-based analysis and energy reconstruction is being used to perform precision measurements
  - Energy scale uncertainties for photons understood to better than 0.1%

- ML-based regressions a critical piece for modern Higgs measurements!



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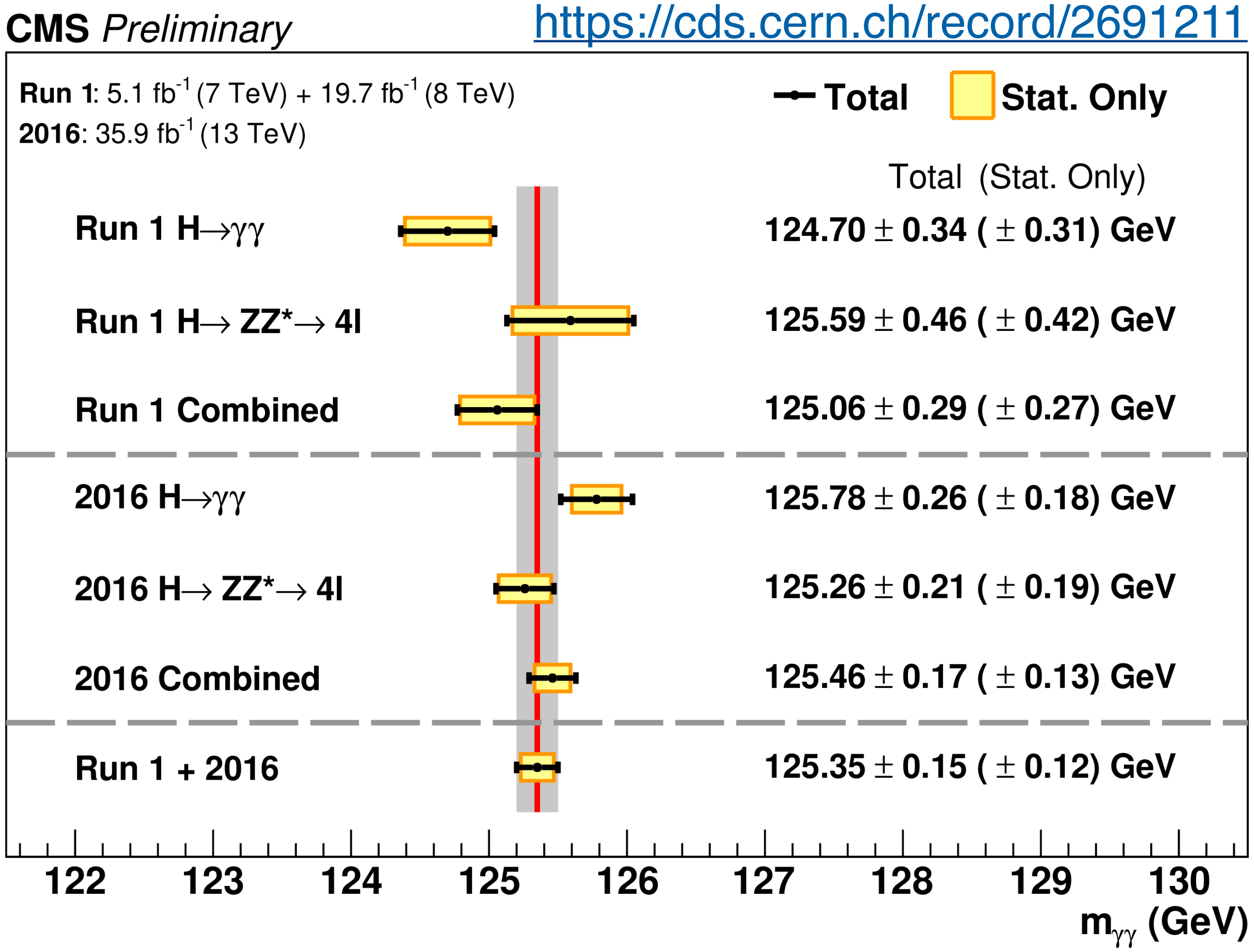
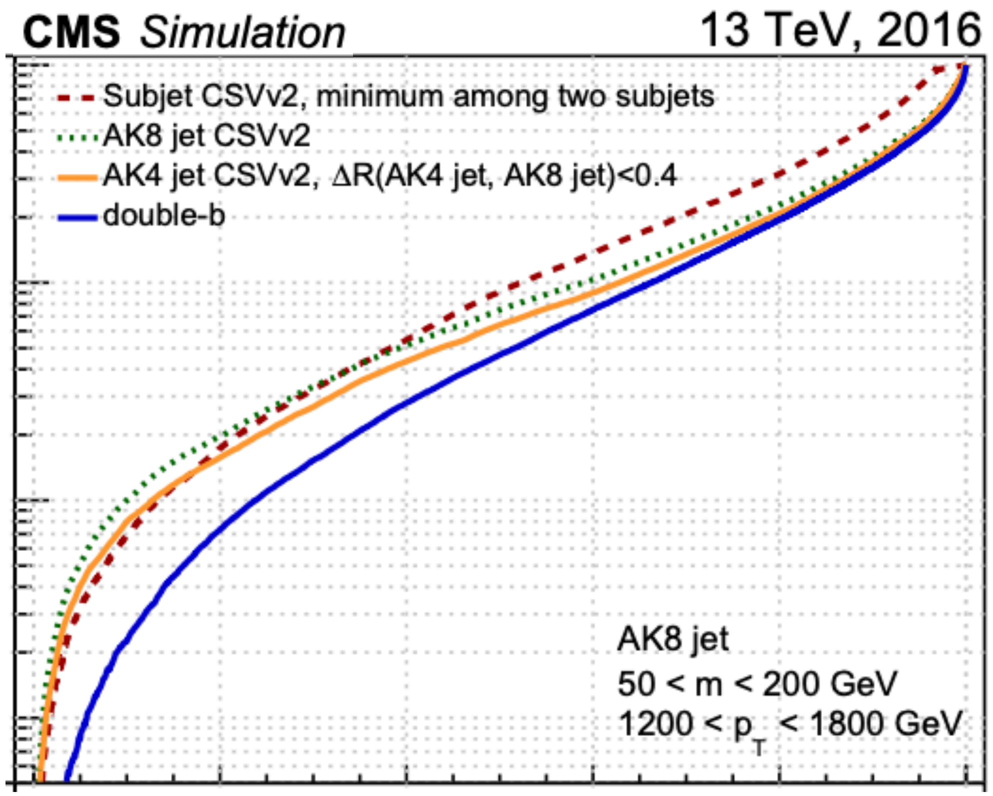
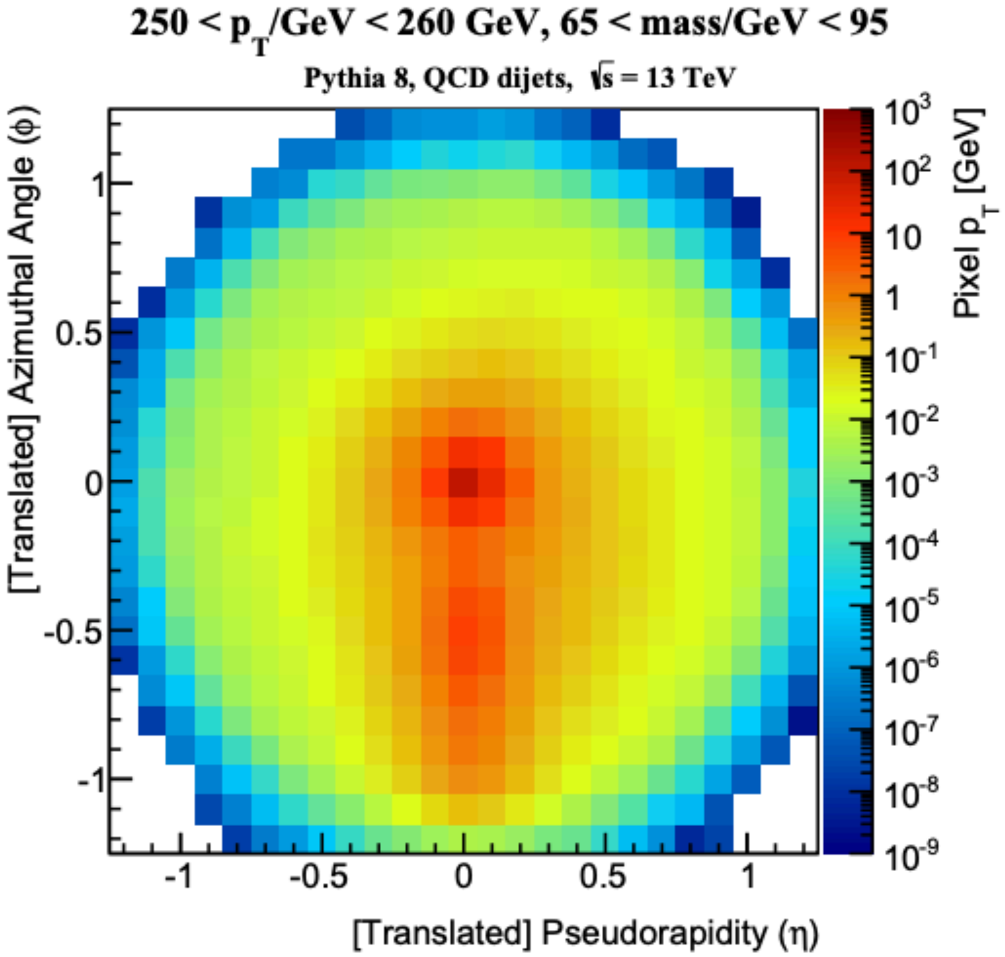


Jet tagging and Jets as images

https://arxiv.org/abs/1511.05190



https://arxiv.org/abs/1712.07158



- Given the complex nature of jets, ML techniques have been commonplace
  - Every particle in a jet has some information about that jet's nature

- Common uses in b-tagging, and more recently merged-jet tagging
  - Evolution from using the original jet clustering very rigidly to allowing the ML algorithm to pick out what relationships are interesting
  - Only possible with modern ML techniques like deep networks or CNNs

Jets aren’t really images though!

- What is seen in the distribution of calorimeters and tracks is the outcome of relationships between hadrons and the QCD fluctuations that made them

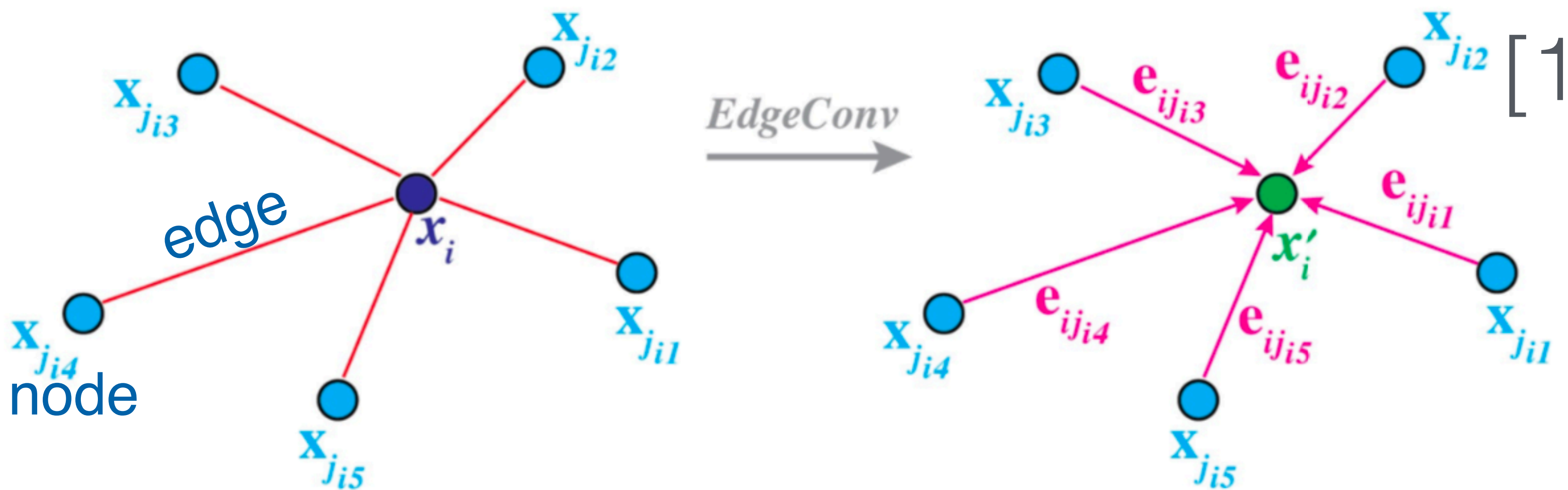
- Jet formation is modeled well by a series of nested branchings of QCD splitting functions
  - This is where the real information about the jet “lives”

- It would be better to try to learn classifying information using this tree of splittings
  - It is more fundamentally related to the physics, a more clear “representation” of the data

- This is a graph, not an image!
  - Moreover, this graph can vary from event to event and jet to jet
  - How can we get around this since the techniques we have so far are static?

- A solution lies in Graph Neural Network (GNN) techniques

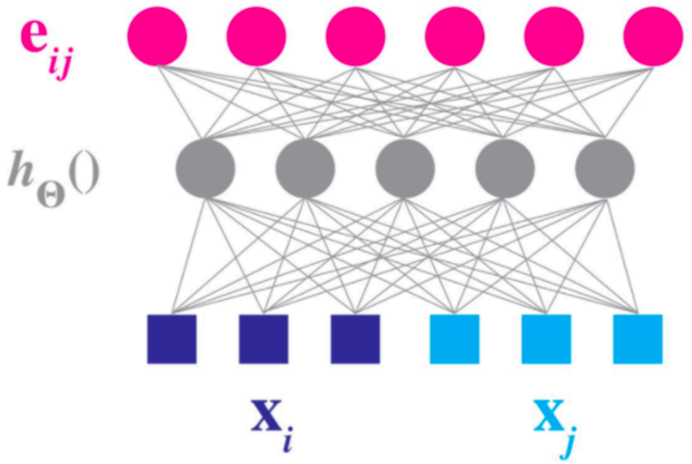
Graph Neural Networks: Edge Convolution



[1801.07829]

- Update $x_i \rightarrow x_i'$ by using **edge features**
  - i.e. learned features of the edges that connects x_i with its neighbors
  - Still independent of ordering of points, but uses **local geometry**
  - '**Convolutional**' as the operation is applied point by point to obtain **x**'
- Calculate edge features simply with e.g. a MLP which takes the node features as input

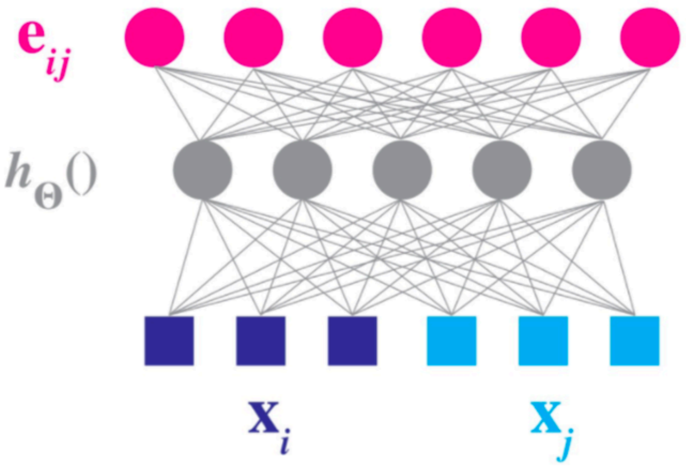
$$\mathbf{x}'_i = \underset{j:(i,j)\in\mathcal{E}}{\square} h_{\Theta}(\mathbf{x}_i, \mathbf{x}_j)$$



Can set dim of edge feature vector

Graph Neural Networks: Dynamic Graph Convolutions

[1801.07829]



$$\mathbf{x}'_i = \mathop{\square}_{j:(i,j)\in\mathcal{E}} h_\Theta(\mathbf{x}_i, \mathbf{x}_j)$$

$$h_\Theta(\mathbf{x}_i, \mathbf{x}_j) = h_\Theta(\mathbf{x}_i)$$ No neighborhood info (only global)

$$h_\Theta(\mathbf{x}_i, \mathbf{x}_j) = h_\Theta(\mathbf{x}_j - \mathbf{x}_i)$$ Only local information

$$h_\Theta(\mathbf{x}_i, \mathbf{x}_j) = \bar{h}_\Theta(\mathbf{x}_i, \mathbf{x}_j - \mathbf{x}_i)$$ Combination of both

- **Dynamic:** Redo kNN after every update
  - The connectivity matrix changes after every update

How graph neural networks are more like general programming

- From the two prior slides - GNNs provide a way to dynamically encode relationships between pieces of data
  - This is the equivalent of loops with nested if-statements, compared to more static fully connected or convolutional networks

- Each operation on the graph drives a new set of decisions based on a ruleset that is learned by the neural network
  - Specifically the network within a GNN making themessages which are passed

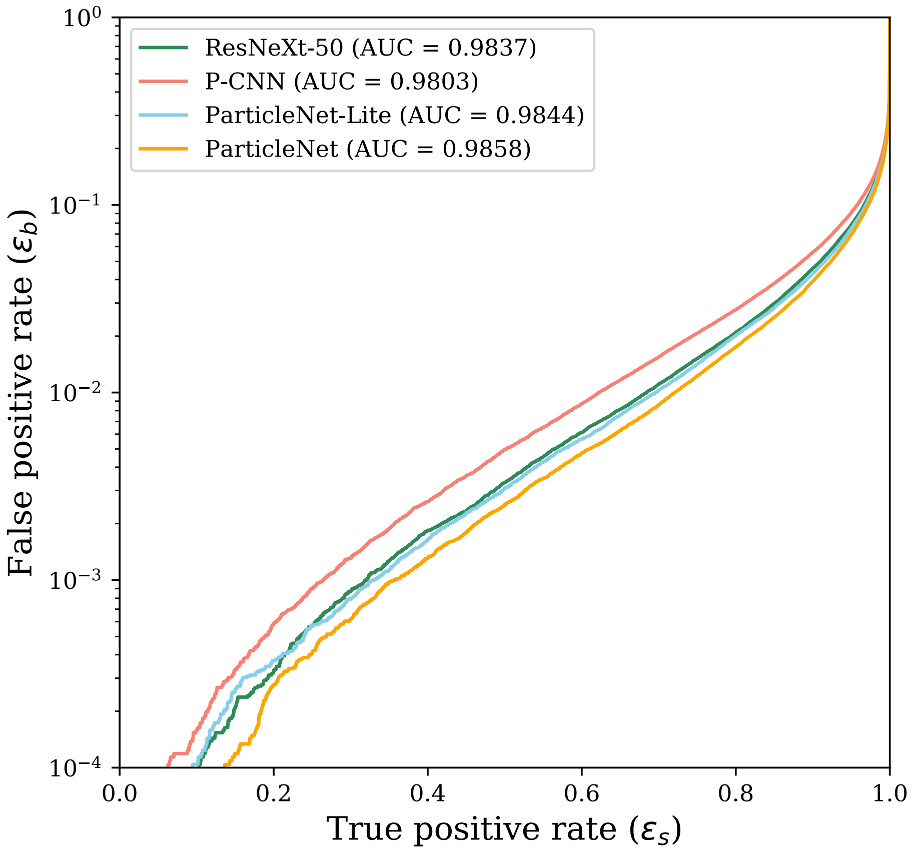
- This means that significantly more complex processes can be encoded more precisely by representing recurrent relationships in the structure of the model itself
  - Rather than having to learn it by example through training.

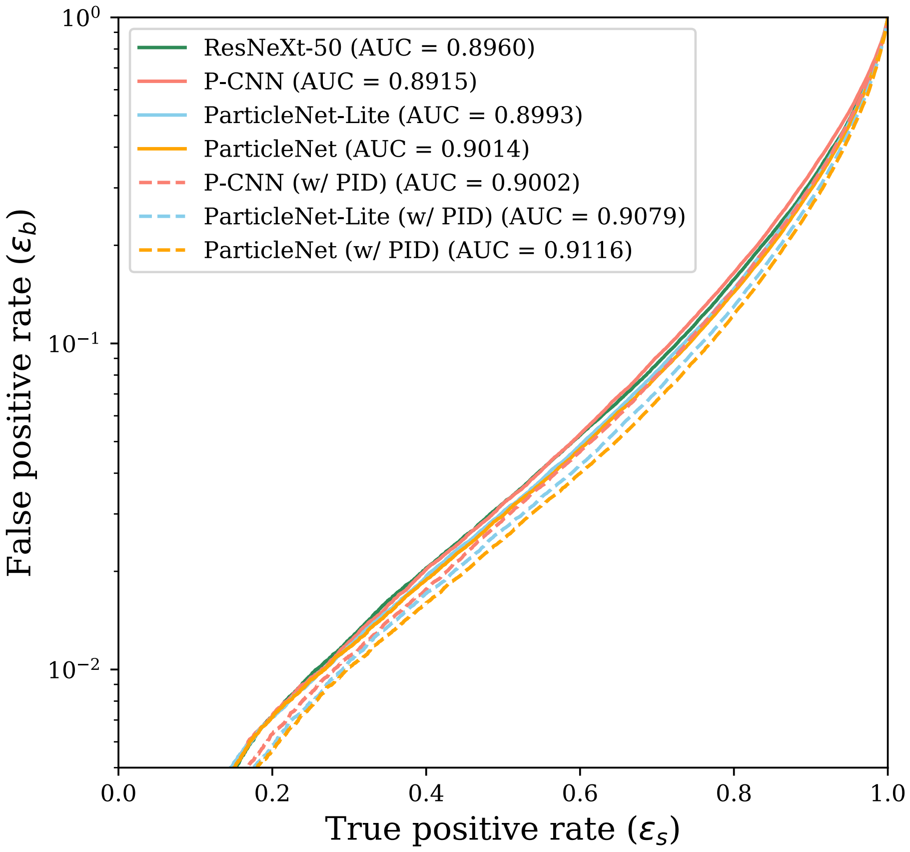
Jet tagging using graphs

- Below are results for using a graph to describe associations in jets
  - Improved performance with respect to image-based architectures!

- Train the classifier to learn what connections between particles are important

- Less need to pre-process the input properties for classification
  - Little to no transformation of data about jet constituents

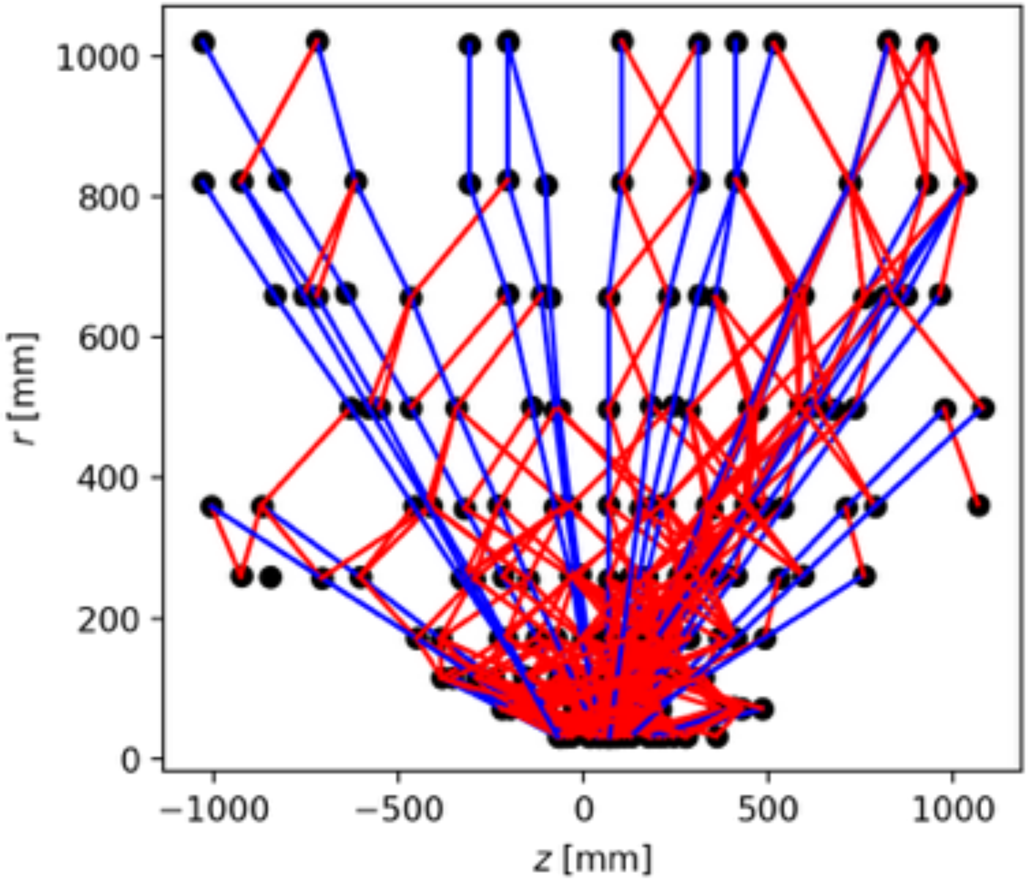




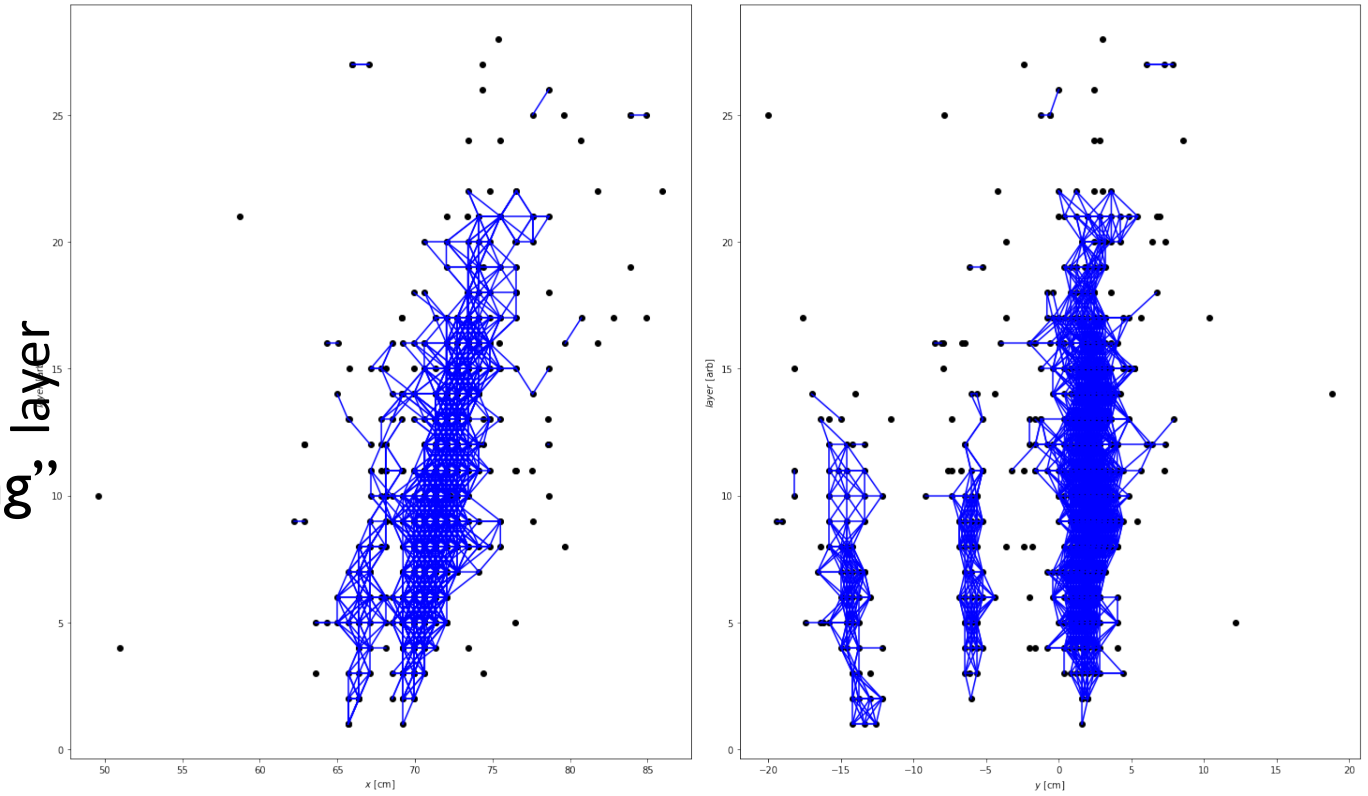
https://arxiv.org/pdf/1902.08570.pdf

From Jets to Tracks and Clusters

- Tracks and clusters can also be described as connections between points
  - Instead of connections between different particles to distill information about a jet, we examine connections between detector hits to distill information about if those points are related
- Finding points comprising helices in tracks is the same as points in calorimeter clusters
  - Can we simplify our lives and find one algorithm which can handle these different cases?



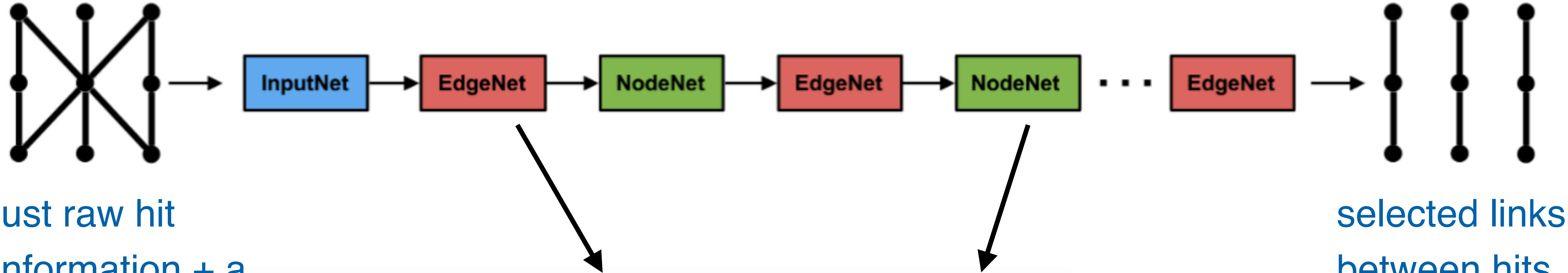
→ “same thing”



Putting it all together: a model for reconstruction

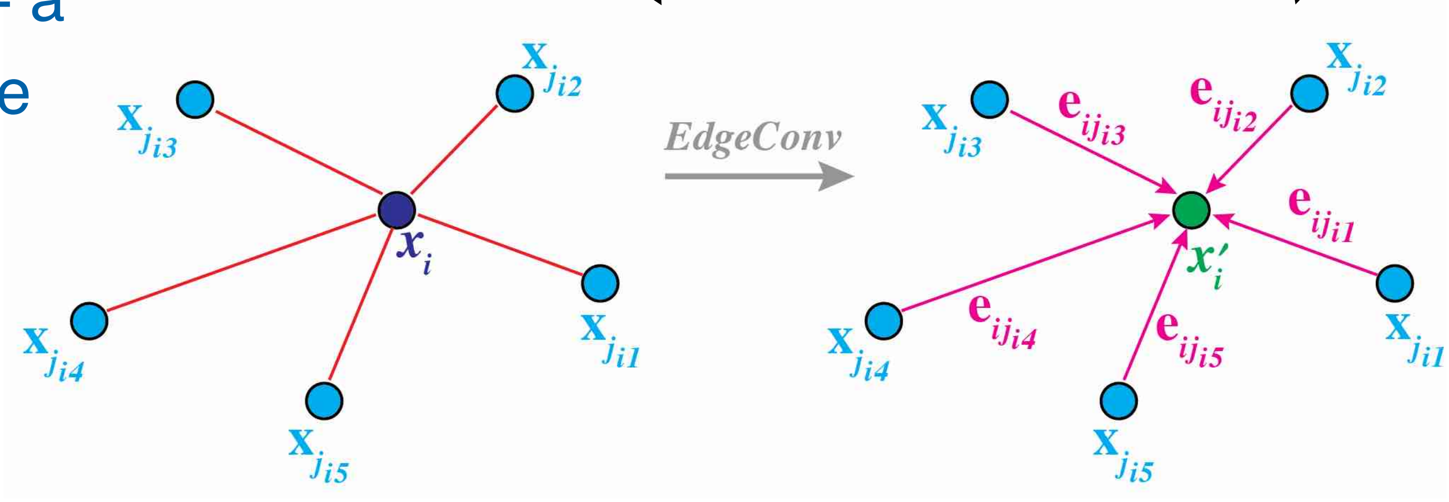
- With an preliminary model the answer seems to be “yes”
  - So long as we are willing to accept some light post processing

- Basic steps:
  - Define an input graph
  - train an ‘edge classifier’ based on information sharing on that graph
  - Apply edge classification scores to yield a subgraph of just the connections of interest



just raw hit information + a “guess” at the graph

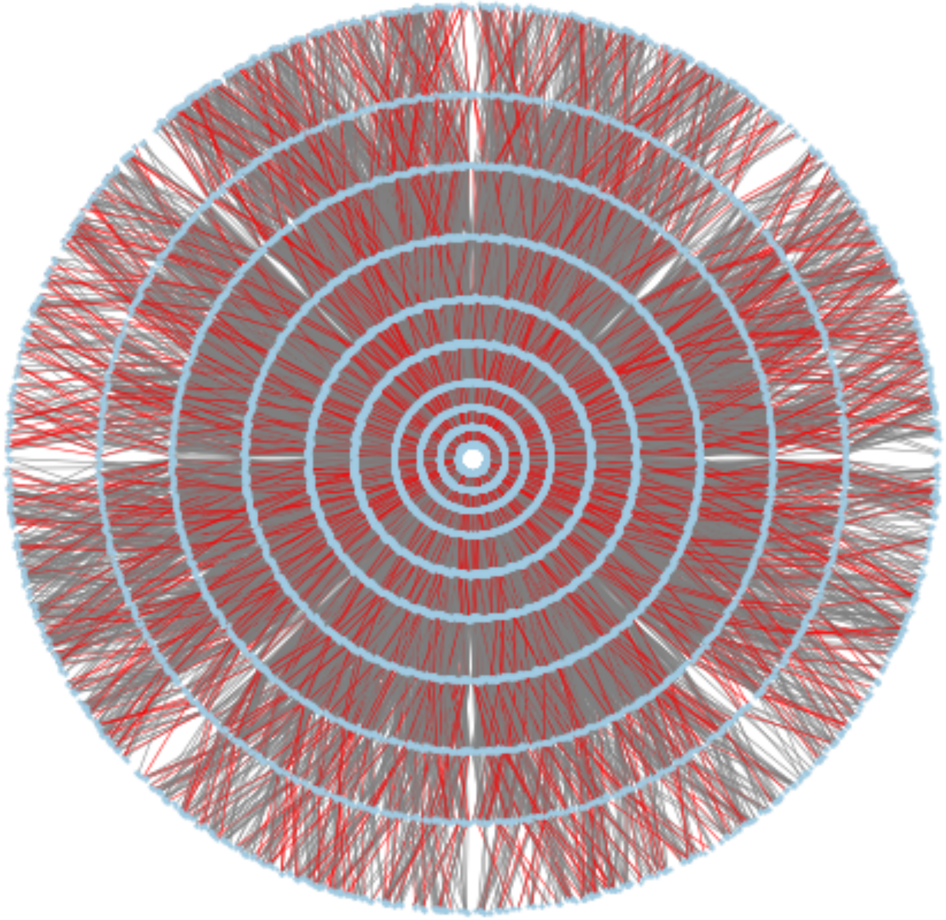
selected links between hits

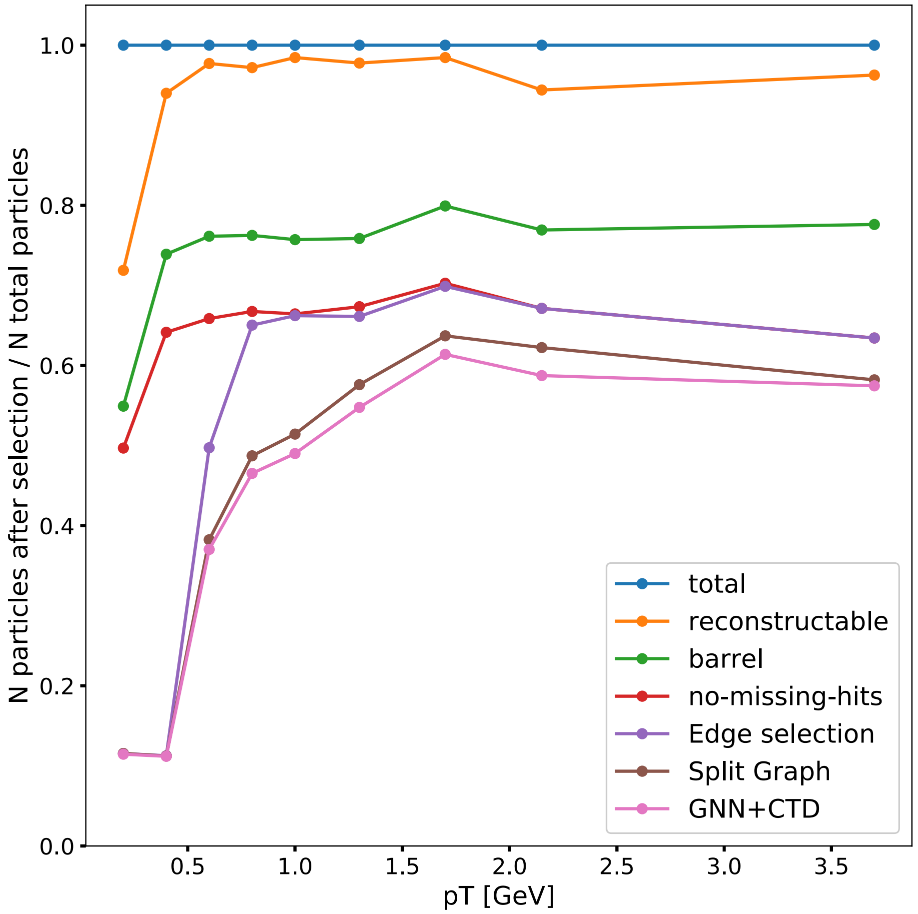


https://arxiv.org/abs/2003.11603

Preliminary Tracking Results with a GNN

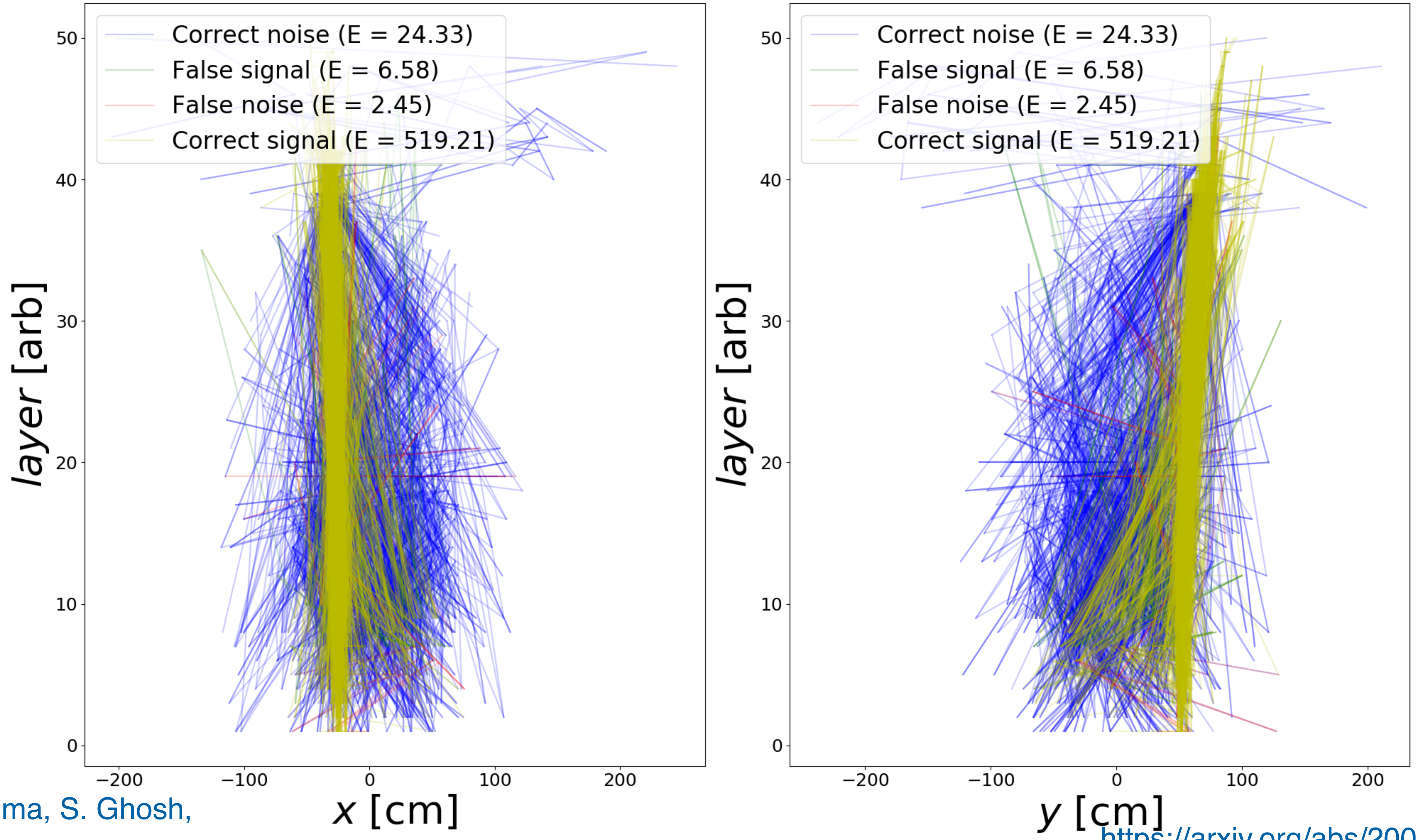
- Many selections applied to yield training set
  - Important: sectorization and no missing hits
- These are “easy” tracks but this also early days for the these kinds of network in HEP
  - Applying GNN, assembling tracks -> 97% efficient relative to preselection
  - Track-segment selection GNN executes significantly faster than Kalman filter





Reconstruction of a charged pion with edge classification

true negatives
true positives
false positives
false negatives



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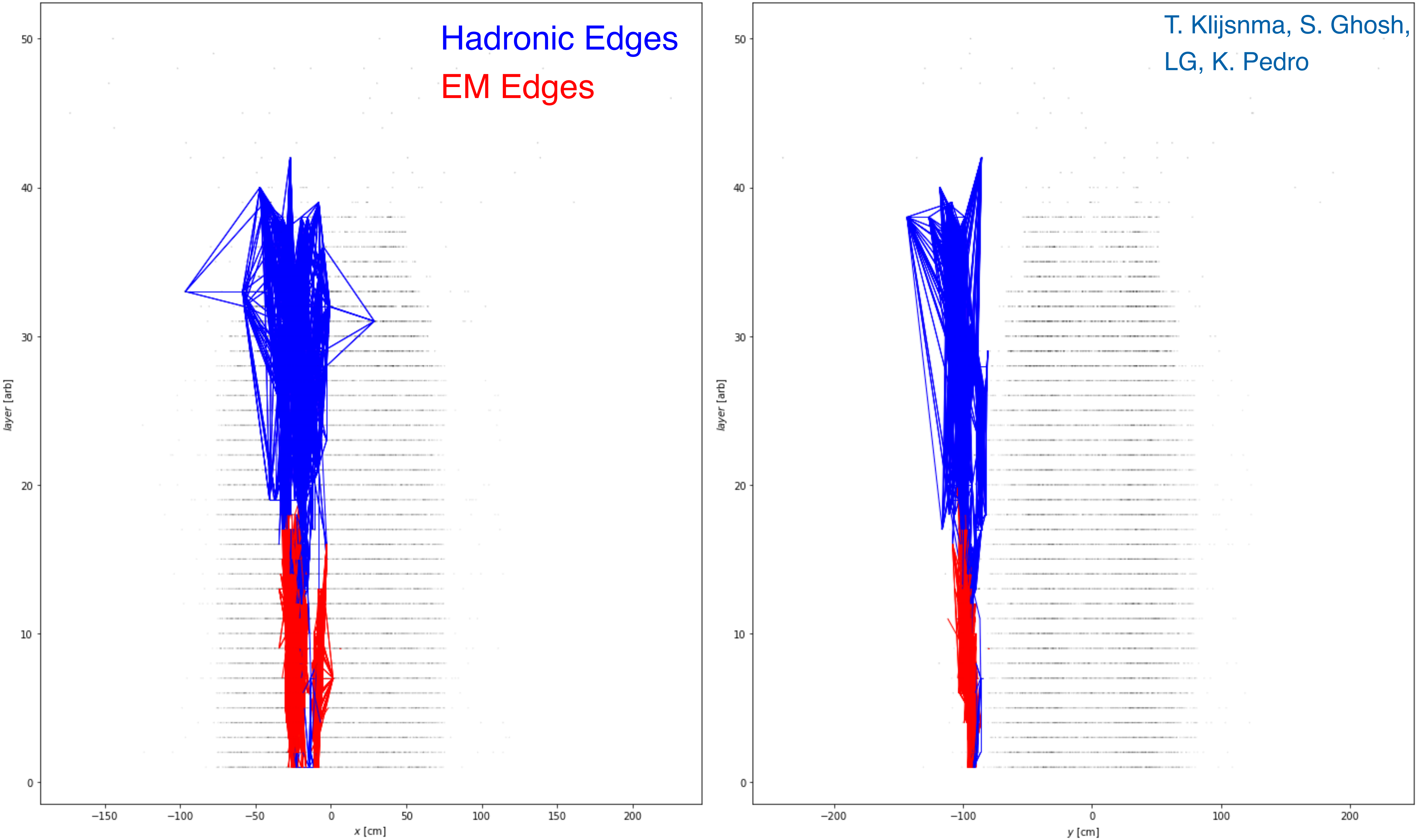
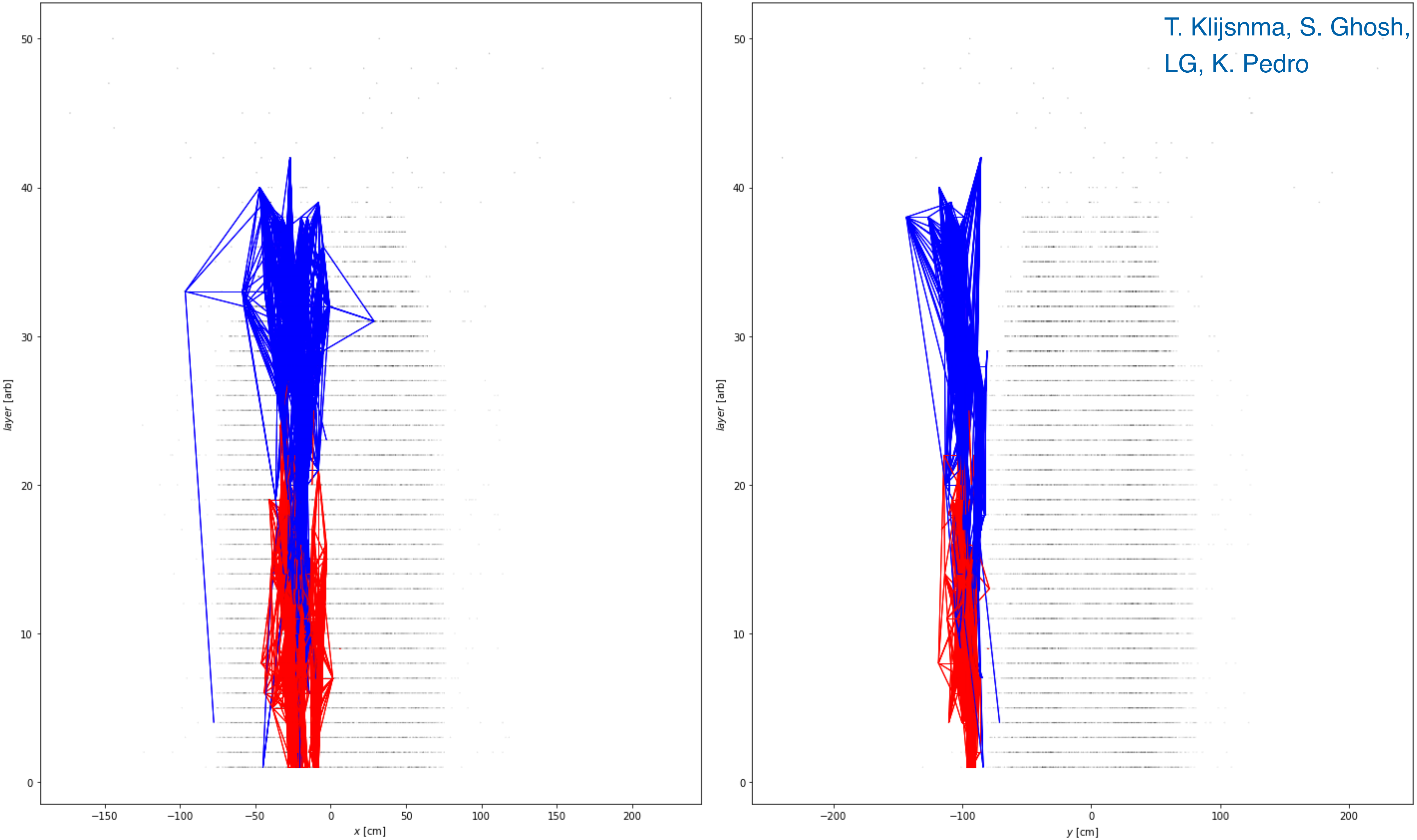
https://arxiv.org/abs/2003.11603

Simultaneous Reco & ID: Tau Lepton Example Prediction



Simultaneous Reco & ID: Tau Lepton Example Truth



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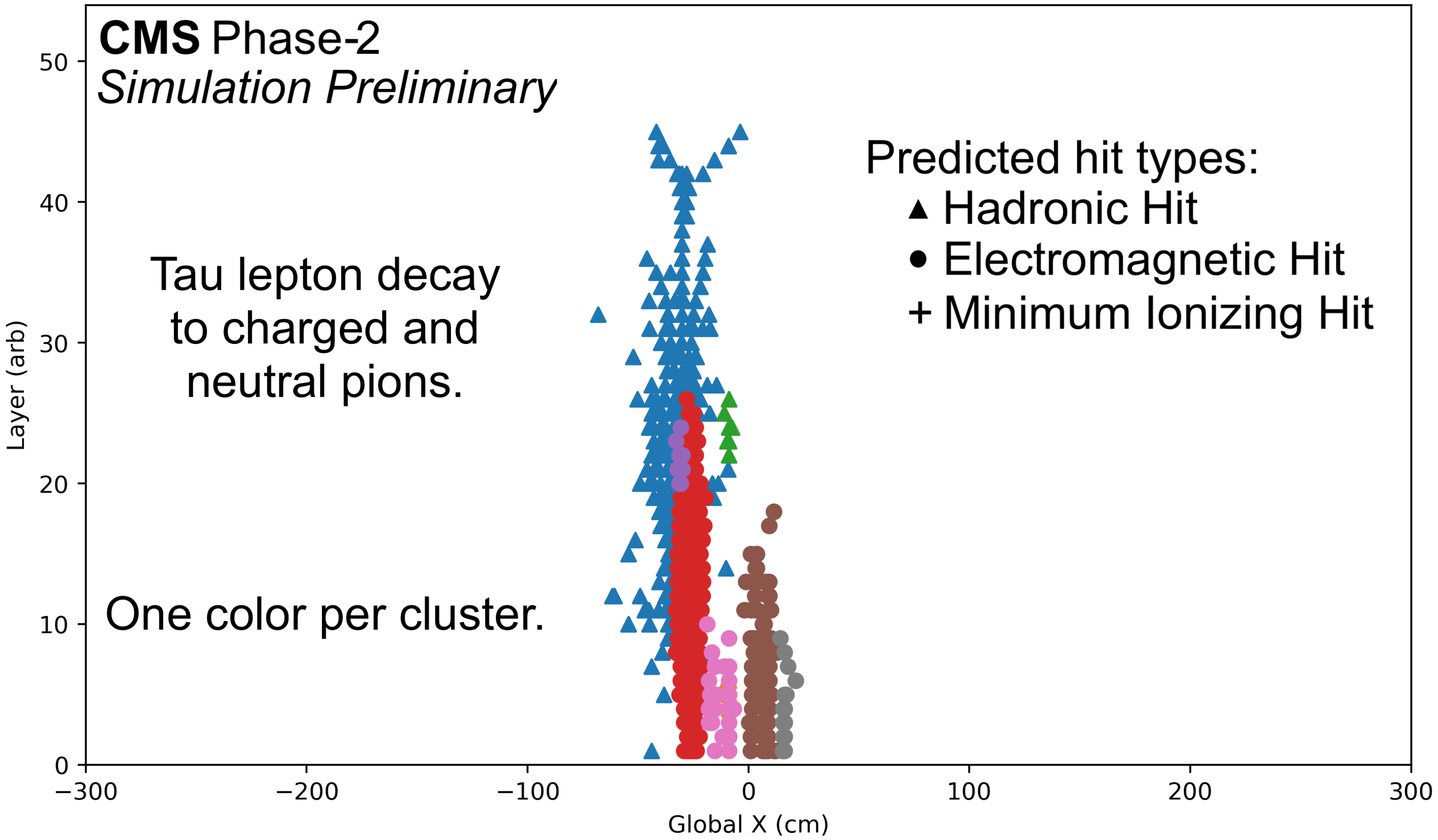
Edge Classification: Making a Clustering (I)

- In order to get calorimeter clusters, need to take the edges and convert to groups of points
  - In this case we just make a union of all the points with common edges of the same type
  - It does a reasonable job already segmenting hadronic energy from electromagnetic
  - We can reconstruct very close-by photons and hadrons effectively

- The same network and processing can also be used on tracking



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Edge Classification: Making a Clustering (II)

- In order to get calorimeter clusters, need to take the edges and convert to groups of points
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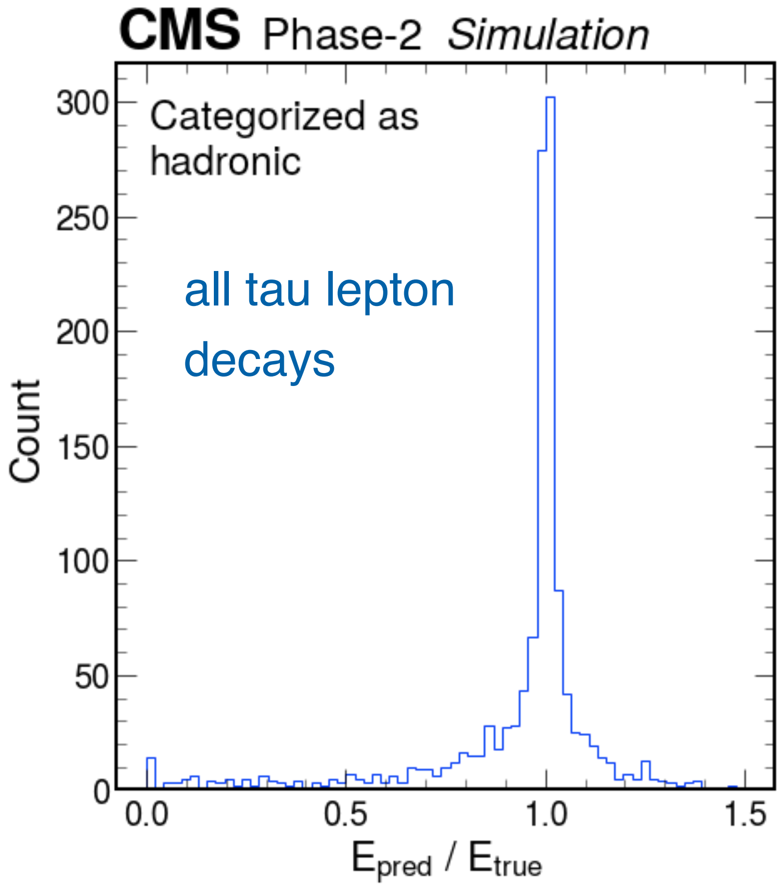
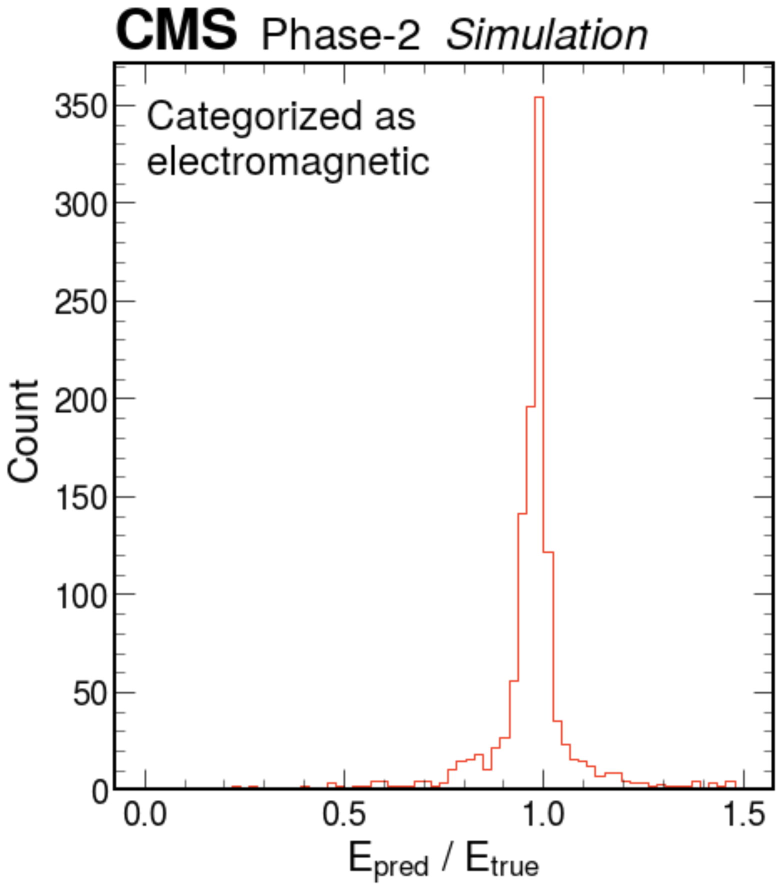
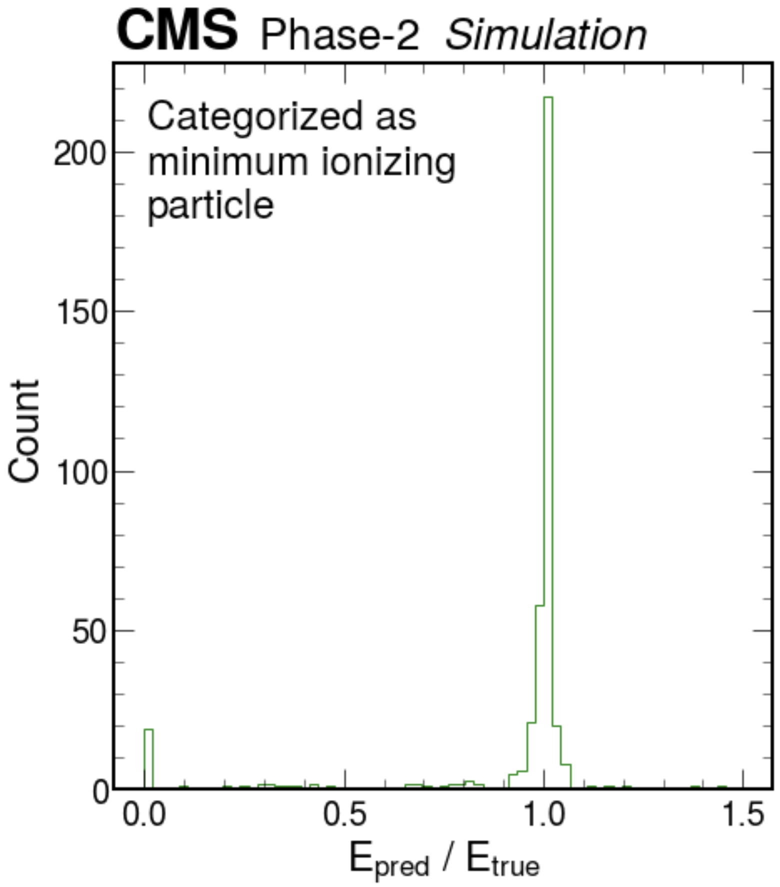
- The same network and processing can also be used on tracking







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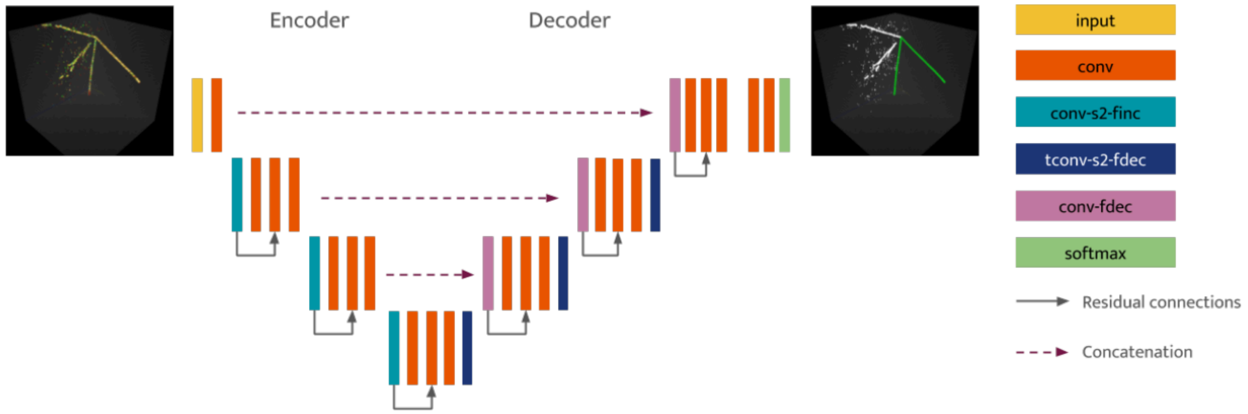
Other methodologies of tackling irregular detectors

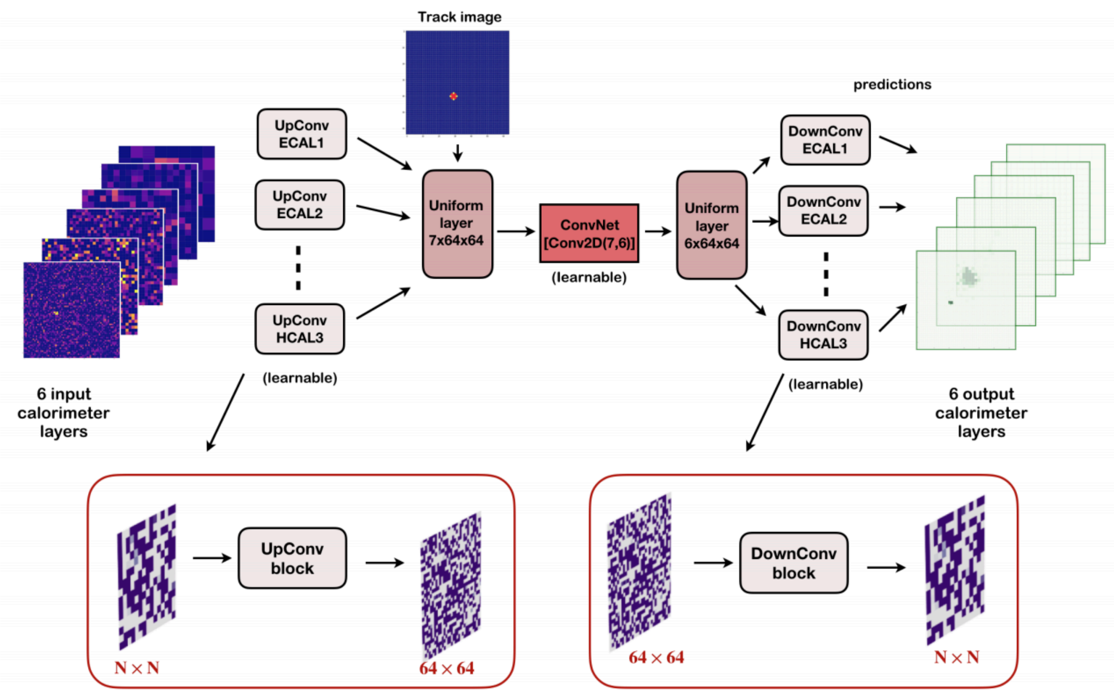
- LArTPCs and current calorimeters are being used to test ML based reconstruction as well
  - Early successes for convolutional based approaches
- ML based approaches starting to take the lead in neutrino physics
- Collider detectors exploring the use of CNNs and Graph techniques to reconstruction particle-level information
  - Similar or improved performance
  - Some issues still left: variable sized outputs

Sparse-CNN clustering for LArTPCs



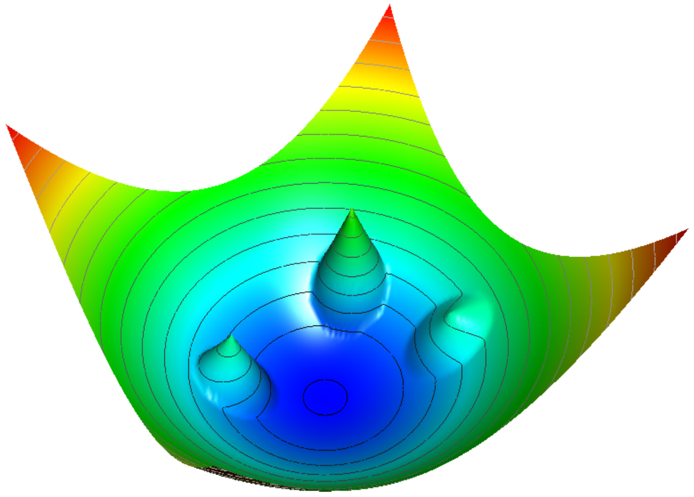
https://arxiv.org/abs/1903.05663

CNN-based particle flow algorithms



https://arxiv.org/abs/2003.08863

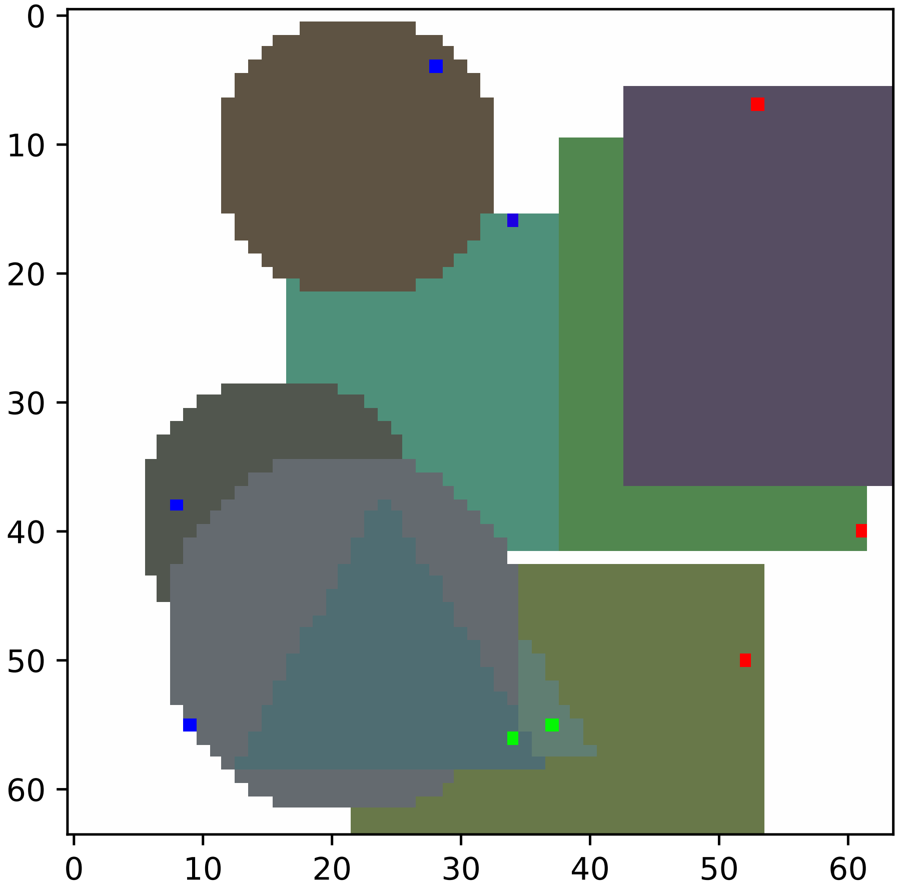
Object Condensation: a loss function for reconstruction



- Physics motivated loss function
  - Potentials with charges
  - like charges attract, opposites repel
  - points that should be associated attract each other
  - variable number of inputs and outputs

- The network is trained to predict the 'condensation points' of the input data
  - The data points closest to a charge barycenter

- The condensation points can then be used to collect points around them into 'segmented' objects
  - at this point we have created particles in an event or clusters in a calorimeter

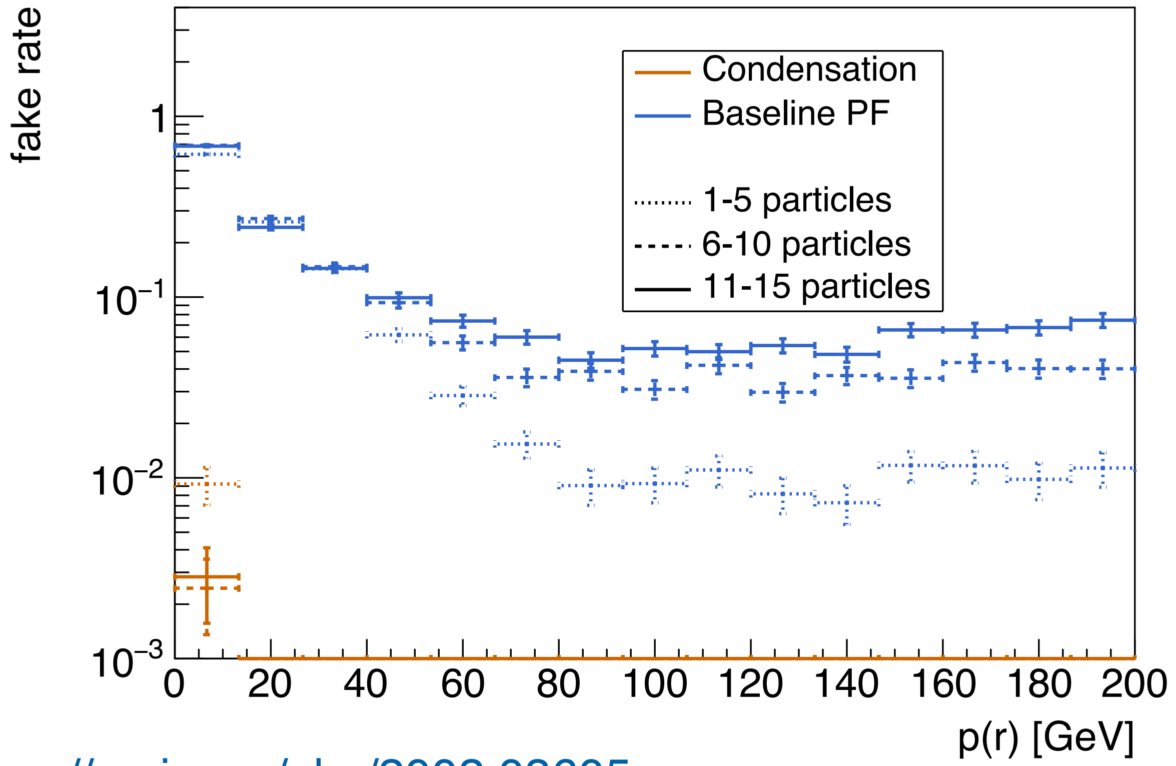


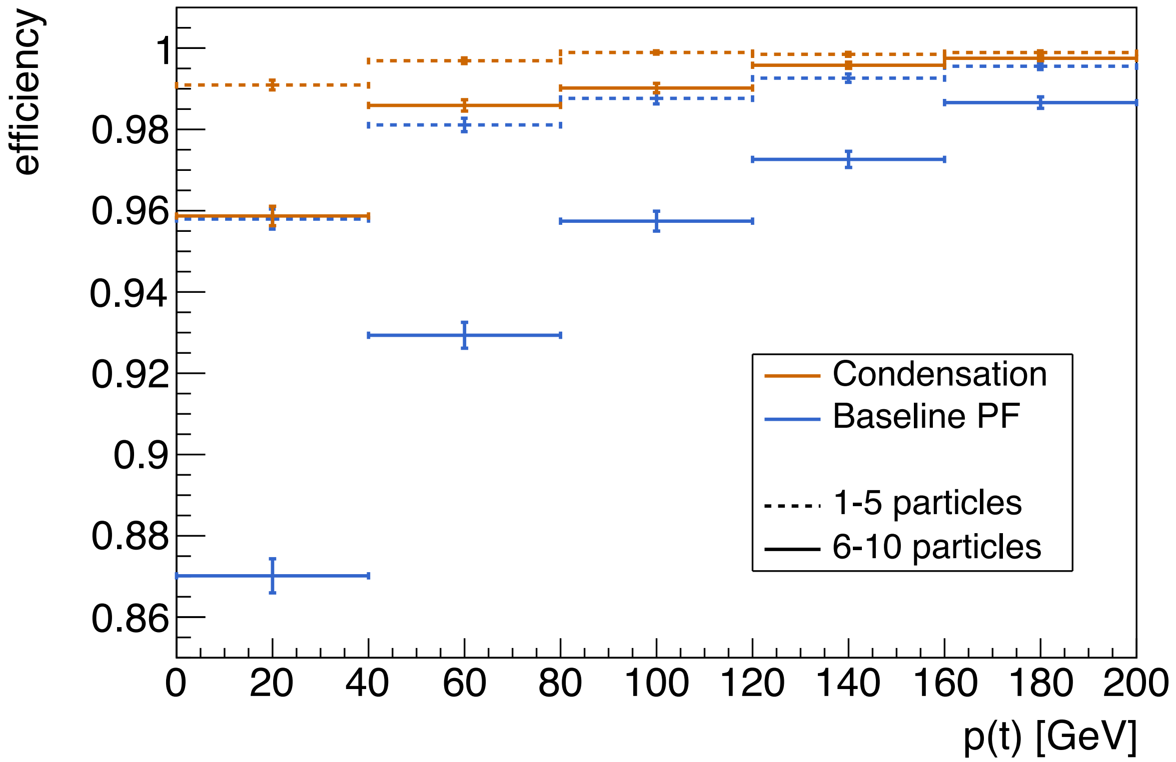
https://arxiv.org/abs/2002.03605

Object Condensation: Results

- A first reconstruction model has been developed and benchmarked
  - Using a toy detector and comparing to a simplified implementation of particle flow
  - Specifically - only a tracker and only an electromagnetic calorimeter

- Particle reconstruction efficiencies significantly improved for object condensation
  - Improved purities and resolutions (backup) across a range of multiplicities as well

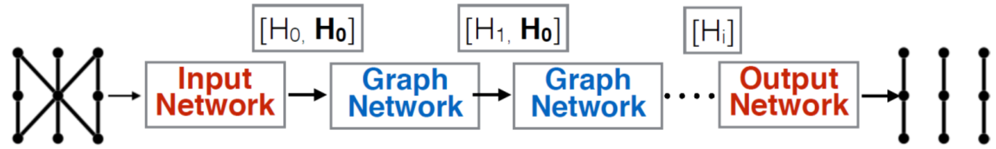




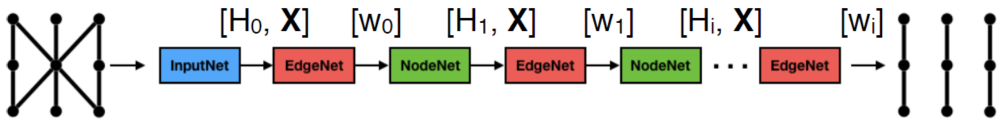
https://arxiv.org/abs/2002.03605

More methods yet to try and refine!

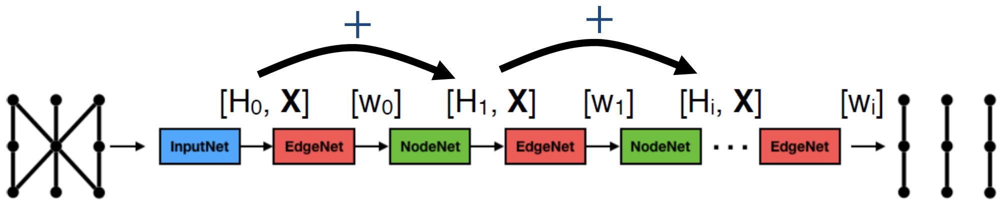
A variety of new message passing schemes (Exa.TrkX)



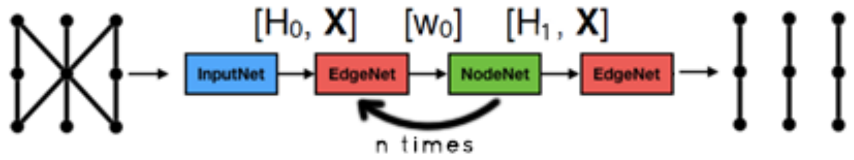
- Message Passing



- Attention Message Passing

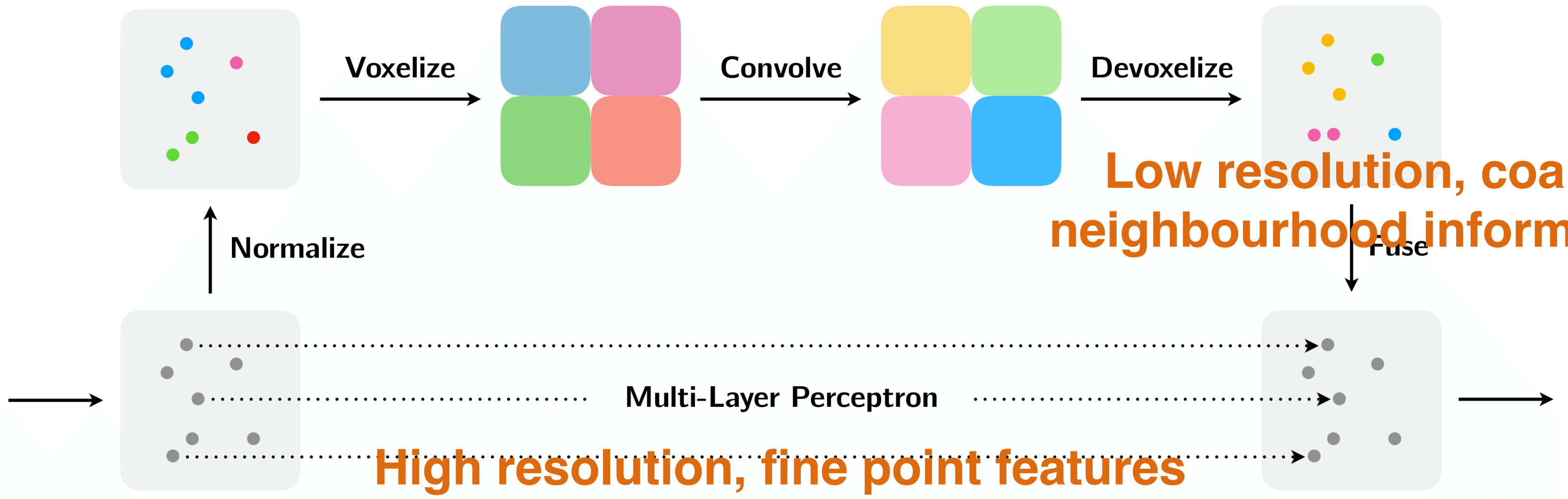


- Attention Message Passing with Residuals



- Attention Message Passing with Recursion

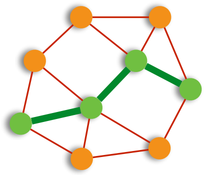
Voxelization for computing efficiency: https://arxiv.org/abs/1907.03739



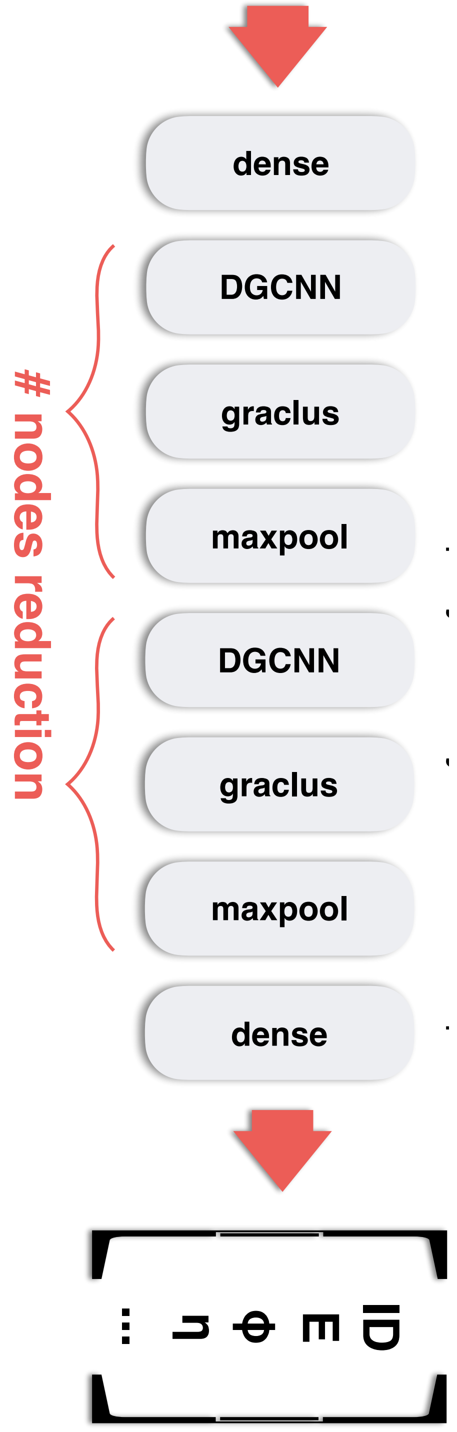
Low resolution, coarse neighbourhood information

High resolution, fine point features

https://arxiv.org/abs/2003.08013



Latent-space clustering



Thoughts on using these techniques in analysis

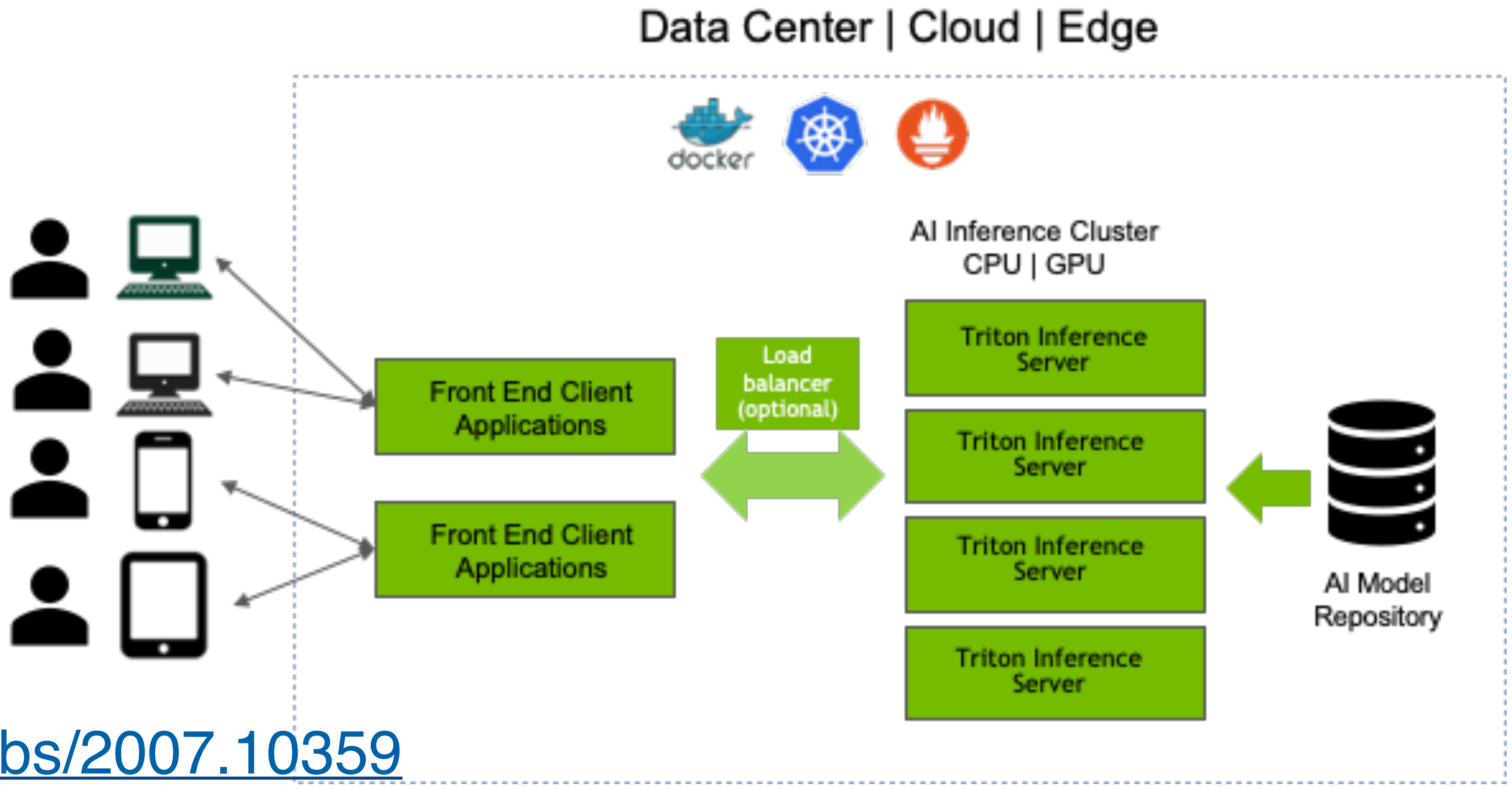
- These GNN-based techniques will eventually be used directly in analysis
- In a very general sense we get the most statistical sensitivity in an analysis by choosing some number of physics-rule based categories
  - e.g. VBF, VH, boosted Higgs
  - Or, as in Higgs to 2 photons, having primary categories based off ML discriminator scores that tend to reflect reconstruction quality and detector performance

- However as the final states become more complex (6-8 jets) it becomes less and less efficient and accurate to do that sorting by hand using some heuristics
  - The probability to choose an improper combination of jets or leptons explodes as final state multiplicity increases

- Using a GNN in analysis to encode relationships of kinematic structure to play off kinematics vs. reconstruction quality vs. sensitivity to then create categories would help mitigate these combinatorial effects
  - For at worst a linear increase in the background (so ~sqrt(2) improvements)

Deploying these techniques in the experiments (I)

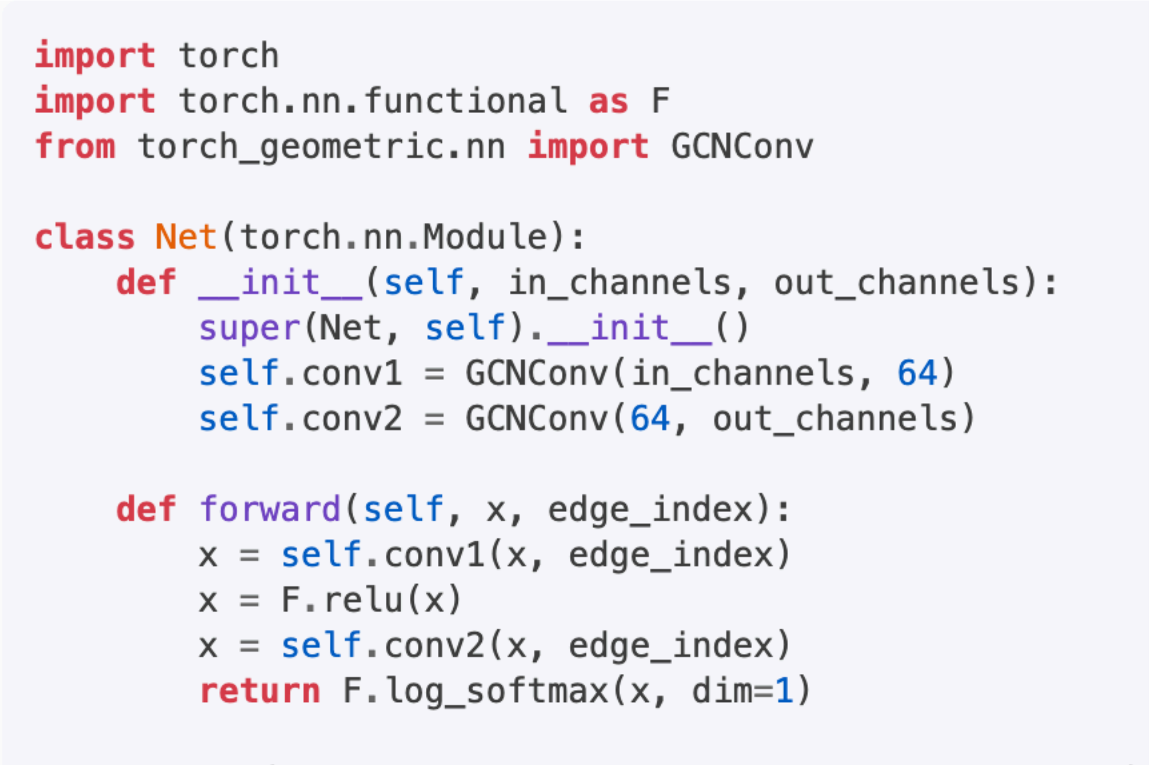
- Experiment software stacks are often difficult to deal with, but are requiring more and more ML inference as part of their standard operation
  - Difficult to update to cutting edge software without expert knowledge
  - Already many moving parts, difficult to maintain
  - Adding machine learning frameworks to this means even more complexity!
- We are exploring decoupling this by using machine learning *as a service*
  - Experiment framework then makes standardized, lightweight api calls to a separate server running a big stack of GPUs and all the models one may require for reconstruction



https://arxiv.org/abs/2007.10359

Deploying these techniques in the experiments (II)

- GNNs, being rather new, were not readily compatible with inference as a service frameworks
  - Often required some contortion or limitation on how you were defining the model
  - Makes the process of model development and maintenance a pain!
- Together with authors of a GNN package for pytorch we developed a way to make the models immediately deployable
  - With no code changes, access to these powerful models to experiments is fairly easy
  - First large-scale tests of GNNs in CMSSW using models from this talk underway



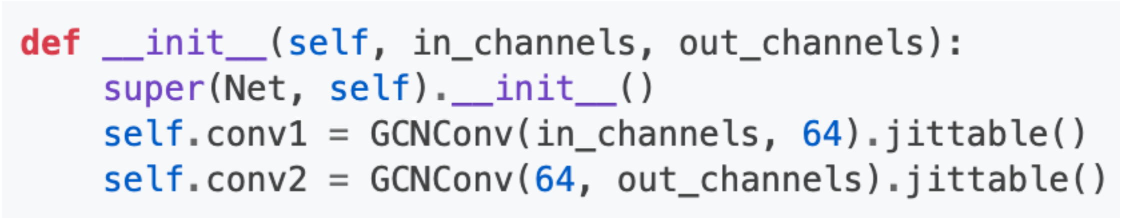
```python
import torch
import torch.nn.functional as F
from torch_geometric.nn import GCNConv

class Net(torch.nn.Module):
    def __init__(self, in_channels, out_channels):
        super(Net, self).__init__()
        self.conv1 = GCNConv(in_channels, 64)
        self.conv2 = GCNConv(64, out_channels)

    def forward(self, x, edge_index):
        x = self.conv1(x, edge_index)
        x = F.relu(x)
        x = self.conv2(x, edge_index)
        return F.log_softmax(x, dim=1)

model = Net(dataset.num_features, dataset.num_classes)
```

change to



```python
def __init__(self, in_channels, out_channels):
    super(Net, self).__init__()
    self.conv1 = GCNConv(in_channels, 64).jittable()
    self.conv2 = GCNConv(64, out_channels).jittable()
```

forward stays the same

```python
model = torch.jit.script(model)
```

serialize jittable model

https://pytorch-geometric.readthedocs.io/en/latest/notes/jit.html

Conclusions and Outlook

- Machine Learning is being used for more and more fundamental tasks in HEP
  - Adoption of ML techniques has led to simplification in analysis definition
  - We have also demonstrated that we can control the process of training and applying these techniques to yield *precision results*
- ML techniques have been evolving to become more dynamic and HEP has been tracking with that
  - We are now at the point where we can perform inference on variable sized inputs with variable sized outputs, which was not possible 4 years ago
- Using the vastly more complex information of new detectors is made tractable by the nature of these more-dynamic Graph Neural Networks
  - We can now implement and use complex reconstruction algorithms end-to-end in ML
- Reconstruction using Machine Learning stands to simplify algorithm design and improve their physics and computing performance
  - Allowing the HEP community to better use the ever-more-complex detectors we are designing now and striving for in the future

Extras

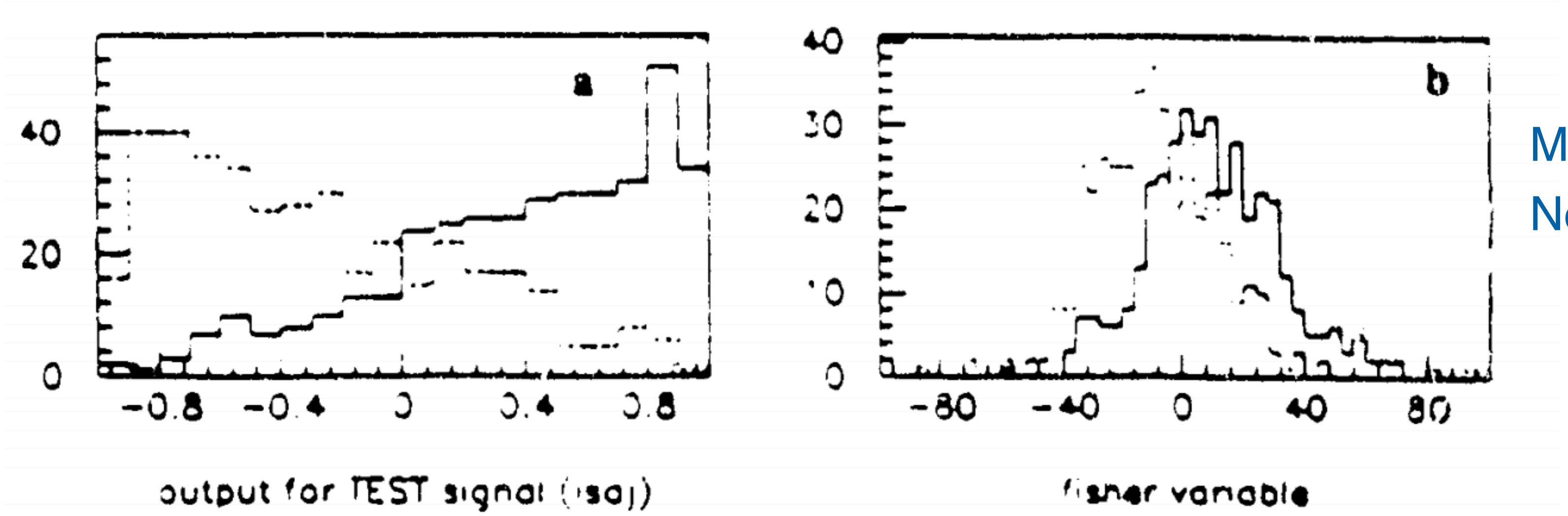
How did we get to where we are going?

- The detectors and challenges, and the tools to address them are the result of a long story in particle physics
  - We always want better discriminators that utilize more information

- HEP Physicists have to demonstrate control over methodologies
  - We can't just separate categories of data from one another
  - Error models and confidence regions are required in order to report our results

- Using ML techniques as reconstruction algorithms is the result of decades of accumulated knowledge within HEP

Figure 2



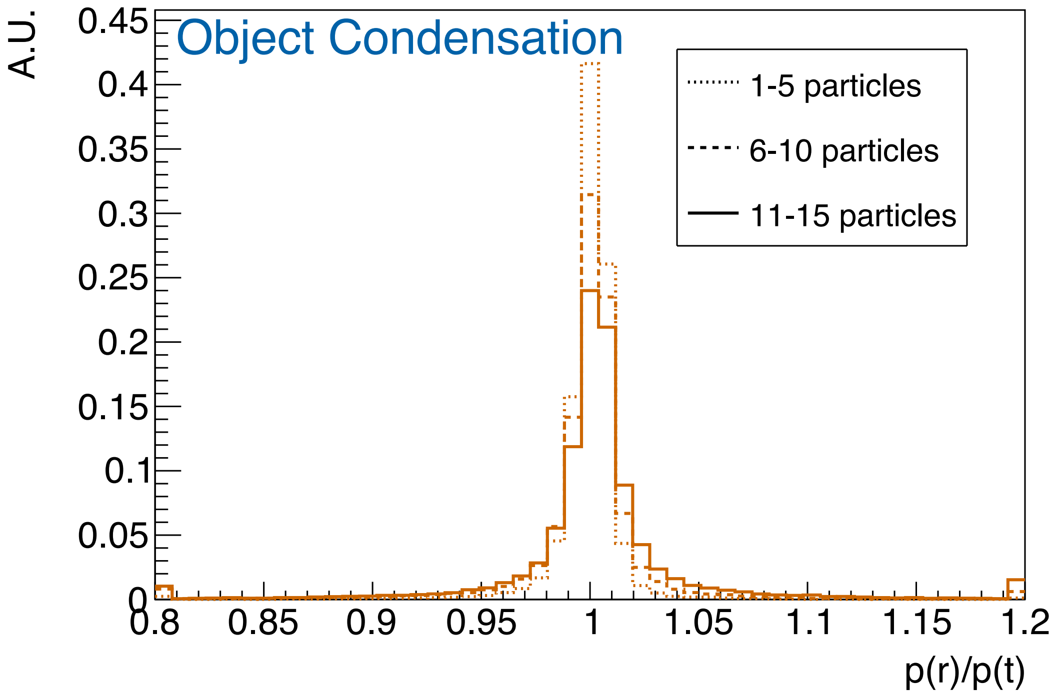
Multijet Top discriminant from 1992

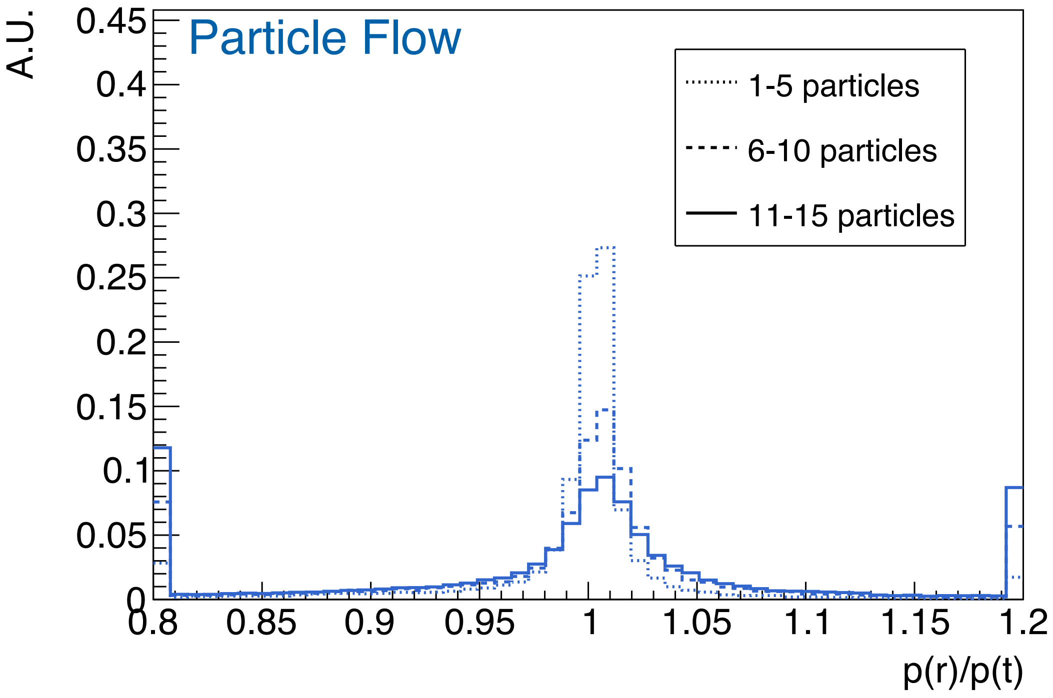
Neural Network (left), Fisher discriminant (right)

https://www.osti.gov/biblio/10110749

Object Condensation Performance

- Object condensation reconstructs individual particles significantly better
  - Even in dense multi-particle environments
  - Significant reduction in outliers





Full results for deep double b-tag