



Machine Learning

Current Projects
@ Belle II



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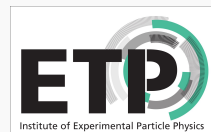


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Belle II MVA**

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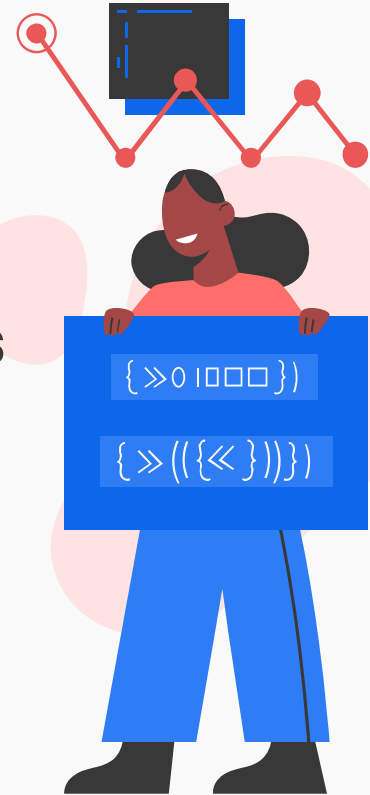
**Object
Condensation for
Reconstruction**

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**Overview over
Belle II projects**

04

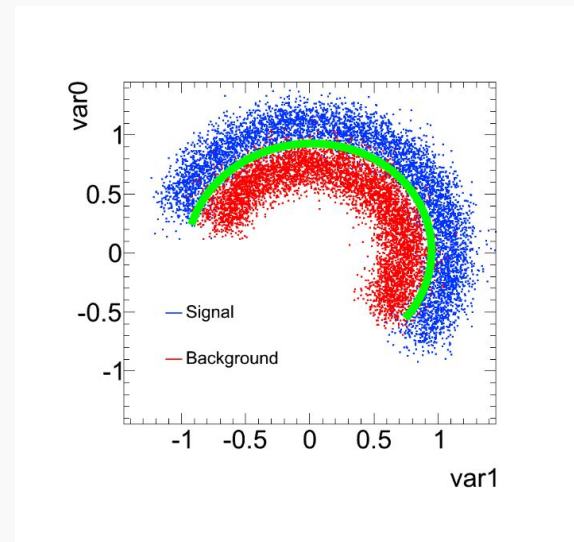
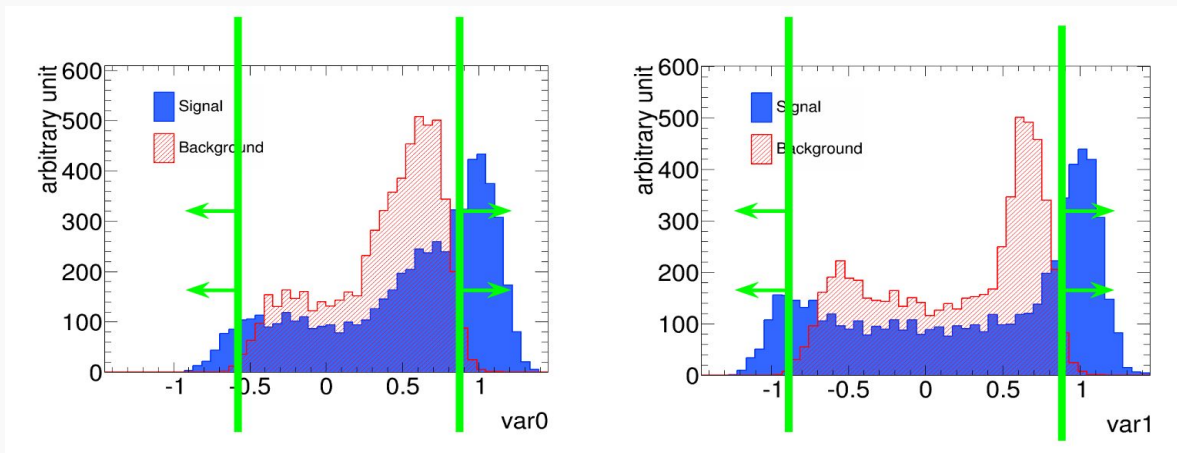
**How can I
participate?**



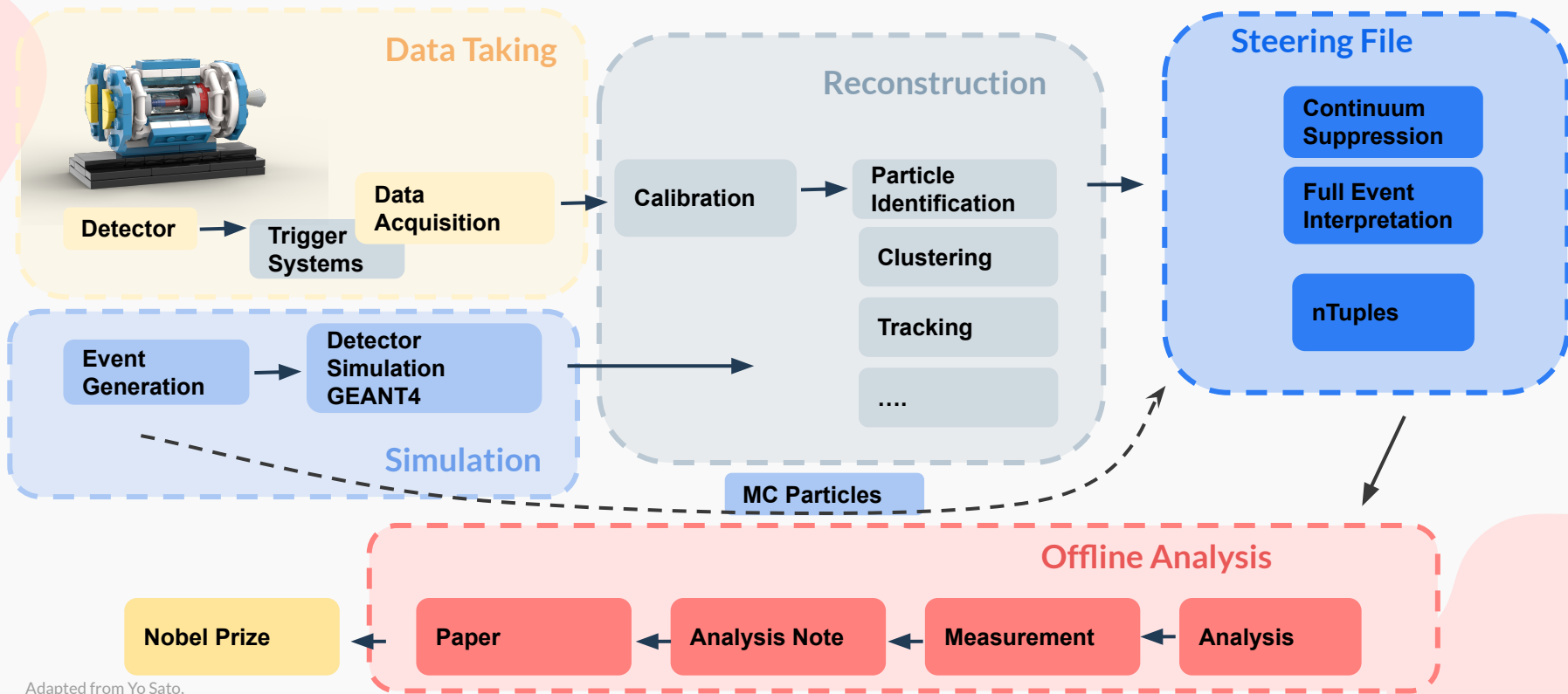
Why Multivariate?

Why not simply cut on variables?

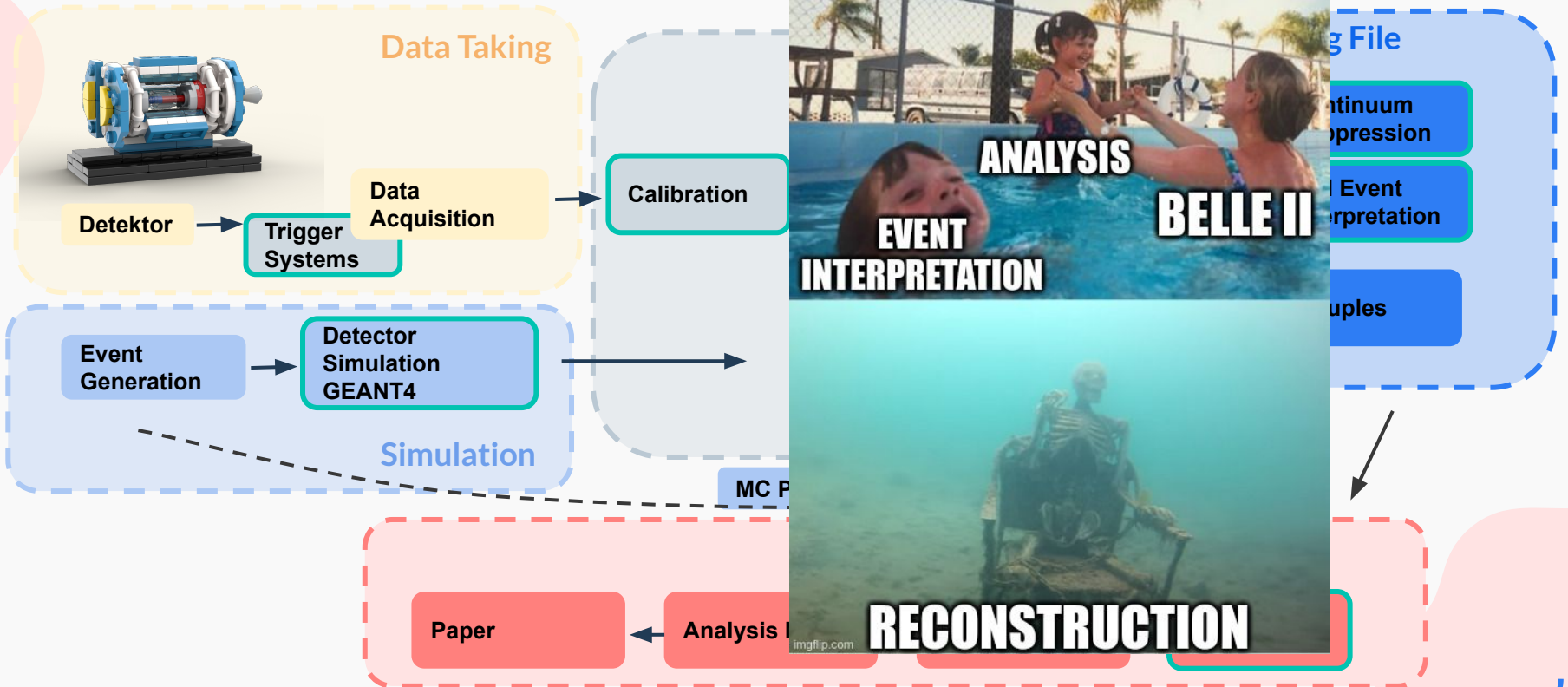
- Correlations not visible



Workflow



Workflow



Belle II Machine Learning

[]	Reconstruction
[]	Event Interpretation
{ }	Analysis
< >	Simulation

{ Every analysis ever }

Boosted Decision Trees

[FEI]
[Fake Photon Suppression]

[PID] { Exploring ML for Analysis }
[Slow Pion Rescue] [Neural Z Trigger]

Classic Neural Networks [Continuum Suppression]
[BGNNet]

Generative Adversarial Networks
< PXD >
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[Deep FEI]
[Hyper Tagging]
Transformers

[Deep Continuum Suppression]

Convolutional Neural Networks

[PIDs with CNNs]
{ New Physics Searches }

Autoencoder { Anomaly Detection }
[graFEI]
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Graph Neural Networks [CDC Tracking]
[graFEI]

[Flavor Tagger] [ECL Clustering]

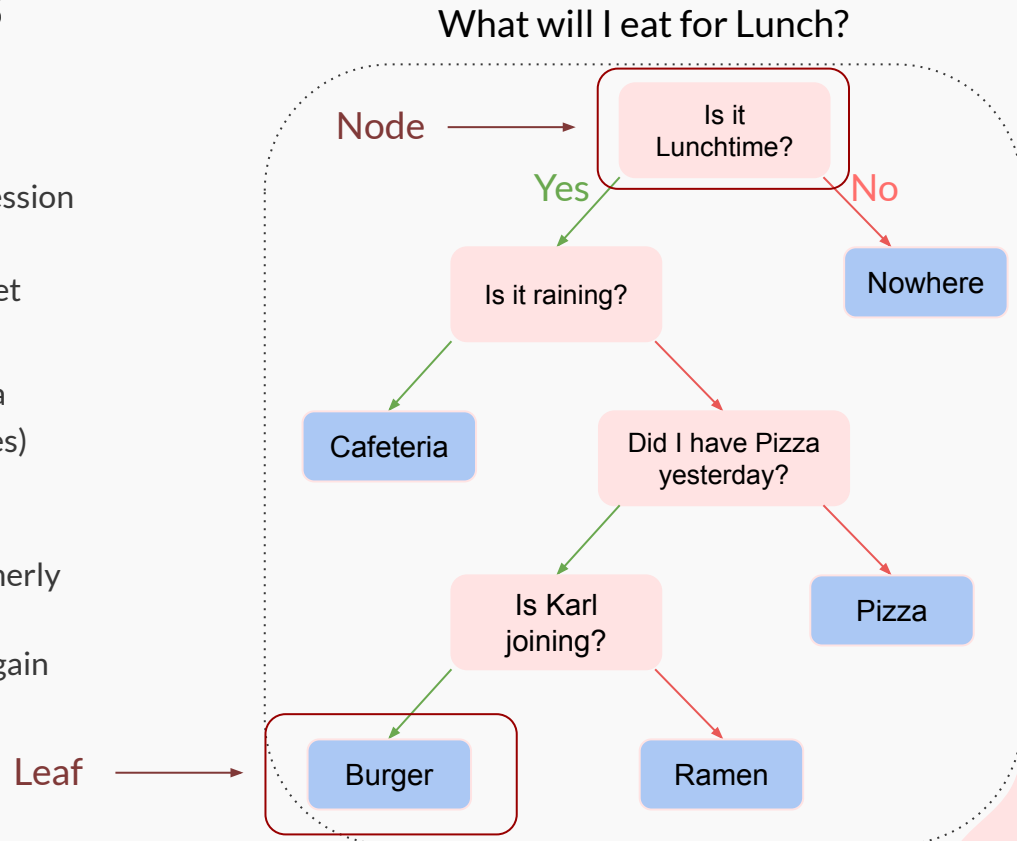


02

Overview over Belle II Projects

Decision Trees

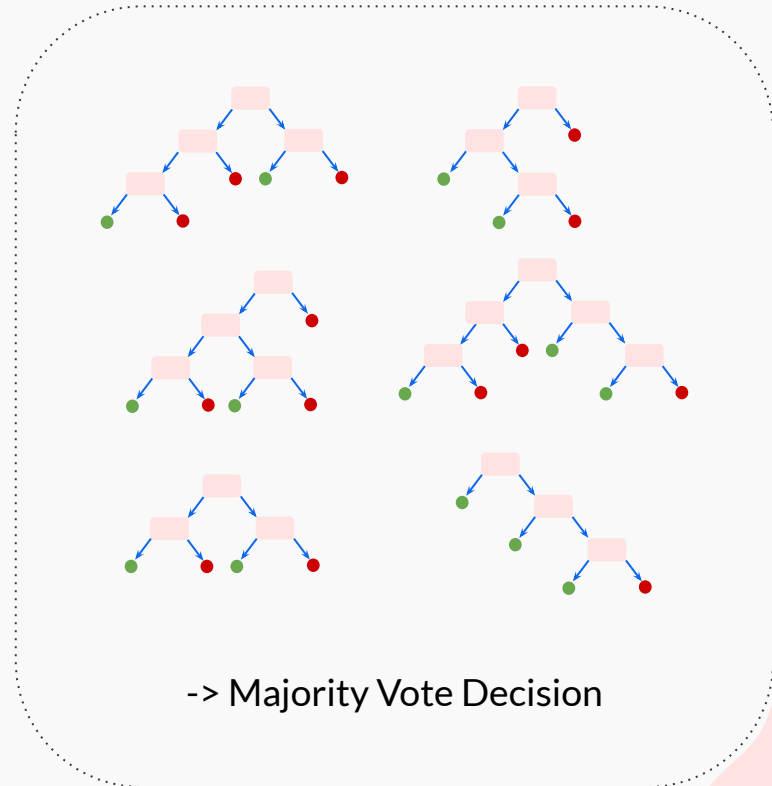
- Popular for classification and regression tasks
 - Easy to understand/interpret
 - Fast training
 - Good with multivariate data
- Consecutive set of questions (nodes)
- Final verdict is reached after given maximum of nodes (leaf)
- Each question depends on the formerly given answers
- Trained on maximizing separation gain between nodes



(Boosted) Decision Trees

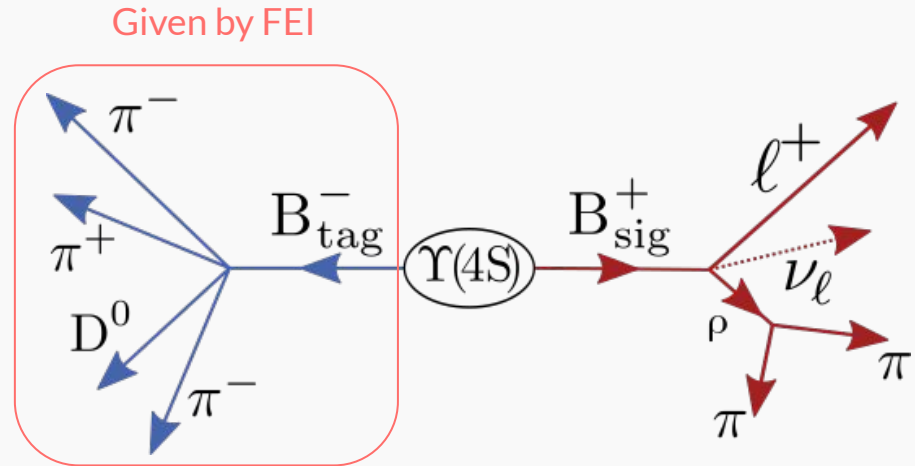
Is it Signal or Background?

- Single trees are often not very strong
- Combination of different trees
 - > Random Forest
- Output is decided by majority vote
- Boosting:
 - Misclassified events are weighted higher
 - Future trees concentrate on misclassified events
 - Easy to overtrain
- Pruning: Reduce tree size by removing redundant nodes



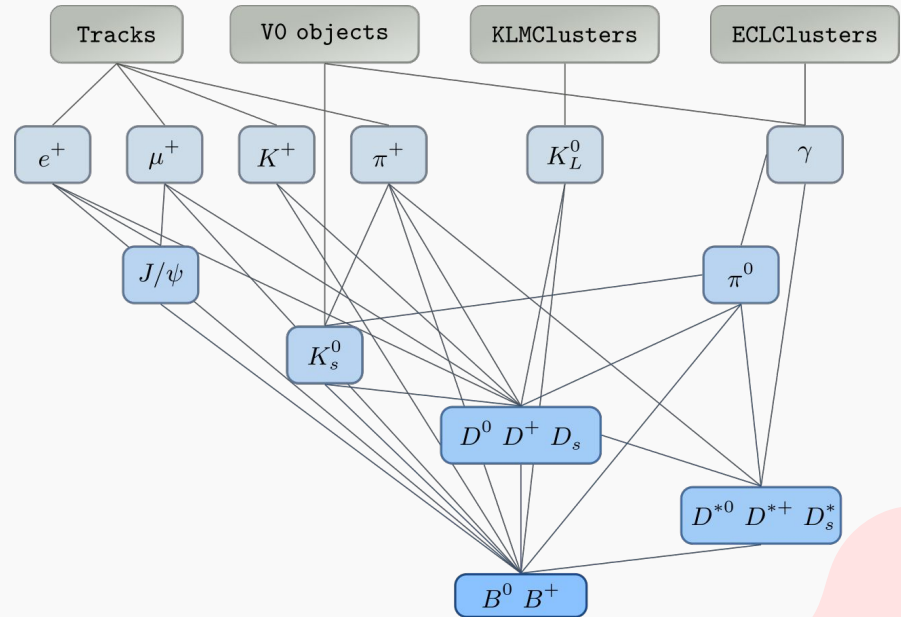
Example: Full Event Interpretation (FEI)

- Idea: Tagging B-meson decay chains through BDTs



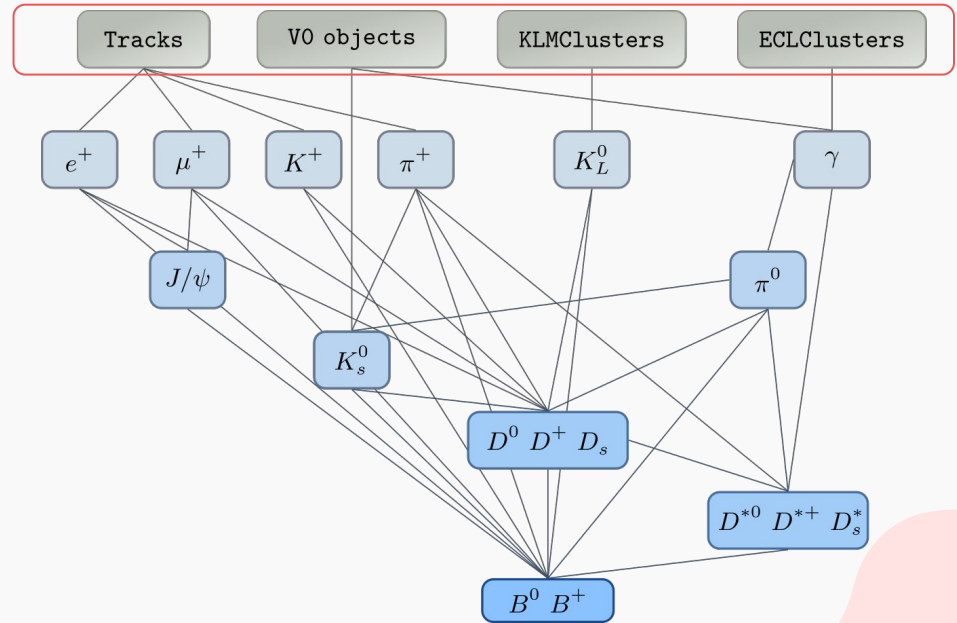
Example: Full Event Interpretation

- Idea: Tagging B-meson decay chains through BDTs
- Hierarchical Structure
- Probability of each candidate being correct is estimated by BDTs



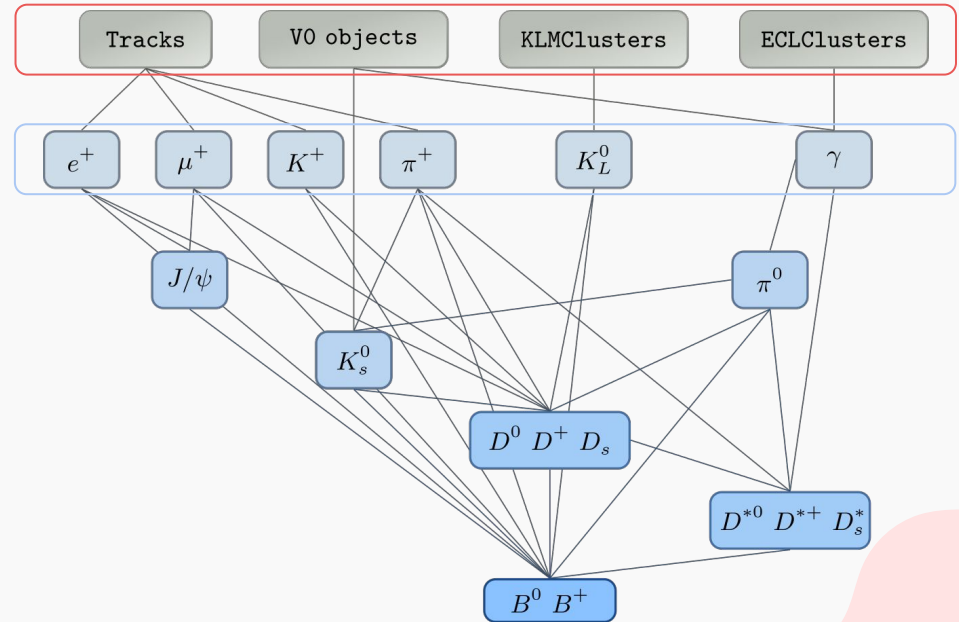
Example: Full Event Interpretation

- Idea: Tagging B-meson decay chains through BDTs
- Hierarchical Structure:
 1. Construction of final-state particles using **reconstructed tracks and clusters**
- Probability of each candidate being correct is estimated by BDTs



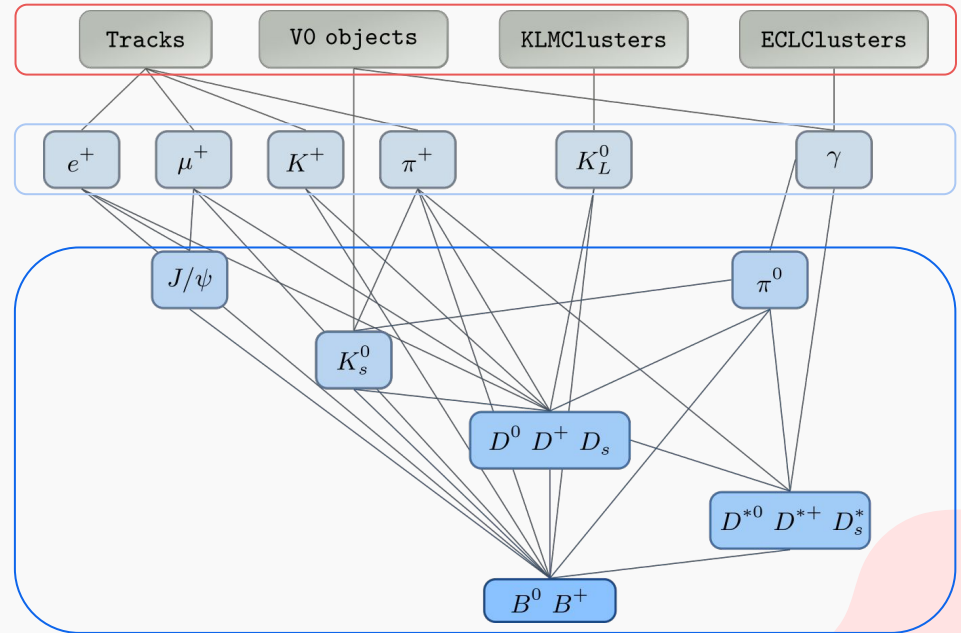
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- Idea: Tagging B-meson decay chains through BDTs
- Hierarchical Structure:
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 2. Combination of **final-state particles** to intermediate particles
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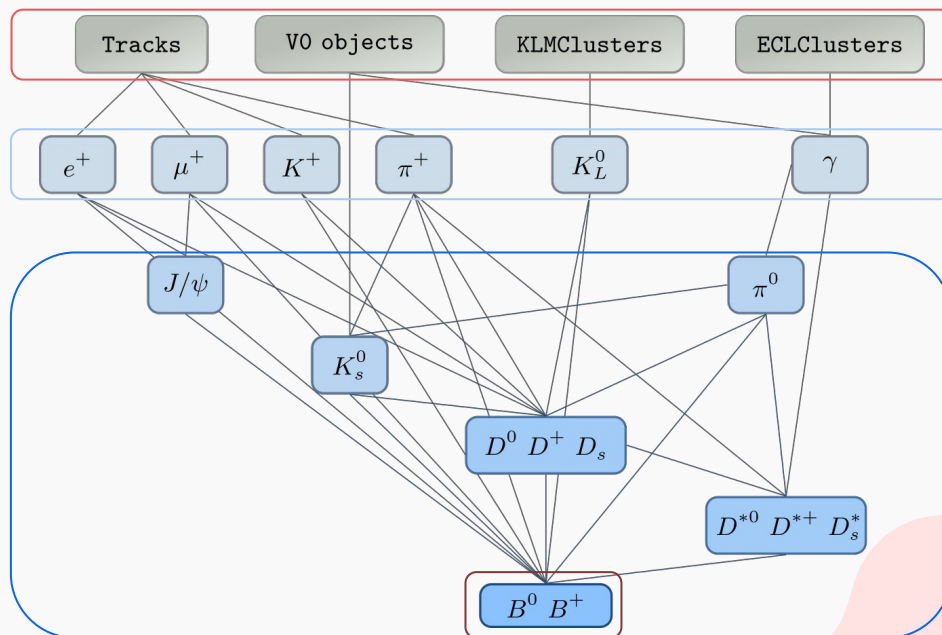
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 - Classifier for **intermediate particles** uses signal probability of daughter particles as input features



Example: Full Event Interpretation

- Idea: Tagging B-meson decay chains through BDTs
- Hierarchical Structure:
 1. Construction of **final-state particles** using **reconstructed tracks and clusters**
 2. Combination of **final-state particles** to **intermediate particles**
 3. Repeat 2. until **final B candidates** are formed
- Probability of each candidate being correct is estimated by BDTs
 - Classifier for **intermediate particles** uses signal probability of daughter particles as input features



BDTs

Measurement of CP asymmetries and branching-fraction ratios for $B^\pm \rightarrow DK^\pm$ and $D\pi^\pm$

with $D \rightarrow K_s^0 K^\pm \pi^\mp$ using Belle and Belle II data

corresponds to $\pm 3\sigma$ around the known K^0 mass [30], with σ being the mass resolution. To improve purity, we reject combinations for Belle [31] and a boosted decision tree classifier for Belle II [32].

Search for lepton-flavor-violating $\tau^- \rightarrow \ell^- \phi$ decays in 2019-2021 Belle II data

Background events are suppressed by a set of requirements on topological and kinematic variables followed by a selection on the invariant mass of the lepton and the photon. The selection also includes requirements on the angle between the lepton and the photon in the production plane.

Measurement of the branching fraction and CP asymmetry in $B^0 \rightarrow K_s^0 \pi^0$ decay

imgflip.com

with σ being the resolution. We suppress contamination from prompt K_s^0 candidates and Λ decays using two boosted-decision-tree (BDT) classifiers [27]. These BDTs rely mostly on kinematic variables of the decay products.

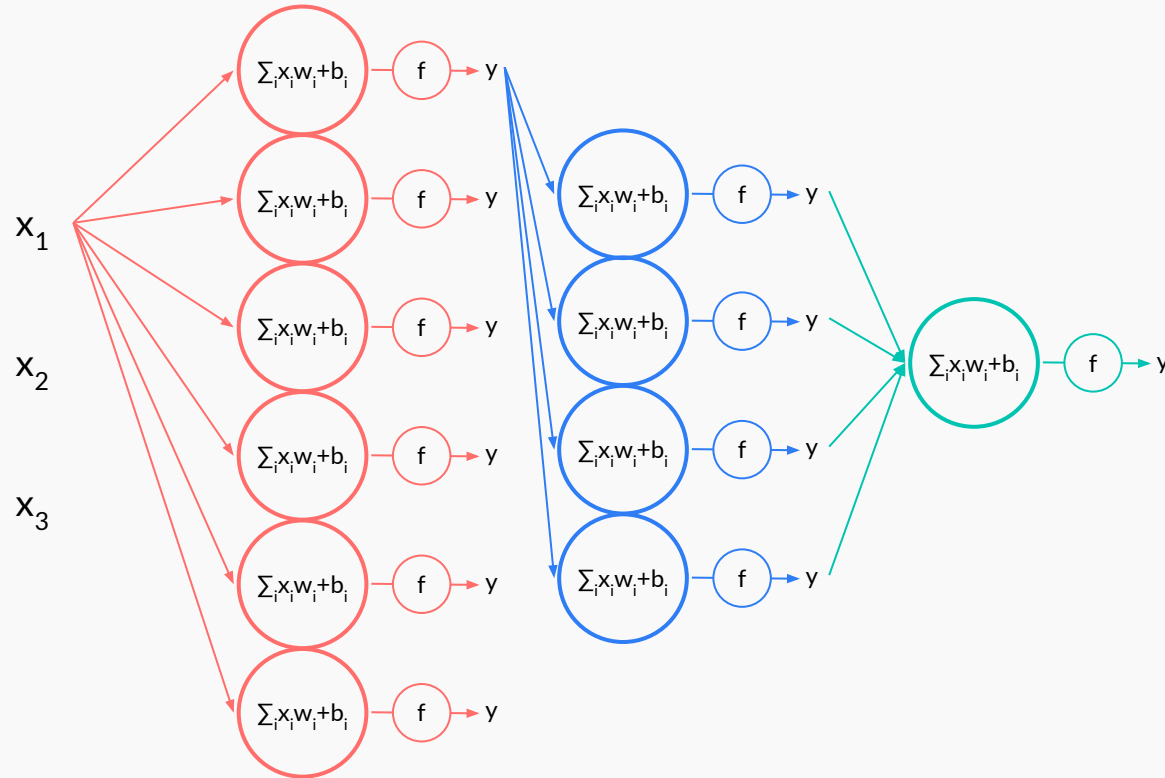
Measurement of CP asymmetry in $B^0 \rightarrow K_s^0 \pi^0$ decay

in the continuum e^+e^- or s quark. The classifier is trained on simulated signal and background events.



Classic Neural Networks

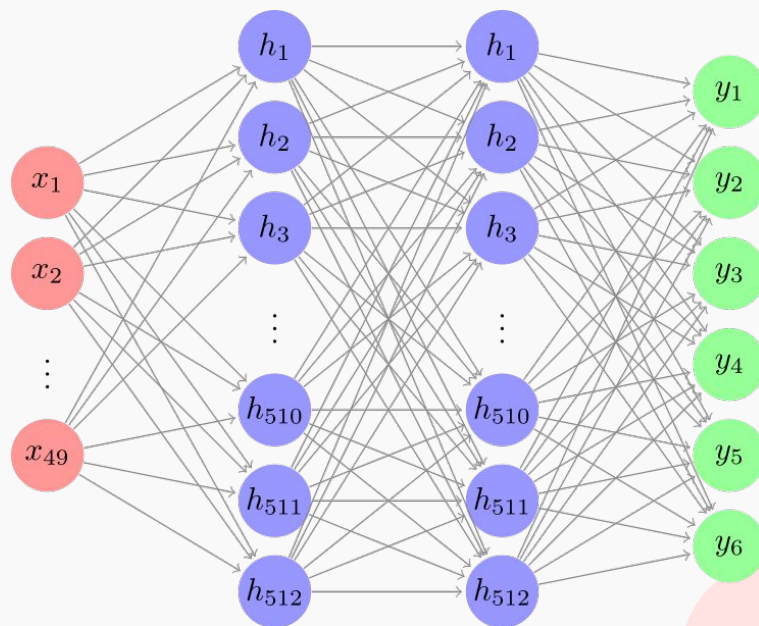
~~Boosted
Decision Trees~~



x_i : Inputs
 w_i : Learnable Weights
 b_i : Learnable Bias
 $f(x)$: Activation function
 y : Output

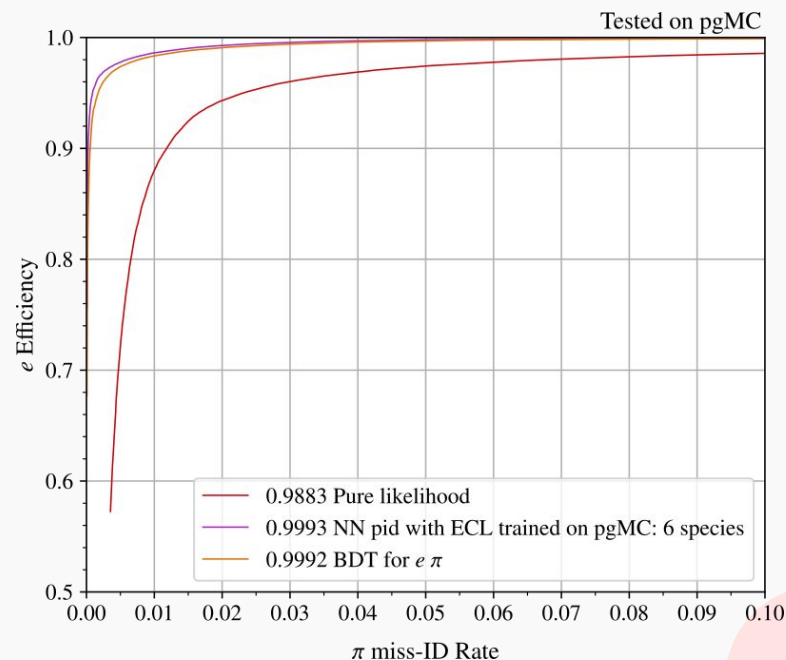
Classic Neural Networks

- Example: Improvement of Particle Identification at Belle II
- Currently likelihood of particle hypothesis is combined out of 36 subdetector likelihoods
 - $\mathcal{L}(h) = \prod_D \mathcal{L}_D(h)$
- NN solution can learn correlations among $\mathcal{L}_D(h)$
- Predict probabilities for all 6 particle species hypothesis (e, μ , π , K, p, d)
- Combination of high-level information as input:
 - $\mathcal{L}_D(h)$
 - Track momentum
 - Track charge
 - ECL Variables



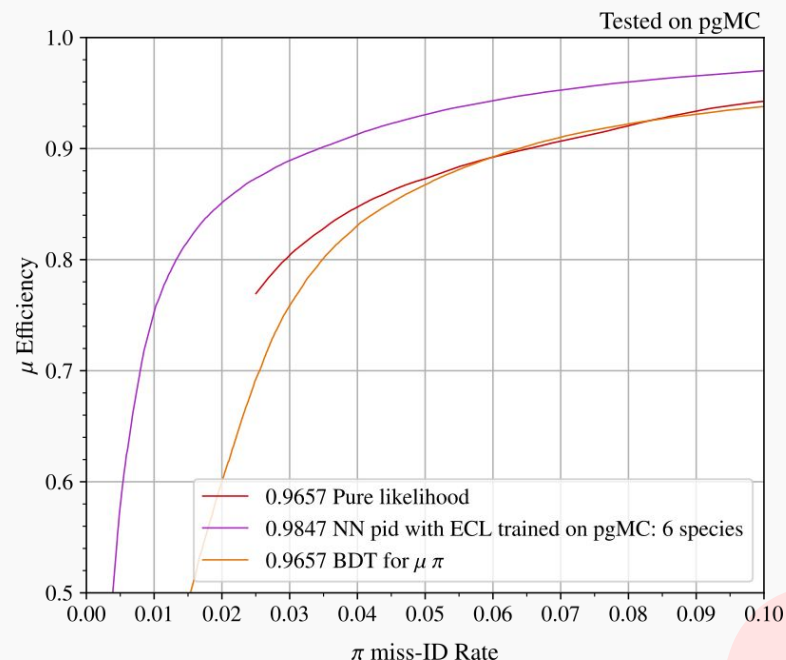
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- Improved performances for all particle hypotheses

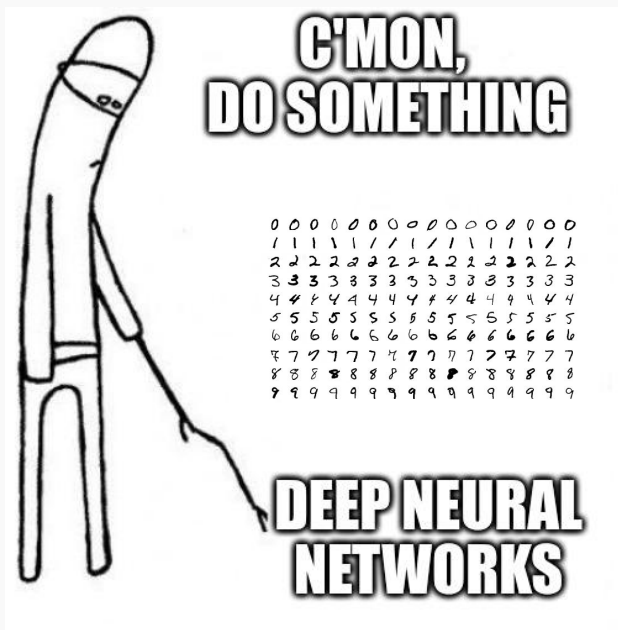


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Convolutional Neural Networks



MNIST Results

Architecture	Test Error	Weights (10^6)
DNN ¹	0.35 %	12.11
CNN ²	0.25 %	5.4

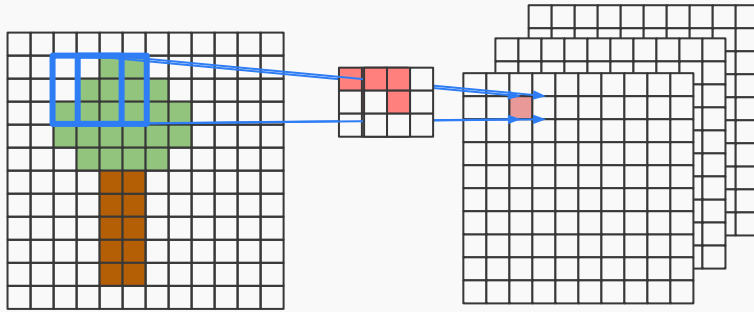
- Deep neural networks scale badly with high amount of inputs
 - Images with 32 pixels already have 1024 inputs
- DNNs don't take locality (nearby pixels are more strongly correlated) and translation invariance (meaningful patterns can occur anywhere) into account

1: <https://arxiv.org/abs/1003.0358>

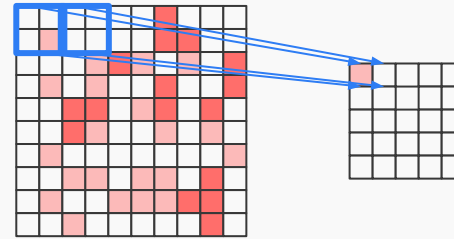
2: <https://arxiv.org/abs/1608.06037>

Convolutional Neural Networks

Convolutional Layer



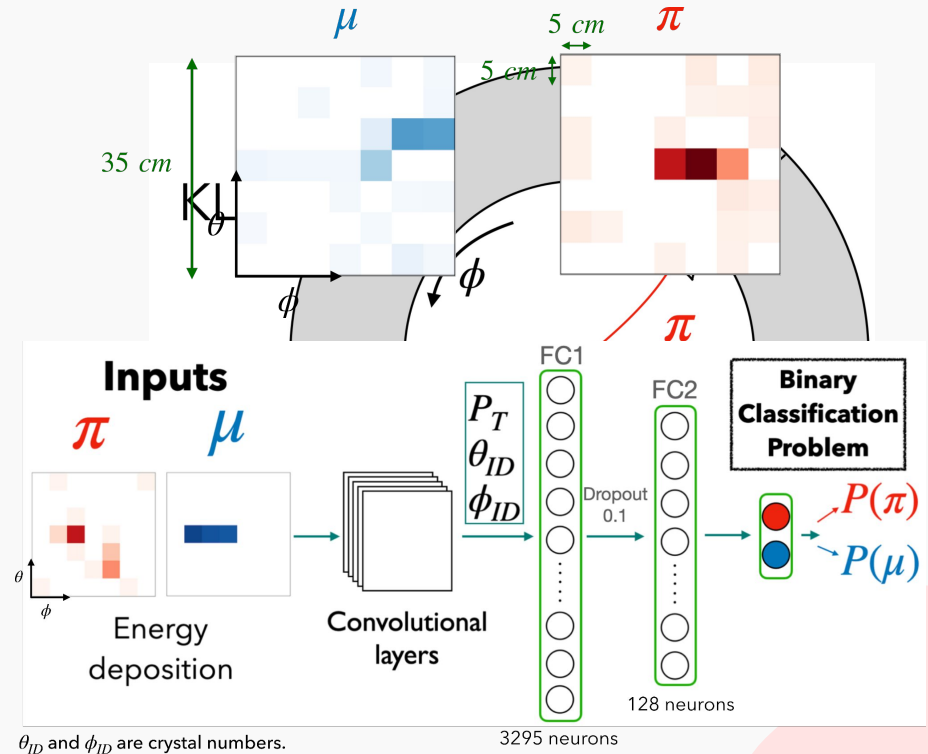
Pooling Layer



- CNNs are very good for image recognition:
 - Input stays in 2D shape instead of being flattened
 - Weights are shared in convolutions -> translational invariance
 - Nearby pixels are more highly correlated due to convolutions in kernels
- Convolutional layer:
 - Apply filter of size $N \times N$ to input
 - Slide filter over entire input layer with fixed stride
- Pooling layer:
 - Reduce layer size by downsampling
 - Different pooling types, such as max or mean pooling

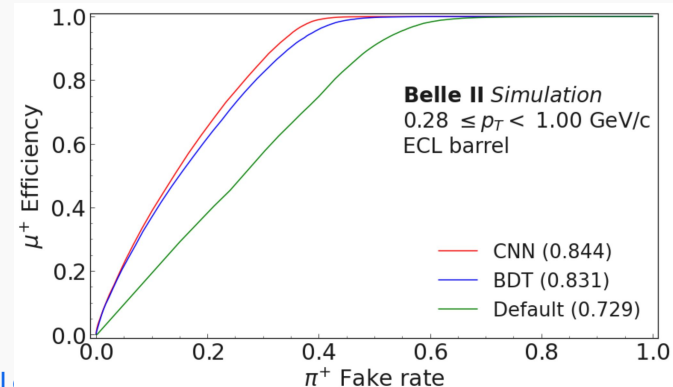
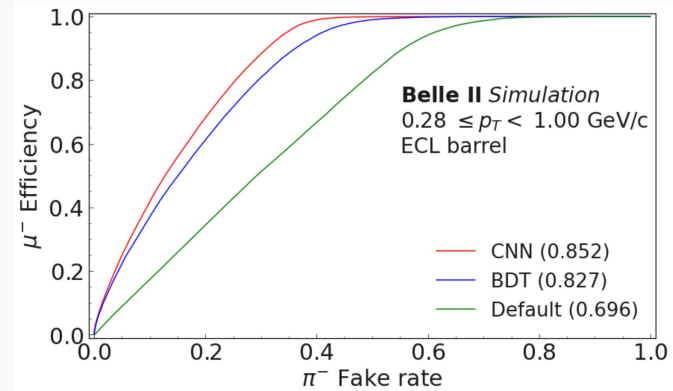
Pion/Muon Identification with CNNs

- Identification of low-momenta muons relies on ECL
 - Better muon-pion separation useful for e.g. leptonic tau decays
- Default PID in ECL uses E/p
 - Not very powerful for low momentum pion-muon separation
- Energy deposition patterns for pions are more dispersed than muons
 - Neural network can employ pattern recognition
- Energy deposition in 7x7 crystals can be treated as images
 - Two separate CNNs for positive and negative tracks
 - CNNs outperform both default and BDT method



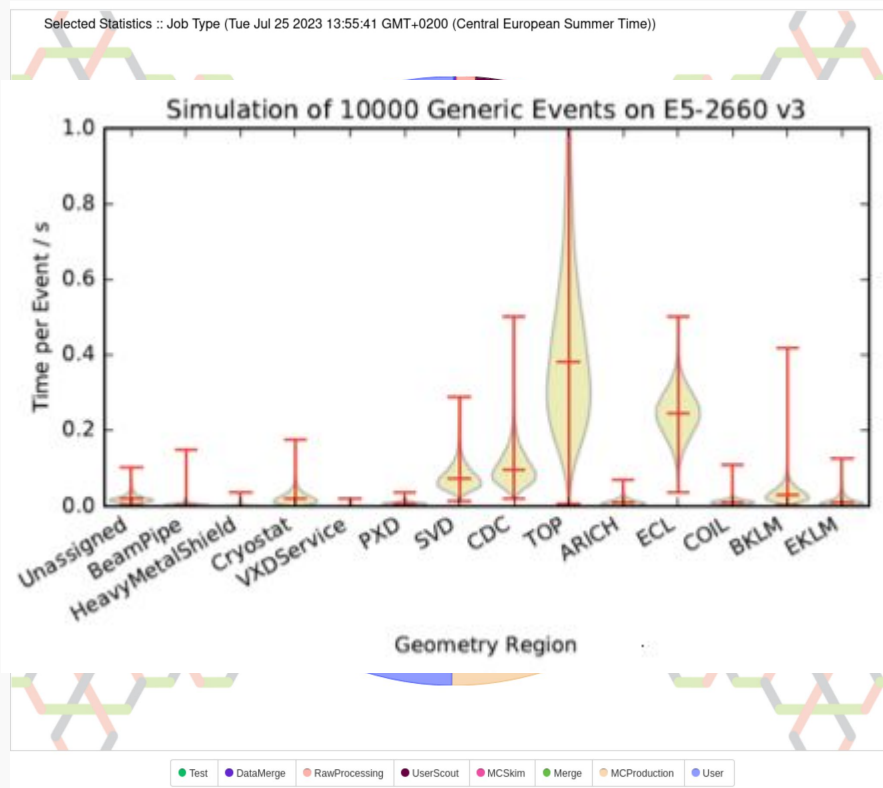
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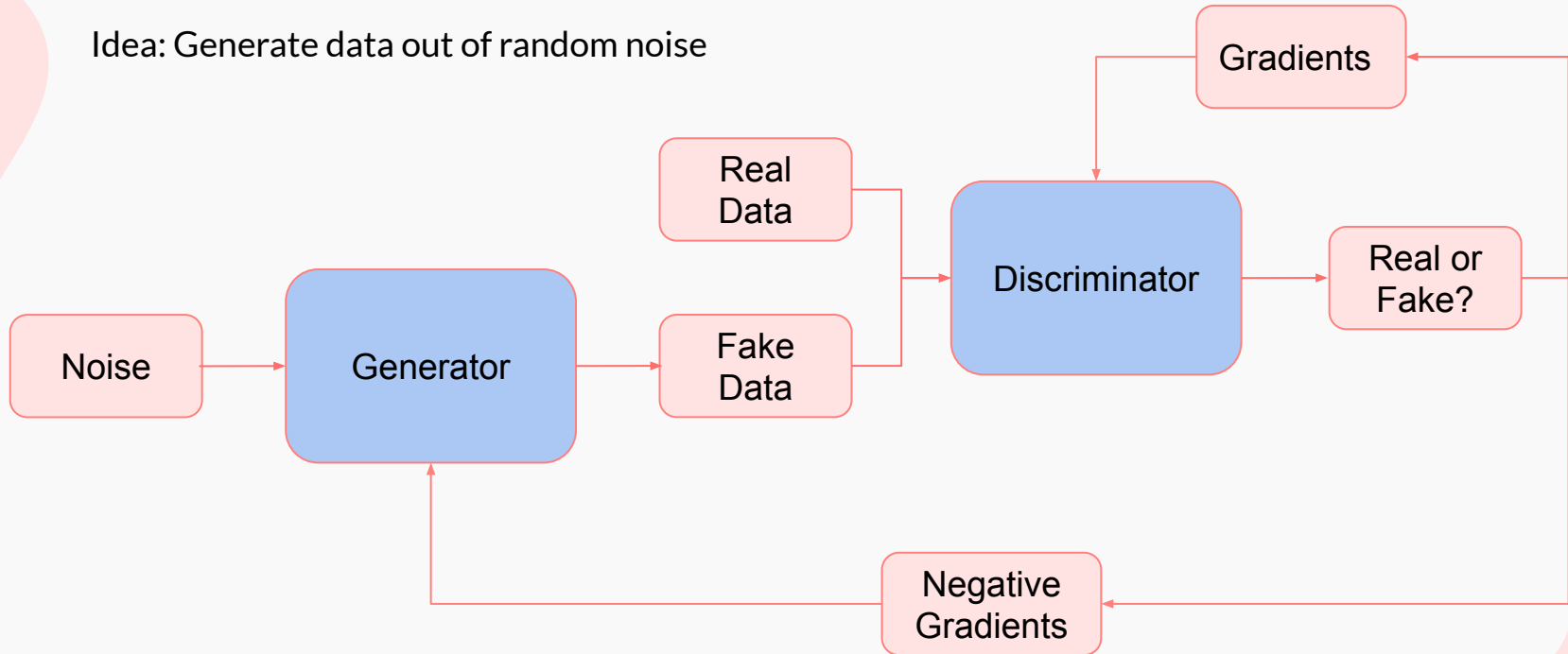
Generative Adversarial Networks

- Big chunk of Belle II computing is MC production
- With higher needs for MC data, computing time and resources might become bottleneck
 - Improvement of MC generation necessary
- TOP and ECL have highest simulation time of all subdetectors
- Improvement of MC simulation through generative ML algorithms
 - Generative adversarial networks
 - Variational autoencoders



Generative Adversarial Networks

Idea: Generate data out of random noise



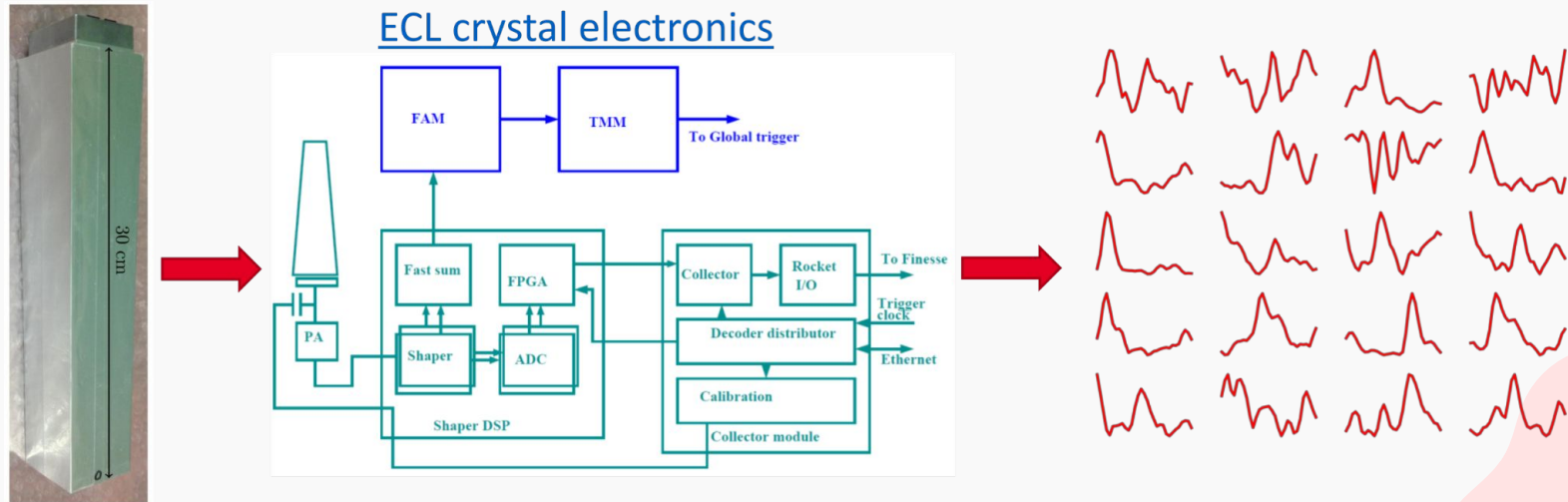
Generative Adversarial Networks

Idea: Generate data out of random noise



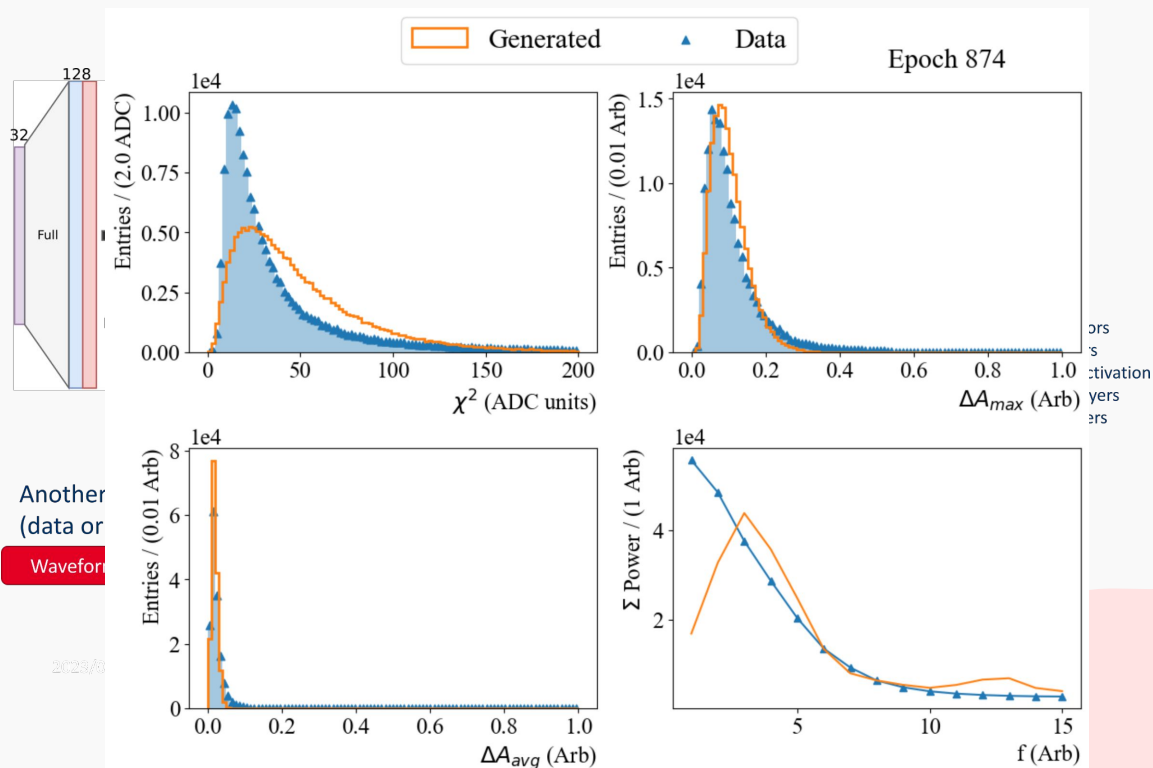
Simulation of Noise Waveforms in the ECL

- ECL consists of ~9000 crystals
- Crystal PMT measurements are digitized and a photon and hadron fit is applied
- Background waveform simulations require much data and bandwidth to store



Simulation of Noise Waveforms in the ECL

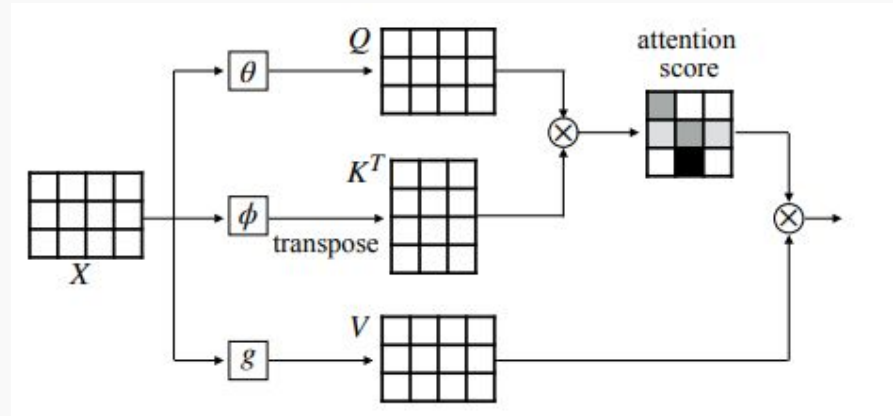
- Strategy: Only keep interesting (high energy, correlated backgrounds) waveforms and simulate the rest
- Train CNN GAN on generating waveforms
- Evaluate network on performance metrics
- GAN shows better performance than Autoencoders or Covariance Matrix Methods



Transformer

Developed for translations:

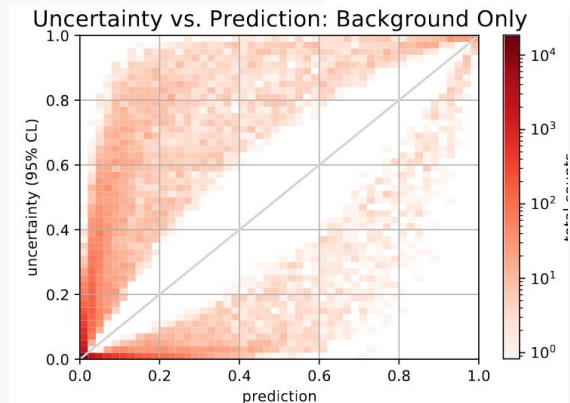
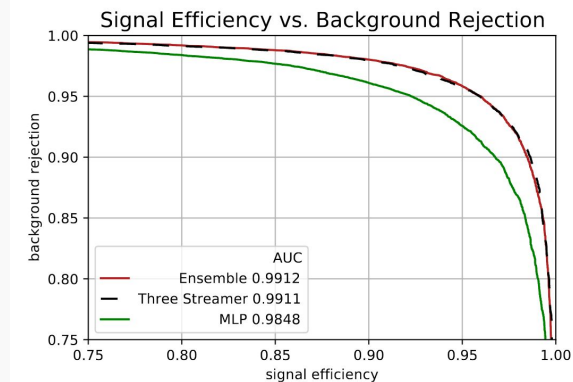
- Positional Encodings
(position in sentence is important for the translation!)
- Attention
(context is important)
- Self-Attention
(synonymous words can have different meanings according to context)



The FBI is chasing a criminal on the run .
The FBI is chasing a criminal on the run .
The FBI is chasing a criminal on the run .
The FBI is chasing a criminal on the run .
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Deep Continuum Suppression

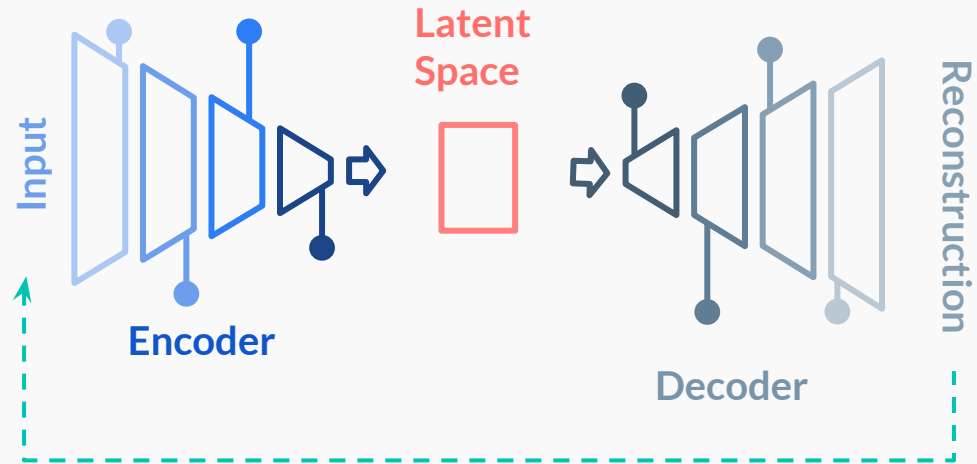
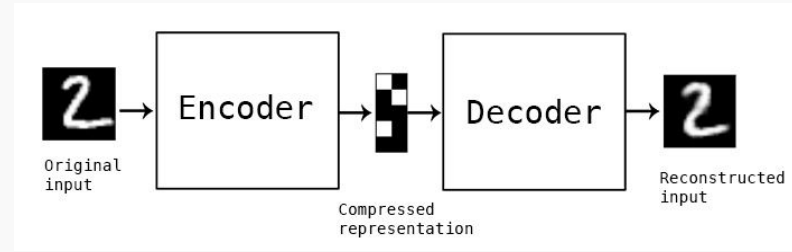
- BDTs and MLPs require fixed order for input particles, so some kind of sorting needed but this is prone to errors
 - Use self-attention-based input for permutation invariance
- Predictive uncertainties for the continuum classifications
 - Use deep ensembles
- Continuum suppression dependent on certain analysis variables, which is introducing a bias for further studies
 - Decorrelation from analysis variables



Autoencoder

- Unsupervised learning to replicate input as output
- Subnetwork **encoder** maps input to embedded representation
- Subnetwork **decoder** maps back to input space
- Lower-dimensional, condensed representation to capture important patterns

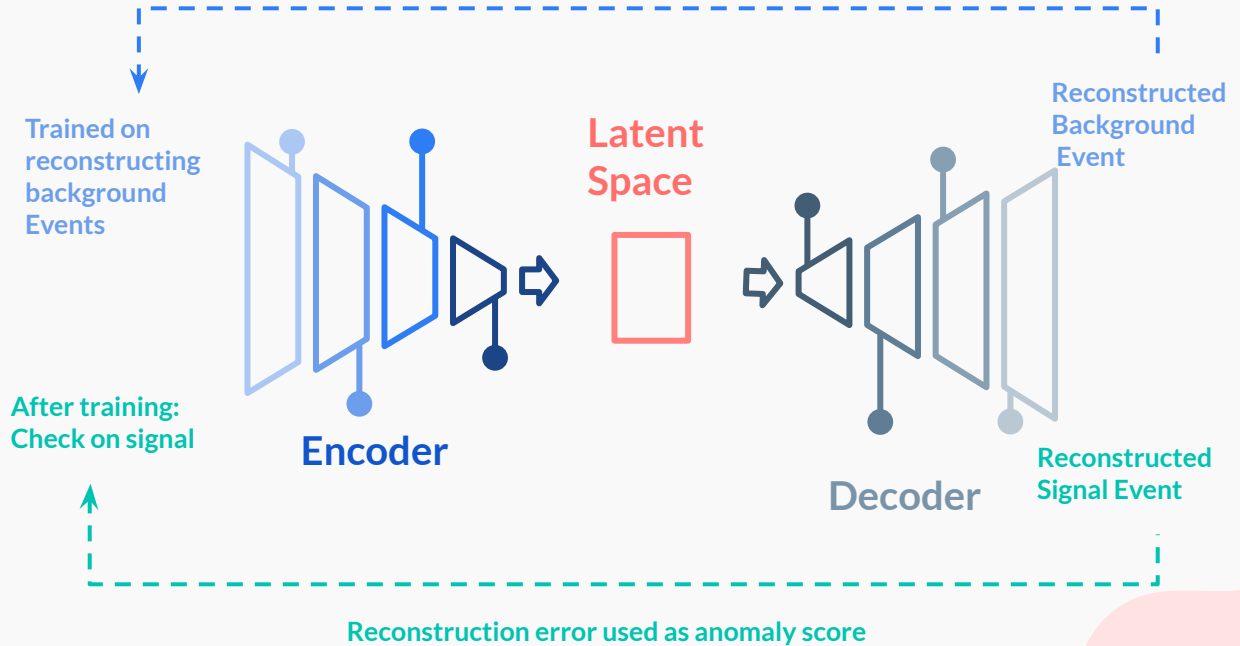
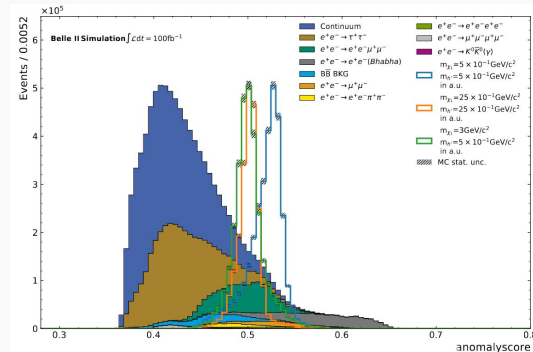
→ Network trained to learn the identity function



No labels required

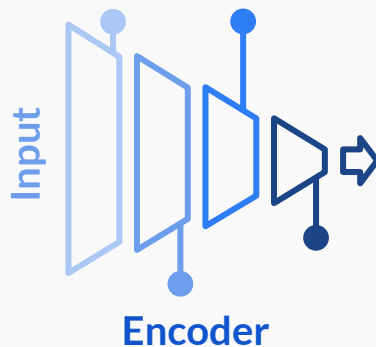
Autoencoder: Anomaly Detection

Goal: Find rare signature of new physics (e.g. dark Higgs searches) through anomaly detection in background dominated regions

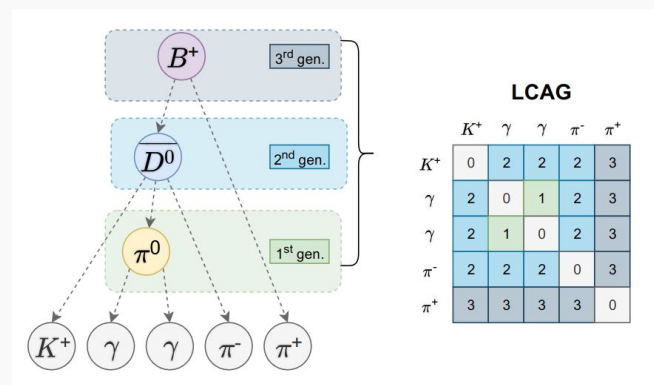
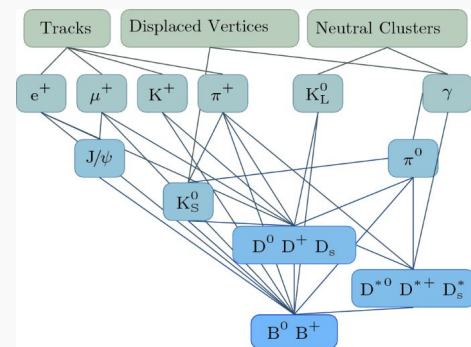


Encoder: graFEI

- Current FEI is restricted by branching fraction coverage (explicit decay structures covering $O(10\,000)$ decays so $\sim 15\%$)
- Use encoder for latent space representation to predict the decay tree
- Permutation invariance



Latent Space



LCAG

	K^+	γ	γ	π^-	π^+
K^+	0	2	2	2	3
γ	2	0	1	2	3
γ	2	1	0	2	3
π^-	2	2	2	0	3
π^+	3	3	3	3	0

Graph Data Structure

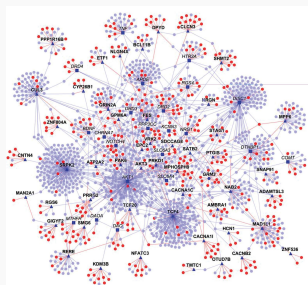
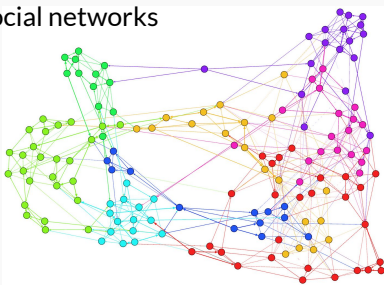
What happens if you have varying input size, for example the different number of particles in Event that are not on grids?

Use Graph Representation:

- Non-euclidian data structure
- Capture both information to the nodes and the relational information (edges)

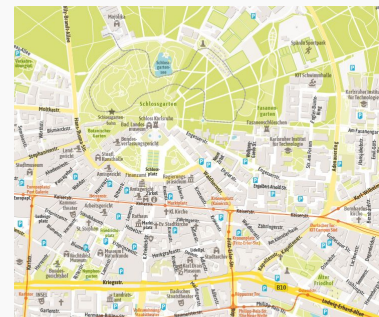
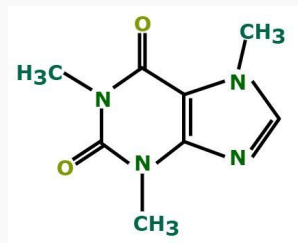
Cannot use CNNs here

Social networks

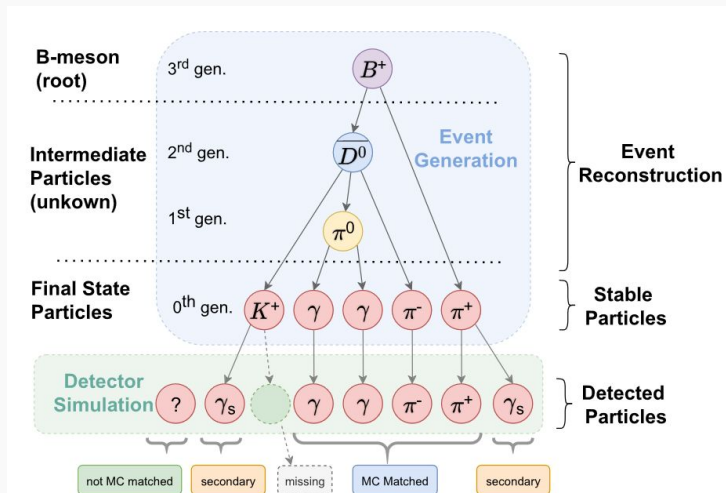


Protein Interaction

Molecules

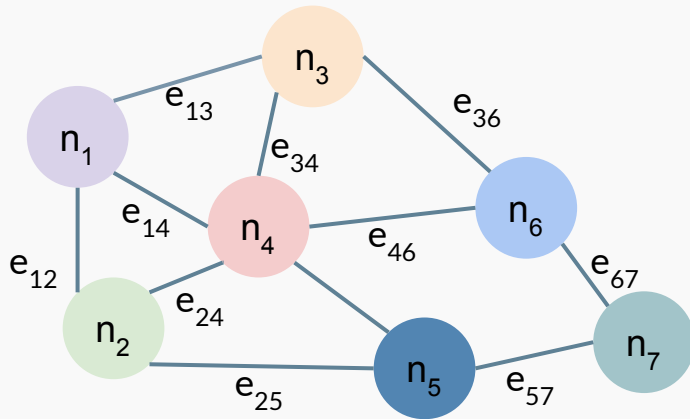


Maps



Particle Decay Trees

Graphs



Graphs are build with:

Nodes n_i

- In our example particles

With node features

- Energy, momentum, charge, PID ...

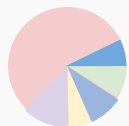
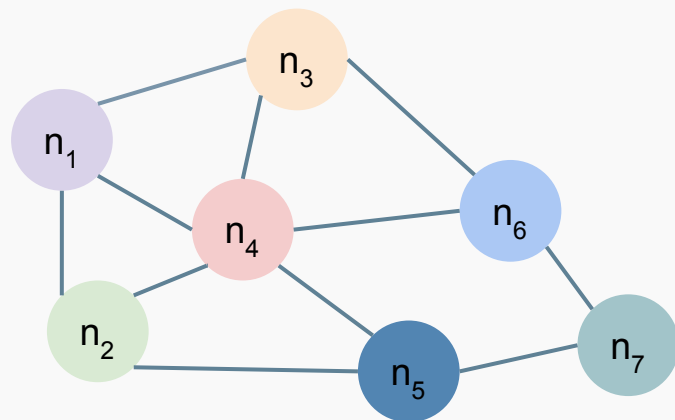
Edges e_{ij}

- Relations between particles

With edge features

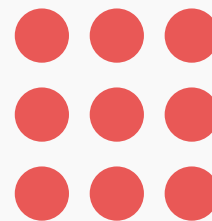
- Angle between two particles, distance, ...

Graph Convolutional Networks



Red node after first update step

- Generalization of Convolutional neural networks to graph-structured data



- Exchange information between nodes
- One-dimensional edge features as edge-weights possible

Current Flavor Tagger

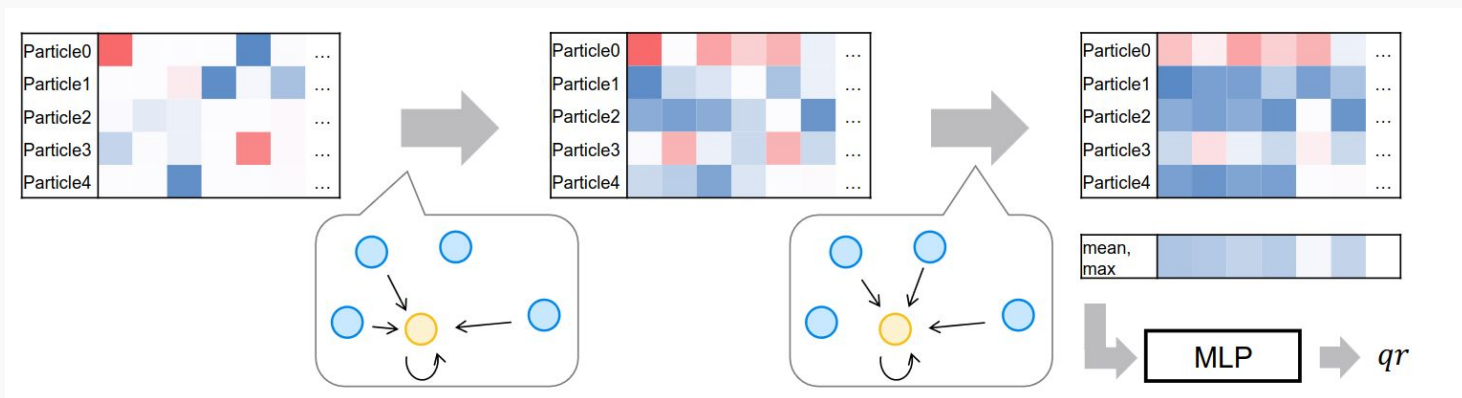
- Identify B-flavor from a single particle in the rest of event *(tag-side) in 13 categories
- Combine the categories output to provide final output
- While each particle has 13 outputs, only the best scores for each category are used
- Information loss
 - Don't know the category score of other particles
 - Don't know which particle has the best score

Event #	Category's output, qp						
	Electron	Muon	Kaon	SlowPion	Int-electron	Int-muon	...
Particle0	0.99	0.00	0.01	0.00	-0.99	0.00	...
Particle1	0.00	0.00	0.12	-0.96	-0.04	-0.51	...
Particle2	-0.01	-0.15	-0.10	0.00	0.00	0.03	...
Particle3	-0.34	0.00	-0.09	0.00	0.80	0.03	...
Particle4	0.00	0.00	-0.94	0.00	0.00	0.02	...
Best	0.99	-0.15	-0.94	-0.96	-0.99	-0.51	...

FastBDT / MLP → qr

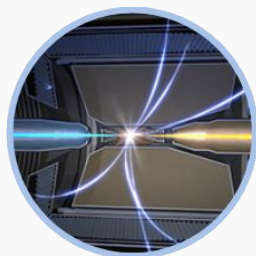
GNN-based Flavor Tagger, GFlaT

- Use Dynamic Graph Convolutional Network
- Update node features using edge information
 - Momentum, relative distance between two particles, 13-category outputs, 6-PID variables as input
- Measured tag-side efficiency with real data: **20 % increase of efficiency** on data



Real Time Application

- Different trigger levels have to reduce data stream to match DAQ limitations
- Level 1 trigger: hardware-based on FPGAs
- High Level Trigger: full reconstruction CPU based
- If data is not triggered here, its not saved → not available



Bunch Crossings:
250 MHz

Level 1 Trigger:
30 kHz, 5 μ s Latency

High Level Trigger:
5-10 kHz, 1.8 Gb/s

→ Bigger is not always better: real time machine learning applications require smart, small networks to be deployed on FPGAs with high throughput rates (e.g. 30 MHz)

Neuro Z-Trigger

CDC Trigger Pipeline

Track Segment Finder

2D Track Finder

3D Track Info

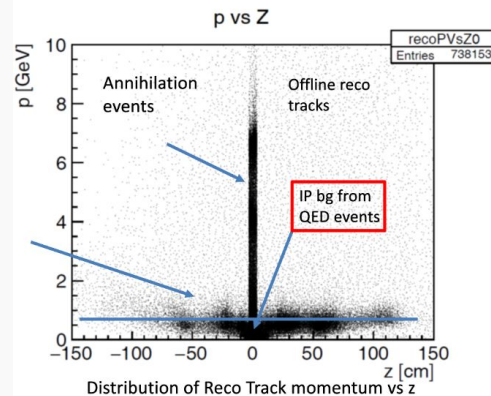
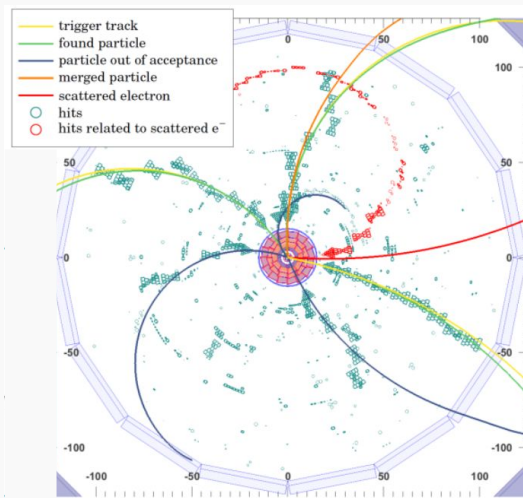
Trigger

Pattern Map

Hough Transformation

Neural Network

27 inputs with 81 hidden nodes and 2 output nodes



- Input of hough transformation used to predict **z-displacement** in respect to Interaction Point and **theta** of track
- Trained on **data** (reconstructed tracks)
- Used to reduce background from QED events (trigger rate too high from only track trigger)

()



}

**Do you have
questions?**



03

Object Condensation for Reconstruction

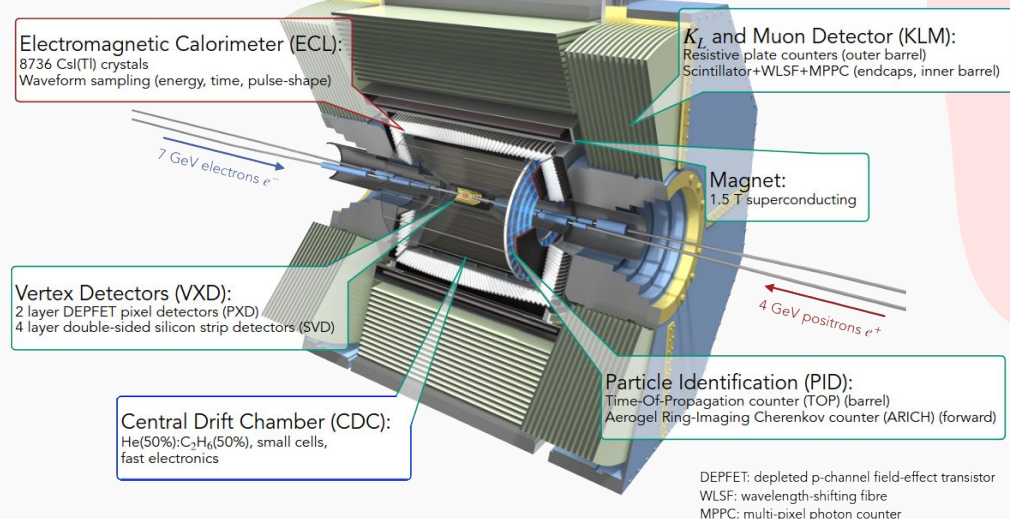


Motivation

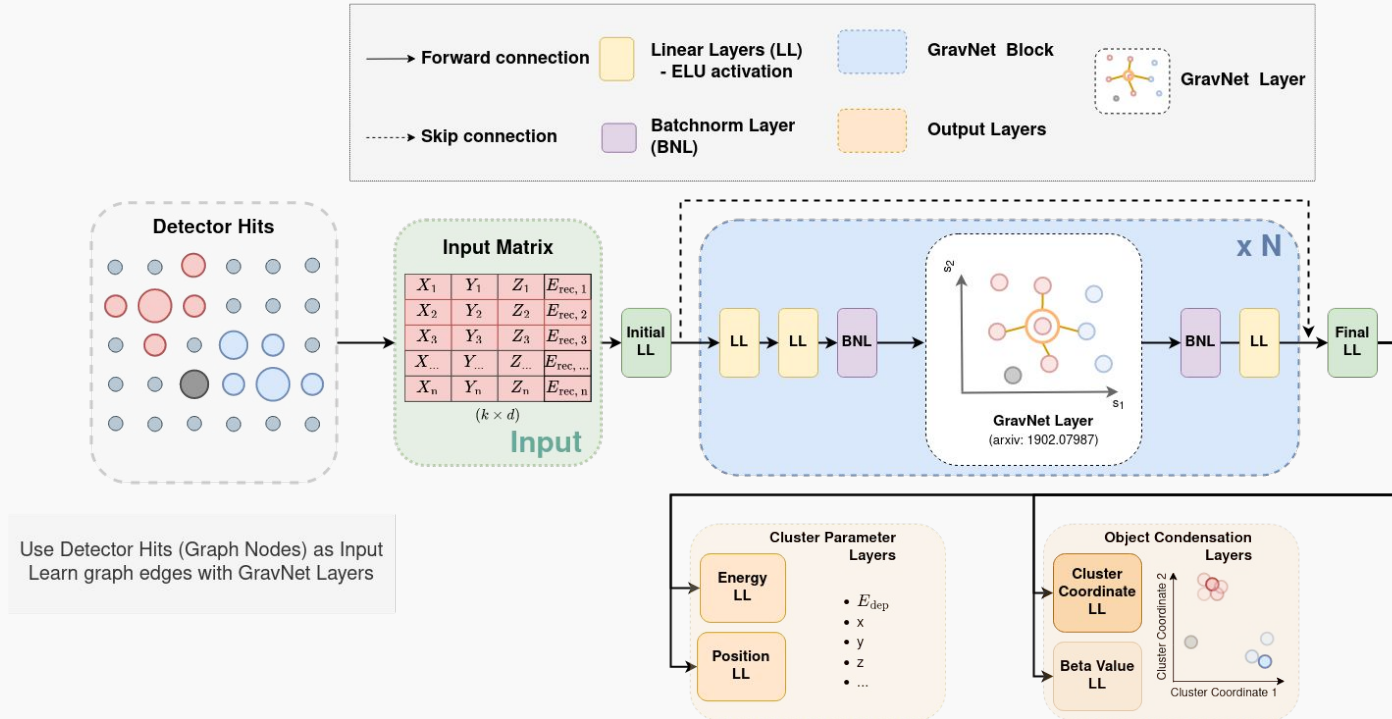
- Searches for new physics for data we did not look at yet
- New tools with Machine Learning to improve trigger level reconstruction
- Improvement of current trigger algorithms

Requirements:

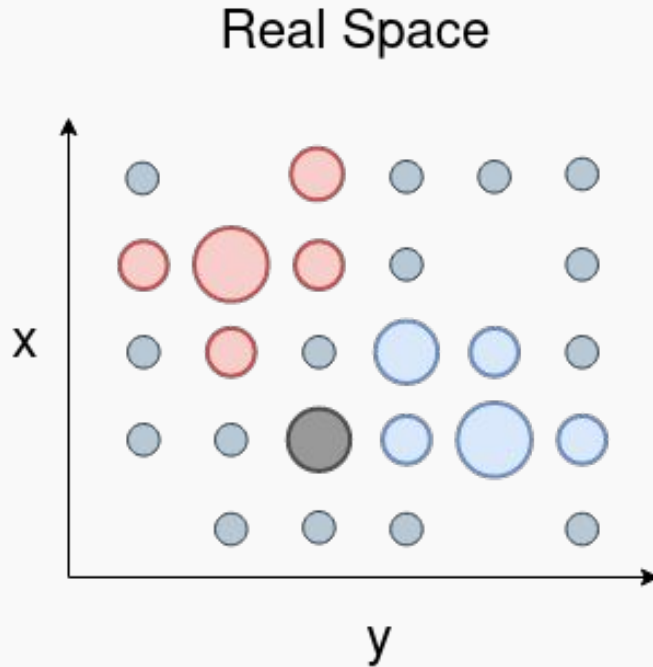
- Varying input sizes due to different number and type of particles in event
 - Use Graph Neural Networks
- We don't know how many clusters/tracks there will be
 - Object Condensation Algorithm¹



Graph Reconstruction Model

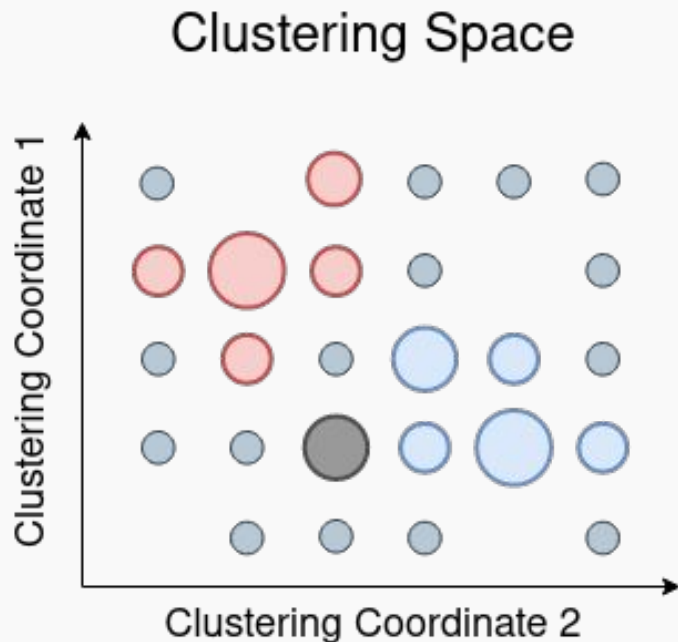


Object Condensation



- OC algorithm takes input vertices (= detector hits) and translates them from real space to a clustering space
- Clustering space is learned by the network
 - In the beginning clustering space = real space

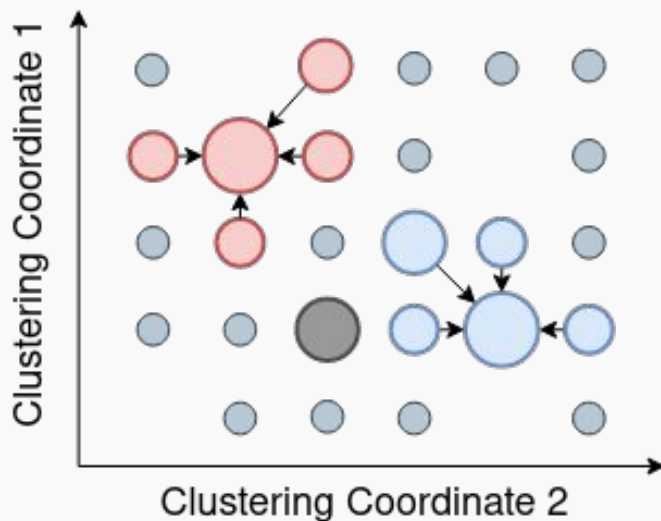
Object Condensation



- OC algorithm takes input vertices (= detector hits) and translates them from real space to a clustering space
- Clustering space is learned by the network
 - In the beginning clustering space = real space
- Dimensionality of clustering space is hyperparameter
- OC algorithm introduces potential that clusters vertices from the same object together

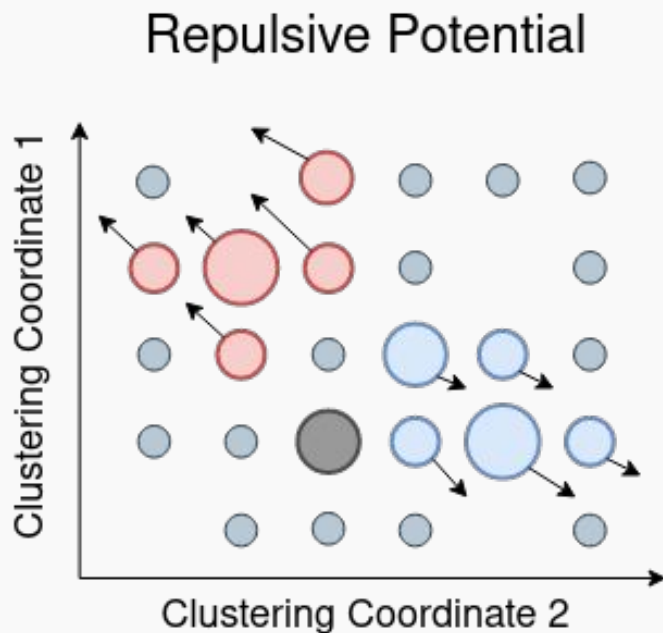
Object Condensation

Attractive Potential



- An attractive potential draws vertices from the same object towards each other
- Background vertices are not influenced by the potential
- Attraction loss favors minimum distance between vertices of the same object

Object Condensation



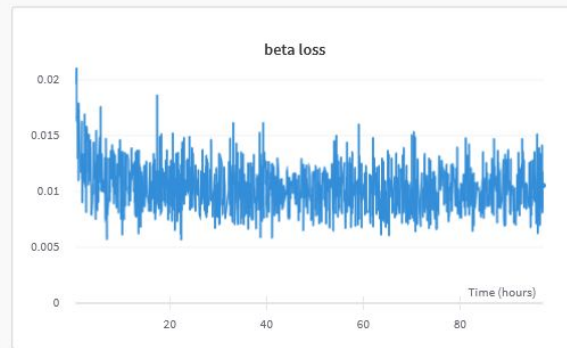
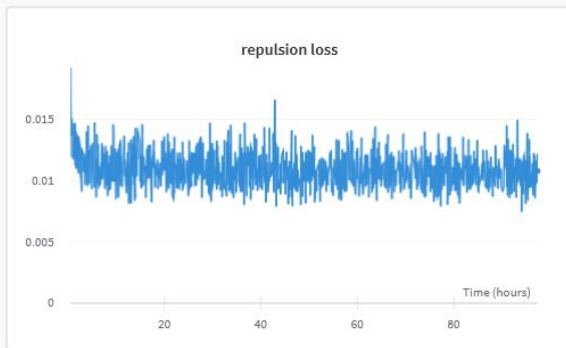
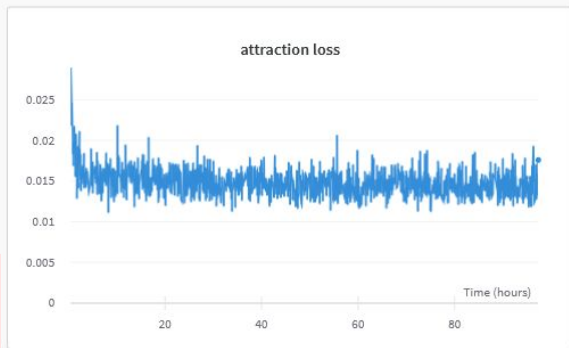
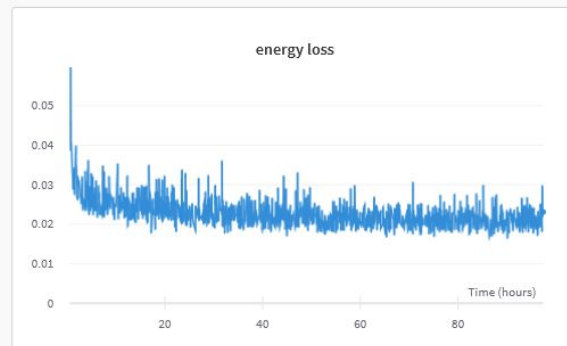
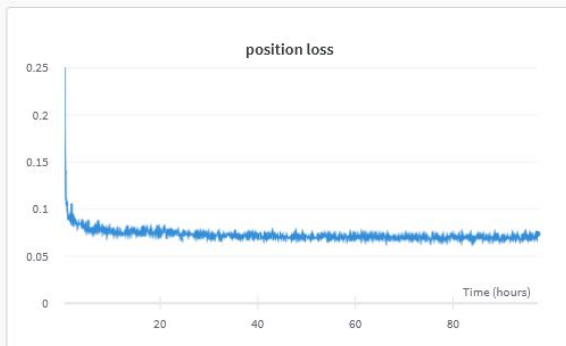
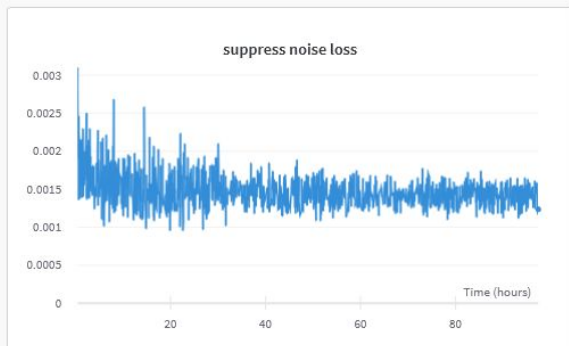
- An attractive potential draws vertices from the same object towards each other
- Background vertices are not influenced by the potential
- Attraction loss favors minimum distance between vertices of the same object
- A repulsive potential draws vertices from different objects away from each other
- Repulsion loss favors maximum distance between vertices of different objects
 - Clustering space is bounded

Object Condensation

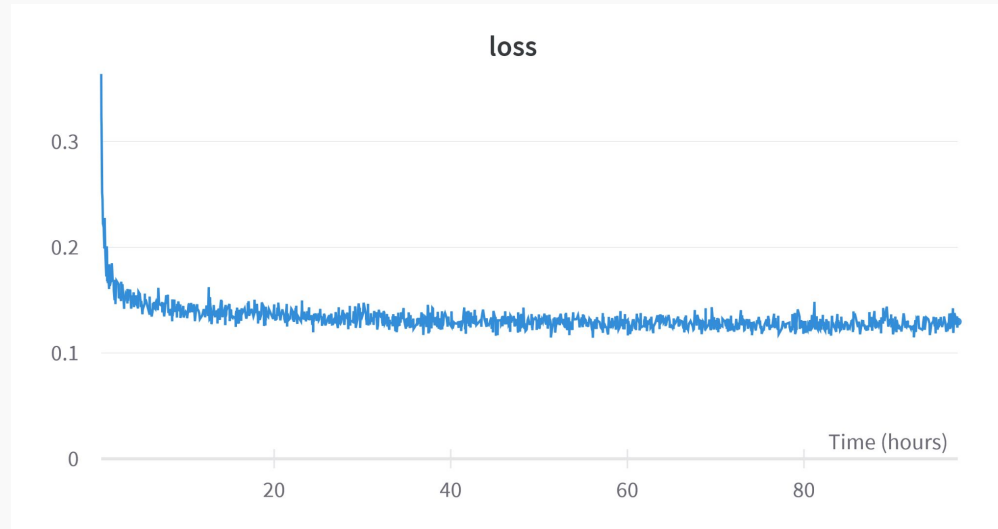


- Each vertex is assigned a β value
- Vertex with the highest β value is called a condensation point
 - Invokes the potential for vertices belonging to the same object
 - β loss favors one condensation point per object
- Condensation points “carry” values for their objects
 - ECL: energy, position, ... of clusters
 - CDC: momentum, charge, displacement, ... of tracks

Object Condensation



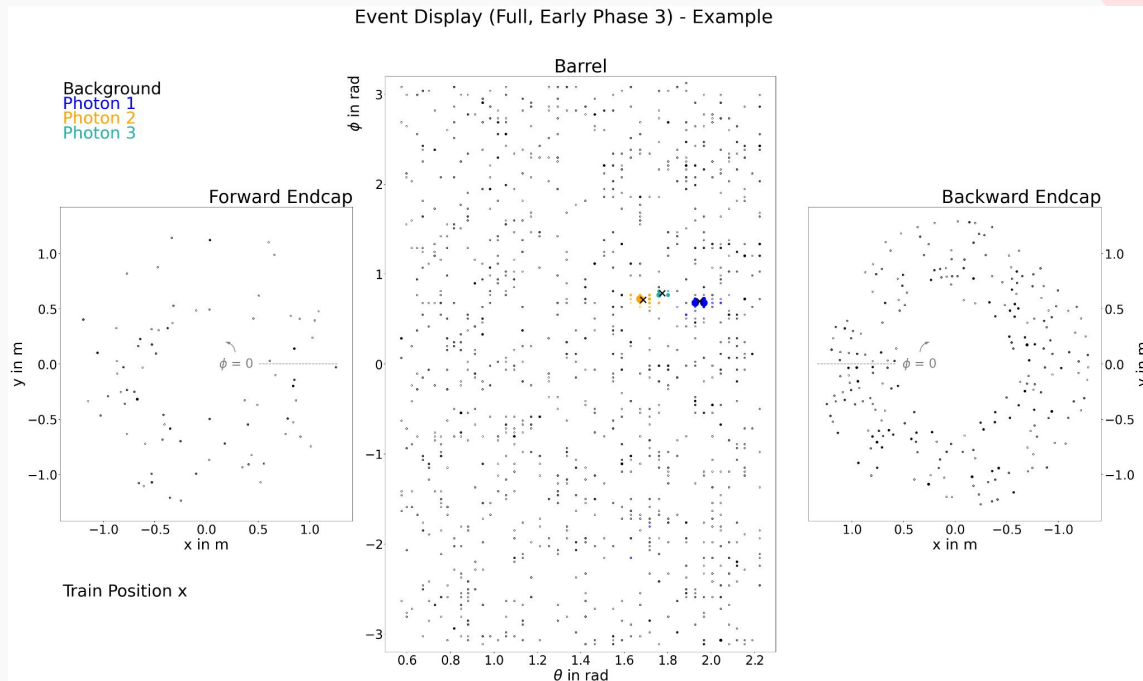
Object Condensation



- Full loss is sum of all sub-losses
- Scaling of losses can be done to improve training

Object Condensation for ECL

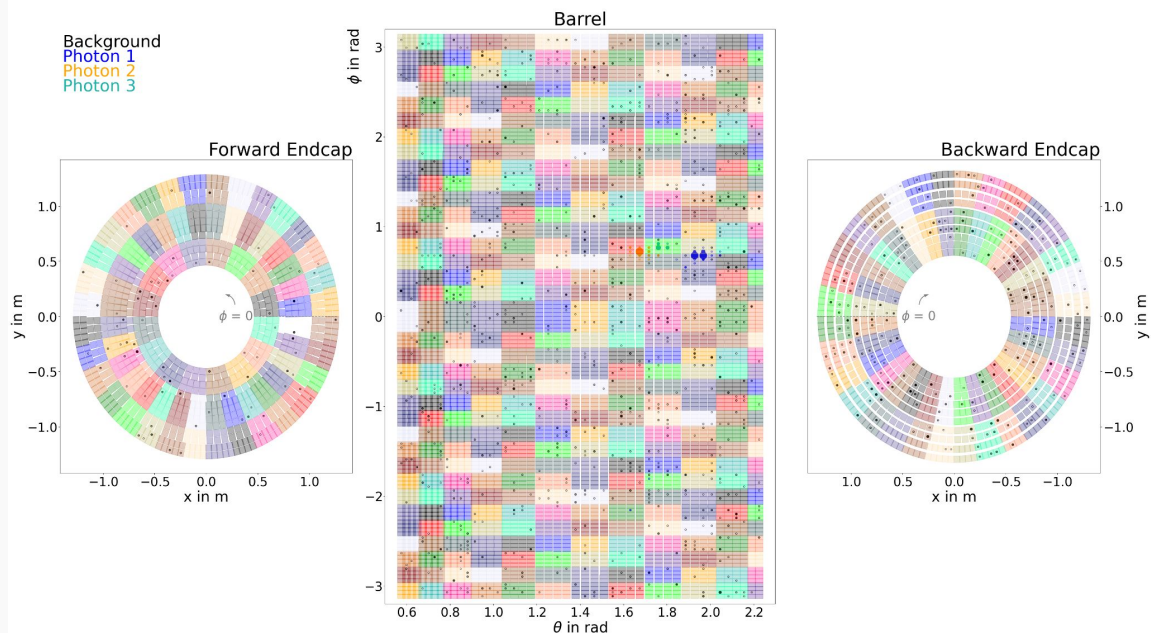
- OC for ECL for both offline and online reconstruction
- For each cluster, predict existence, position and deposited energy
- Offline: Use every crystal with $E > 1$ MeV as input



Object Condensation for ECL

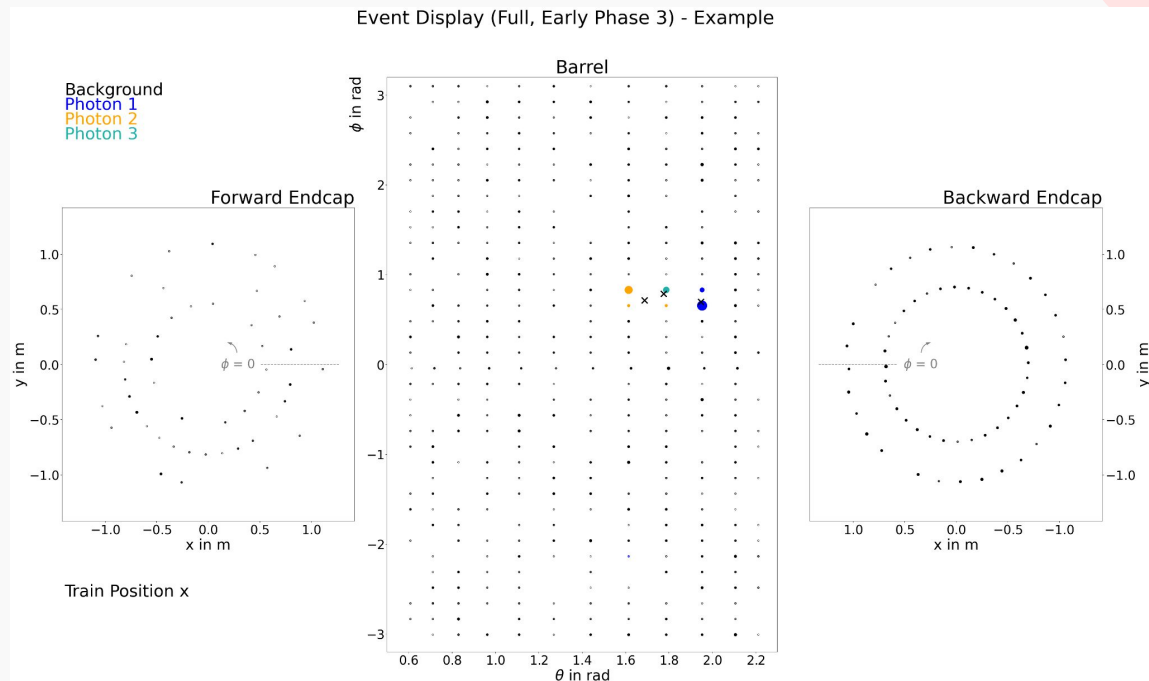
- OC for ECL for both offline and online reconstruction
- For each cluster, predict existence, position and deposited energy
- Offline: Use every crystal with $E > 1$ MeV as input
- Online: Use current trigger mapping (4x4 crystals = triggercell) with energy cut as input

Event Display (Full, Early Phase 3) - Example



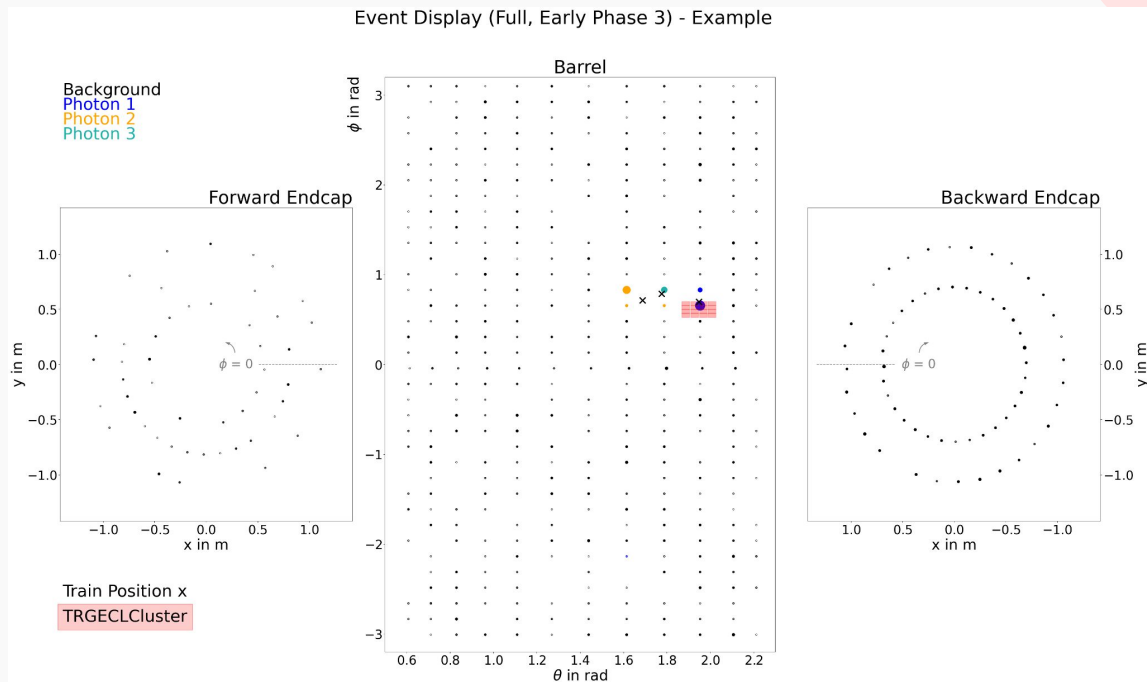
Object Condensation for ECL

- OC for ECL for both offline and online reconstruction
- For each cluster, predict existence, position and deposited energy
- Offline: Use every crystal with $E > 1$ MeV as input
- Online: Use current trigger mapping (4x4 crystals = triggercell) with energy cut as input



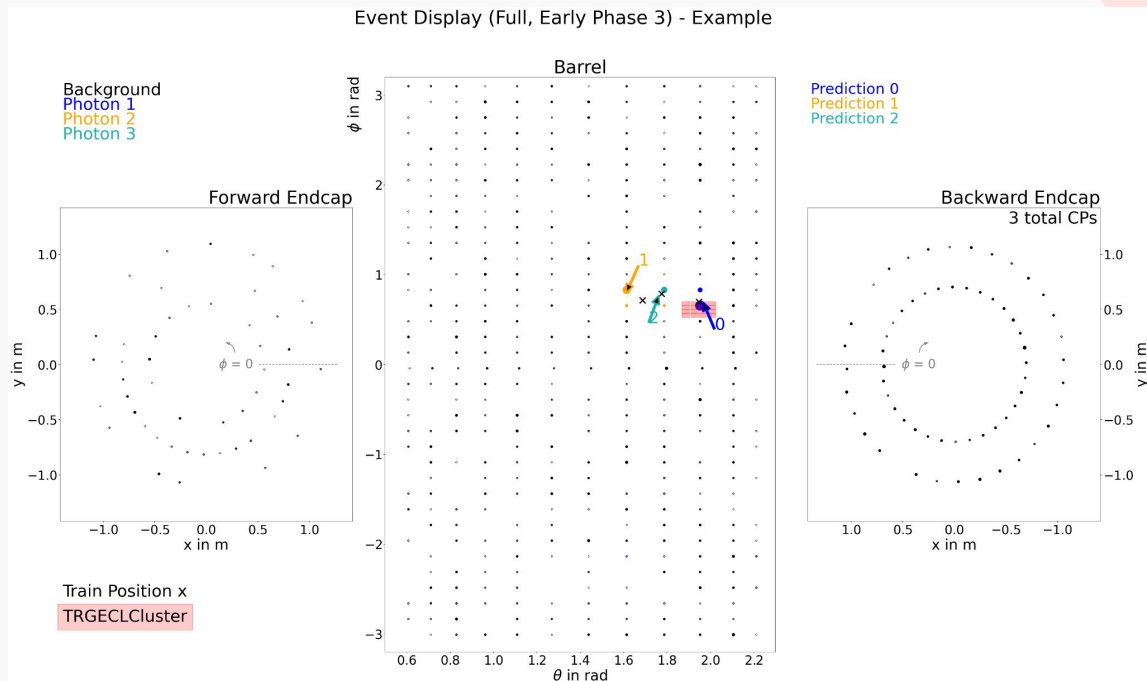
Object Condensation for ECL

- OC for ECL for both offline and online reconstruction
- For each cluster, predict existence, position and deposited energy
- Offline: Use every crystal with $E > 1$ MeV as input
- Online: Use current trigger mapping (4x4 crystals = triggercell) with energy cut as input
- Improve efficiency and resolution of ECL Trigger algorithm
 - Current ECL Trigger has low efficiency for overlapping clusters

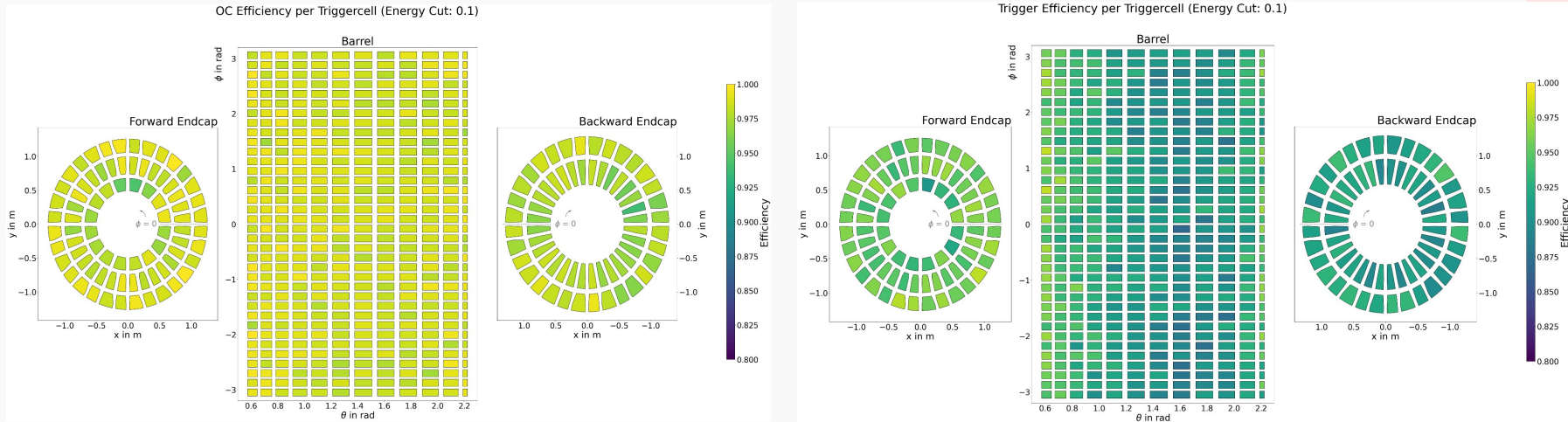


Object Condensation for ECL

- OC for ECL for both offline and online reconstruction
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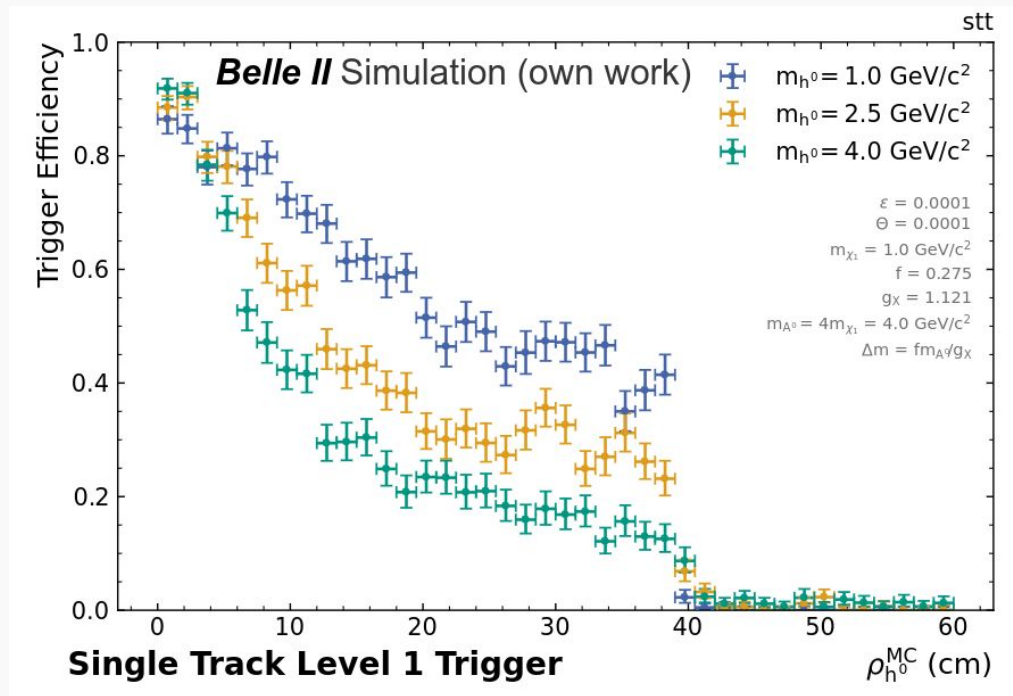


Object Condensation for ECL

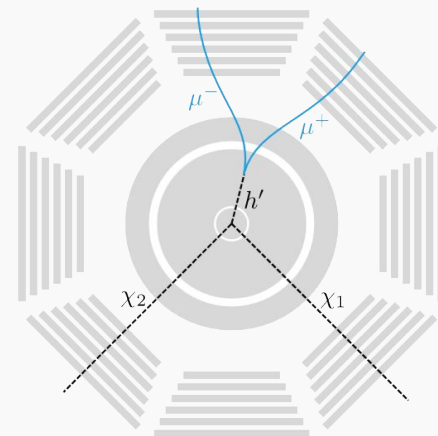


- OC algorithm trained on 1-6 photons with generated energy between 0.1 GeV and 2 GeV
- Energy of triggercells > 100 MeV (modelling of current trigger algorithm)
- Improvement in efficiency for full ECL
- Current model has ~40000 parameters

Object Condensation for CDC

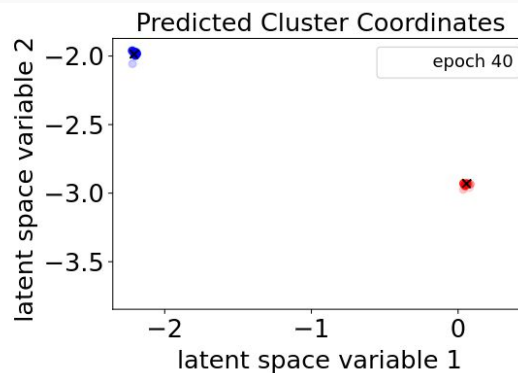
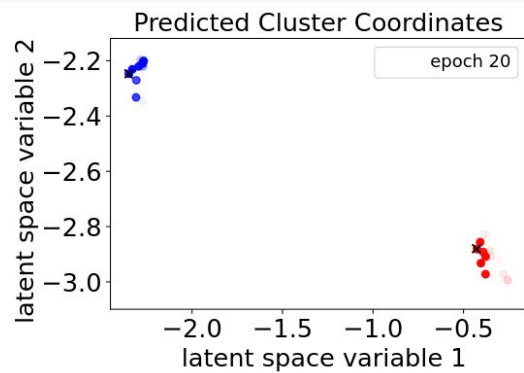
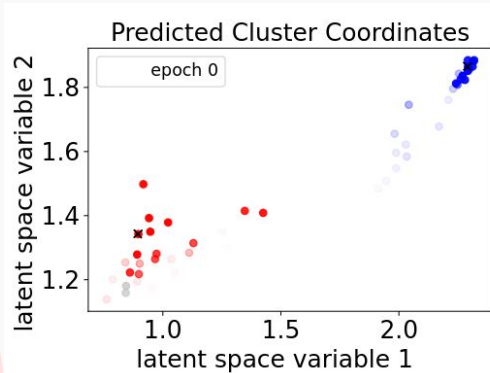
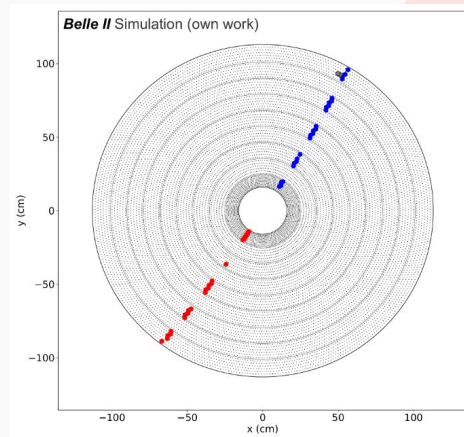


- Displaced vertices important signature in searches for new physics
- Improve both real time and offline reconstruction

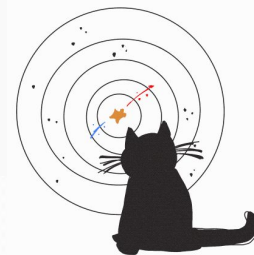


Object Condensation for CDC

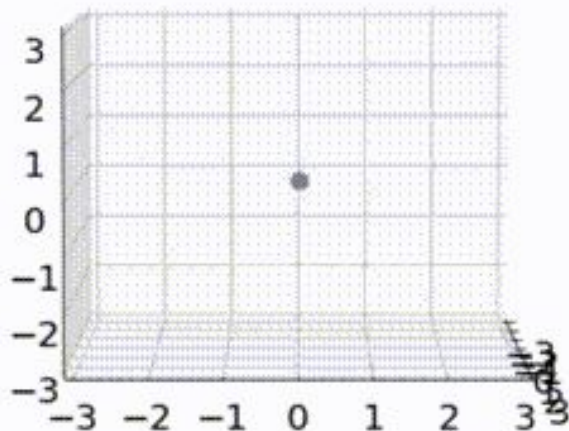
- Use CDC hits in the detector as input for the OC GNN
- Predict number of tracks
 - For each track, predict starting position, momentum and charge



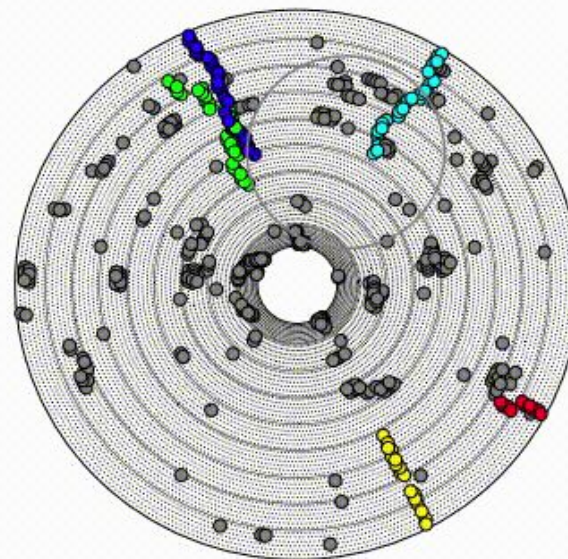
Object Condensation for CDC



Epoch 0

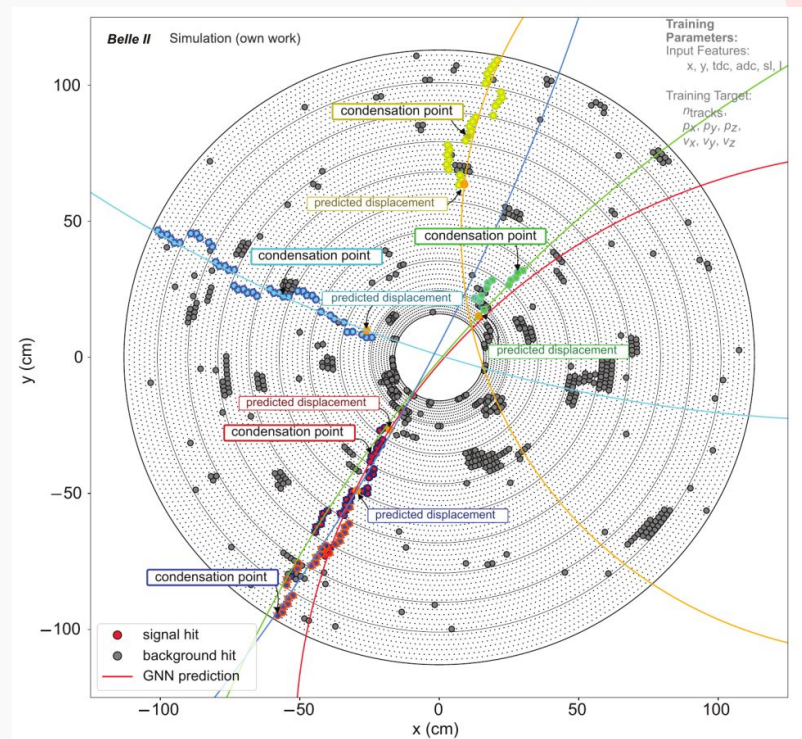
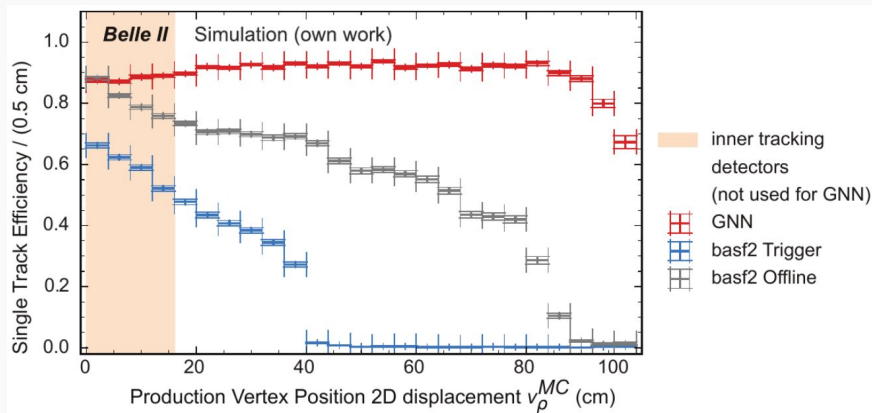


Epoch 0



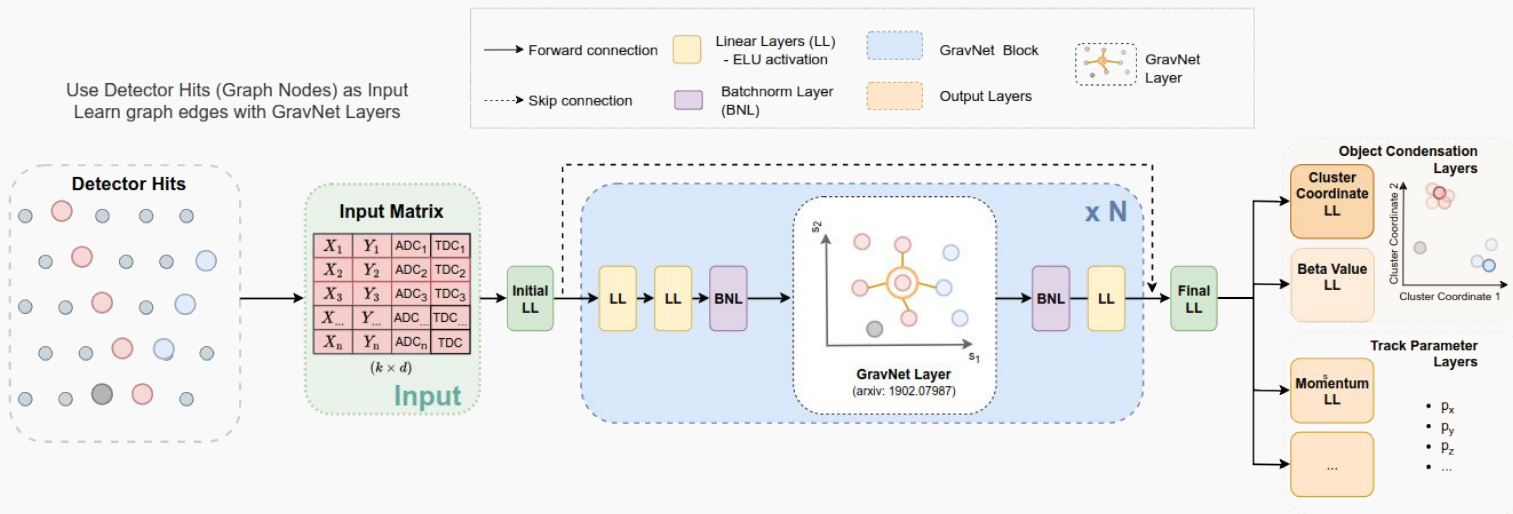
Object Condensation for CDC

GNN achieves 96.68% efficiency on displaced vertex samples $X \rightarrow \mu^- \mu^+$



Graph Reconstruction Model

Use Detector Hits (Graph Nodes) as Input
Learn graph edges with GravNet Layers



Adjustable Parameters:

General Parameters:

- dimension **dim1**, **dim2** of Linear Layer
- number of Graph Blocks **nblocks**

GravNet Parameters:

- number of **k**-nearest neighbors in GravNet
- GravNet space dimensions (currently 4)

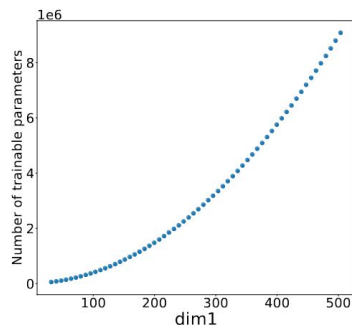
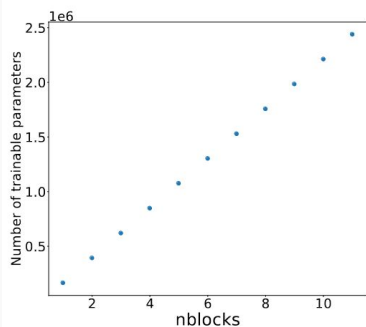
Output:

- Dimension of Cluster Coordinates for OC **coord**
- Number of output layers according to Track Parameter Predictions

Hyperparameter

This starting setup has ~669000 trainable parameters!

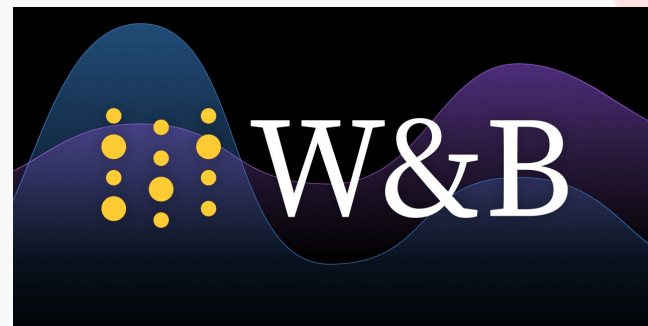
Model Parameters need to be greatly reduced to fit FPGA and gbasf2 CPU requirements



Hyperparameter	Current Value
Number of Neighbors k	9
Number of GravNet Blocks nblocks	3
Number of Nodes 1 dim1	128
Number of Nodes 2 dim2	32
Momentum	0.6
CC Space ccoords	3
Learning Rate lr	0.001
Optimizer optim	Adam

Training Documentation wandb.ai

- Machine Learning Platform for developers
- Cloud based ML experiment tracking tool
- Features:
 - Experiment Tracking
 - Hyperparameter Tuning
 - Data and Model Versioning
 - Model Management
 - Data Visualization
 - Collaborative Reports
 - Integration for **PyTorch**, Keras, PyTorch Lightning etc.
 - Private-Hosting



Overview Reports **Projects** Likes

Projects Create new project

Search 1-12 of 12 < >

Name	Last Run	Runs	Entity	
validation_triggercells	2023-07-23	133	ihaide	...
validation_ep3	2023-06-13	3	ihaide	...
triggercells	2023-07-17	132	ihaide	...

```
wandb.log({'full loss': loss,
          'repulsion loss': reploss,
          'attraction loss': attloss,
          'energy loss': energyloss,
          'beta loss': betaloss,
          'suppress noise loss': suppressloss,
          'pos loss': posloss})
```

Training Documentation wandb.ai

Very simple to use!
Everything at one place!

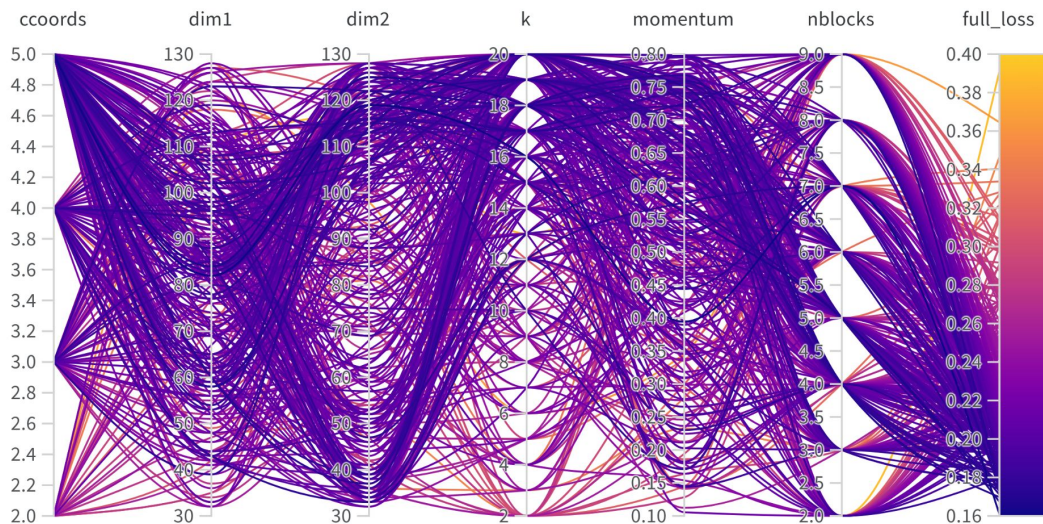
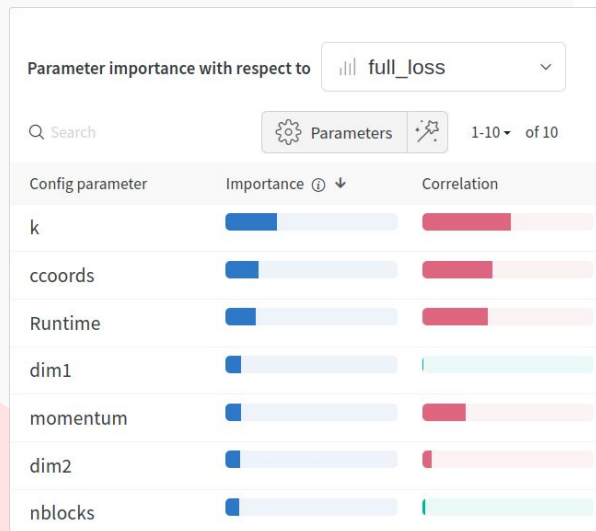
- Save configs and models to keep track of multiple trainings and version control
- Monitor training
- Log weights and biases for deep learning trainings (confirm that not only last layers get updated while training!)



Have to monitor more than 7 sub-losses for Object Condensation!

Hyperparameter Optimization

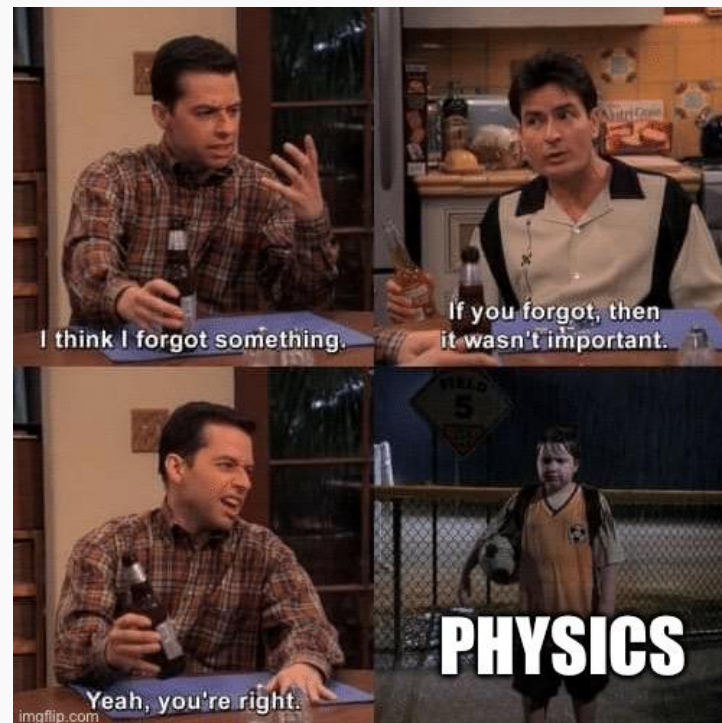
- Runs easily on one or more gpus (start a new sweep on another gpu with the same sweep agent)
- Optimizes model parameters



ECL OC model down to 40,000 parameters

Quality Control

- Machine learning very dependent on training samples
 - Know what is included in the simulated samples and make comparisons with data
 - Be careful about training sample composition (if training samples are 99% background its very efficient to just predict background)
 - Enrich dataset with rare cases
 - Introduce class weights
 - Check how your model will perform on other cases (empty events, background events..)
 - Check for biases in physics distributions for predictions
 - Use meaningful metrics for evaluation
 - Often loss/accuracy is not showing the whole picture





04

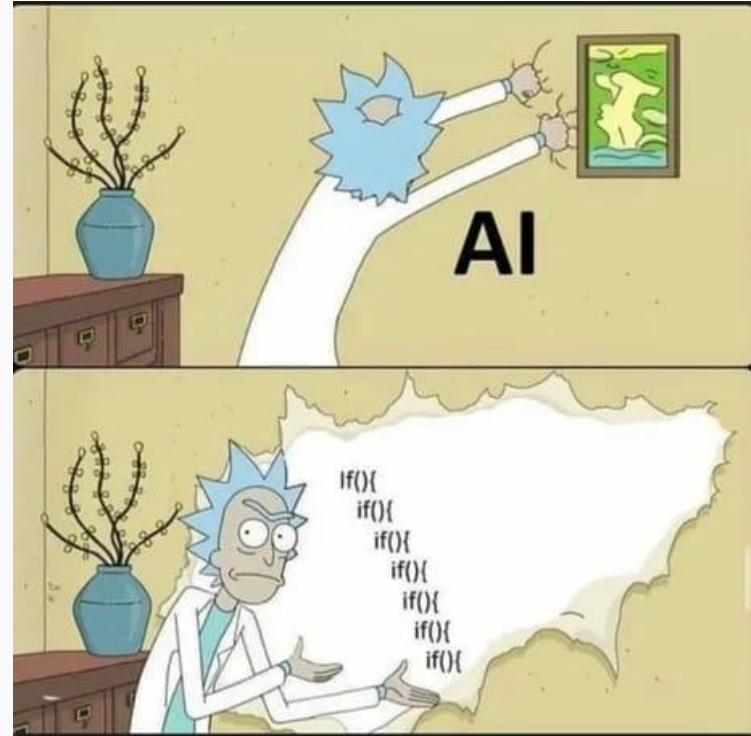
How can I Participate?

Find the right problem

- Lots of challenges in HEP can be tackled with ML algorithms
- Signs for possible improvement through ML:
 - High number of input variables
 - High correlations between variables
 - Unknown or difficult physical model

But:

- Not everything can be improved with ML
- Analytical functions, if known, will often perform better and with less computing resources



Join our MVA/ML Meeting!

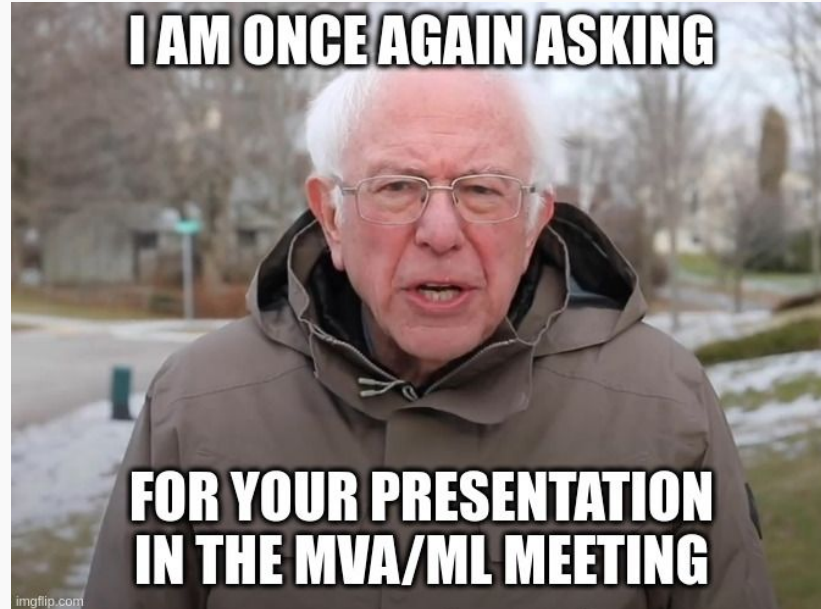


We want
YOU!



Indico: <https://indico.belle2.org/category/167/>

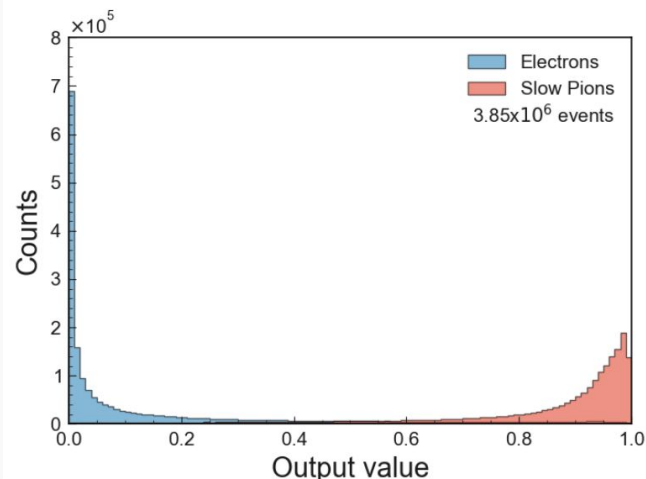
Meetings every 2 weeks, American friendly time every 4 weeks!



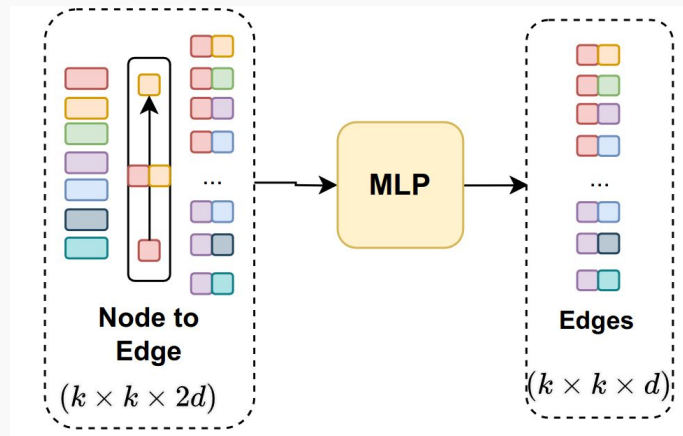
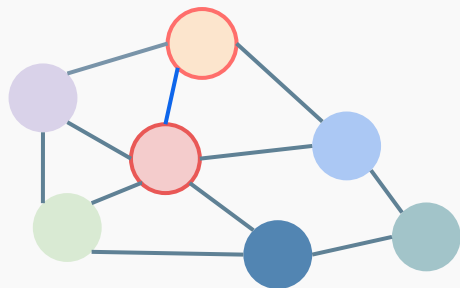
Backup

Slow Pion Rescue

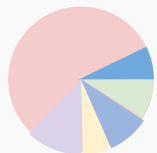
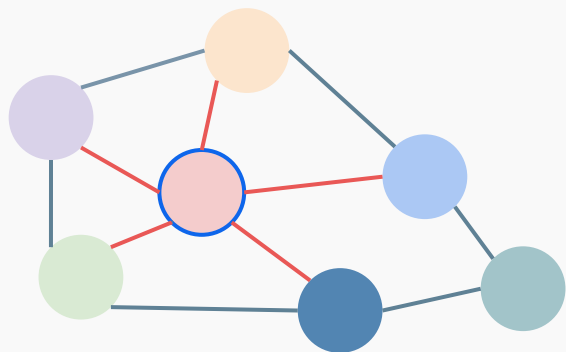
- Around 26% of slow pions are not reconstructed by SVD, need to reconstruct slow pions from the PXD
 - PXD data rate may have to be reduced after shutdown
 - PXD cluster not associated to a track are dropped by region-of-interest algorithm
 - Loose PXD cluster
 - PXD hits are dominated by QED (2000 electrons per 1 slow pion)
 - **Goal:** Discriminate QED background from slow-pion using a neural network
 - 1 hidden layer with 100 nodes
 - PX cluster properties as input: size, shape position, ...
- Tested various network models, achieved 89% efficiency for 90% electron rejection on simulated samples



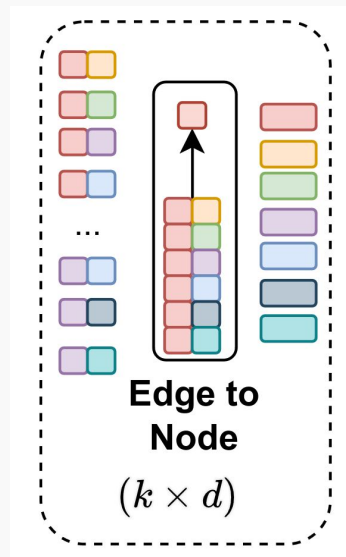
Message Passing: Update Edges



Message Passing: Update Nodes



Red node updated with information of neighbouring nodes and edges

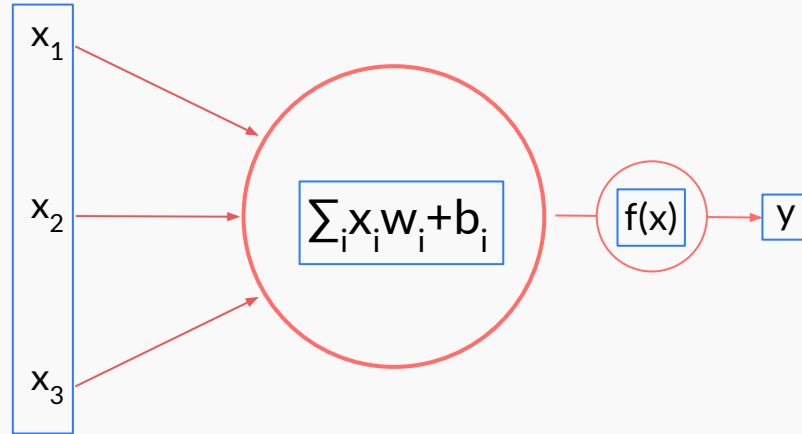


Classic Neural Networks



Inputs:

- Data often encoded in floats
- Best normalized to $[0, 1]$
- Fixed Ordering



Weights and Bias:

- Learnable Parameters
- Often adapted through backpropagation

x_i : Inputs
 w_i : Learnable Weights
 b_i : Learnable Bias
 $f(x)$: Activation function
 y : Output

Activation Function:

- Nonlinear function, such as $\tanh(x)$ or $\max(0, x)$
- Necessary to compute nontrivial problems

Output:

- Classification or regression
- Best scaled to $[0, 1]$
- Input to loss function, evaluation of the network's performance