Machine learning applied to EM showers of the OPERA experiment

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Introduction

Problem statement

Problem: identify all showers in the ECC(Emulsion Cloud Chamber) brick and for each shower reconstruct its energy, initial position and direction.

Setup: $\sim 3 - 5 \cdot 10^6$ background basetracks and 50-200 showers in one ECC brick.

Metrics:

Energy resolution:	$\Delta E / E$
Quality of initial position reconstruction:	MAE over $x_{start}, y_{start}, z_{start}$
Quality of direction reconstruction:	MAE over θ_x, θ_y
Ratio of recovered showers:	recovered showers / total showers
Track classification(indirect metric):	ROC-AUC and PR-AUC

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Data

Each basetrack from ECC brick is described by 6 variables: $x, y, z, \theta_x, \theta_y, \chi^2$, i.e. position, direction and fit quality.

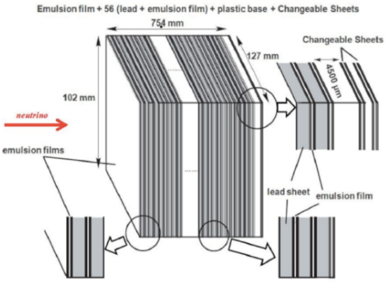
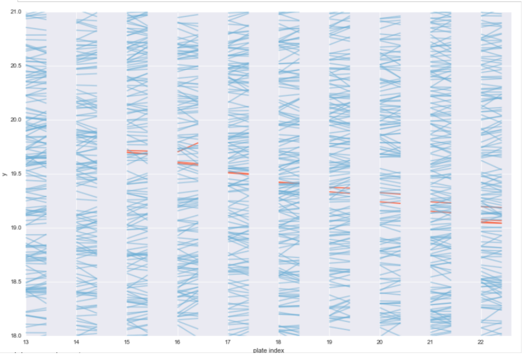
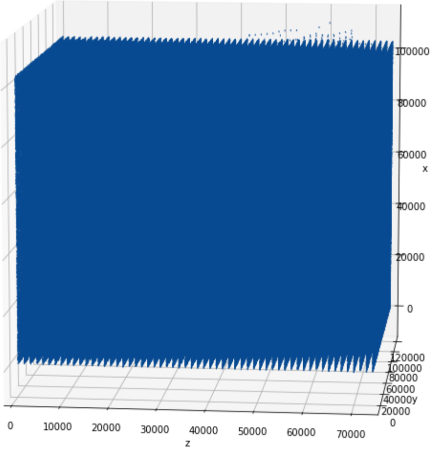
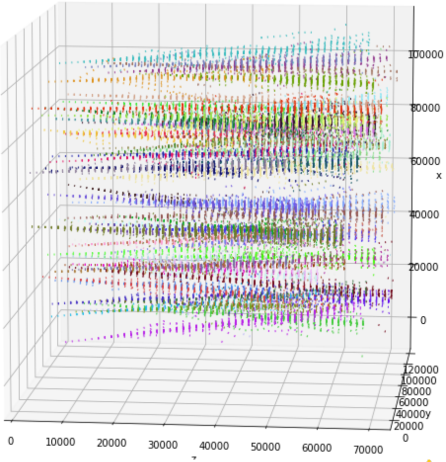


Figure 2.4 – Schematic structure of an ECC brick.



Brick example.





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Previous works

- ‘Search for Tau Neutrinos in the $\tau \to e$ Decay Channel in the OPERA Experiment’ B. Hosseini
  - only one shower with **known** origin;
  - $\sigma(\Delta E/E) = 0.20$
- ‘Machine-Learning techniques for electro-magnetic showers identification in OPERA datasets’ A.Ustyuzhanin, S. Shirobokov, V. Belavin, A. Filatov
  - only one shower with **unknown** origin;
  - $\sigma(\Delta E/E) \sim 0.27$

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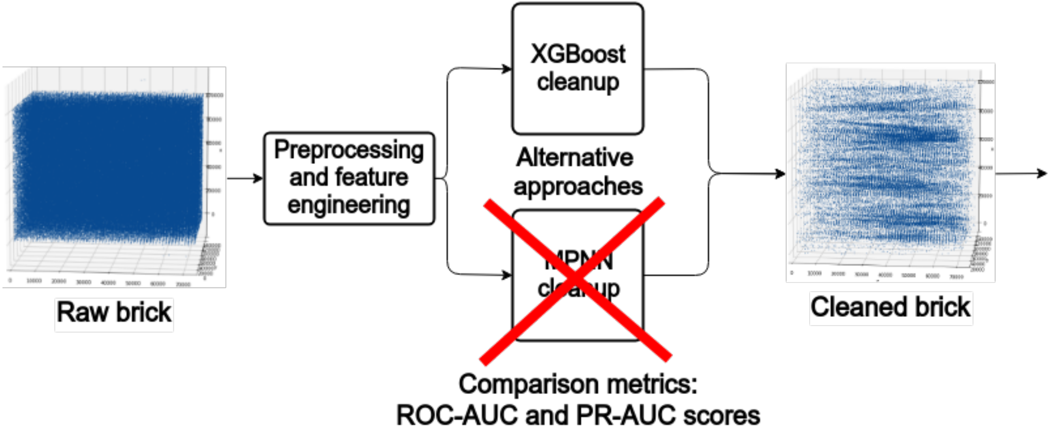
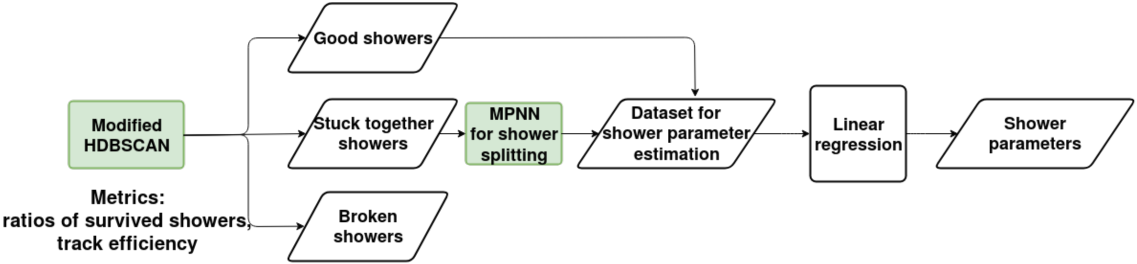
Methodology

Pipeline


Raw brick
Preprocessing and feature engineering
XGBoost cleanup
Alternative approaches
MPNN cleanup
Cleaned brick
Comparison metrics:
ROC-AUC and PR-AUC scores

Pipeline (continued)



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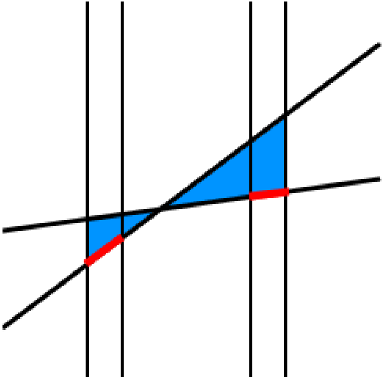
Cleanup

Preprocessing

In preprocessing I am building graph with nodes represented by basetracks. Two nodes(basetracks) are connected with the edge if and only if:

- between them less than 3 layers;
- one of the basetracks lies in the cone of 16 (mrad) with origin in another basetrack;
- integrated distance(blue area on the pic) between tracks less than threshold.



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Feature engineering and XGBoost cleanup

For cleaning XGBoost is applied.

For each basetrack 63 features have been constructed. 3 original basetrack features:

- $\theta_{x,y}$ and χ^2

60 pairwise basetrack features for 4 nearest(with lowest integrated distance) neighbors:

- $\Delta\theta_{x,y}$ and Δx, Δy, Δz between tracks;
- $IP_{x,y}$ for both tracks;
- integrated distance;
- $\theta_{x,y}$, χ^2 of neighbor;
- energy-like feature and likelihood induced from multiple scattering theory(details in backup slide).

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XGBoost cleanup

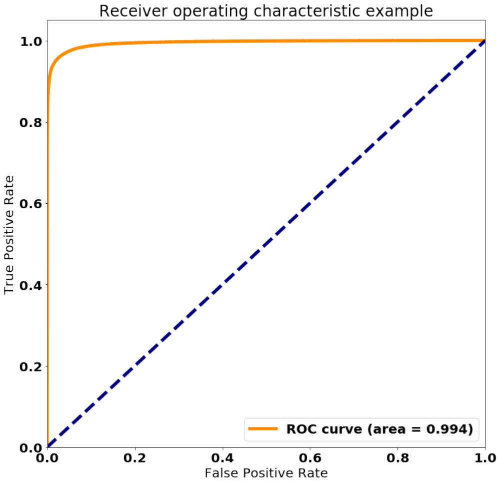

Figure 1: ROC-AUC=0.994

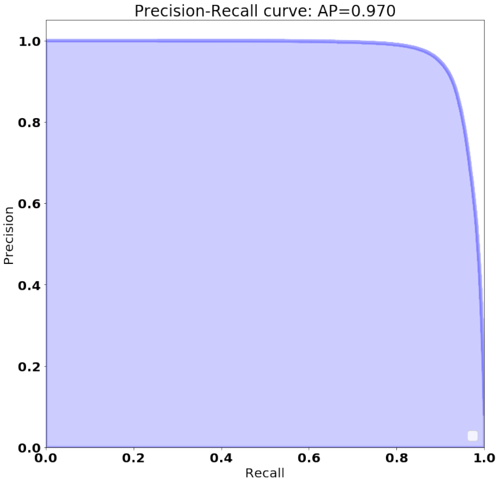

Figure 2: PR-AUC=0.97

Clusterization

Modified HDBSCAN. Algorithm

Step 1. Calculate all pairwise distances.

I.e. calculate all $d(i, j)$. In our case, $d(\mathrm{basetrack}_i, \mathrm{basetrack}_j) =$ integrated distance from preprocessing step;

Step 2. Define mutual reachability distance with parameter 'k'.

$d_{mreach-k} = \max\{core_k(\mathrm{basetrack}_i), core_k(\mathrm{basetrack}_j), d(\mathrm{basetrack}_i, \mathrm{basetrack}_j)\}$.

Where $core_k(\mathrm{basetrack}_i)$ is a distance from $\mathrm{basetrack}_i$ to the k-nearest neighbor.

At this point you have complete graph of distances.

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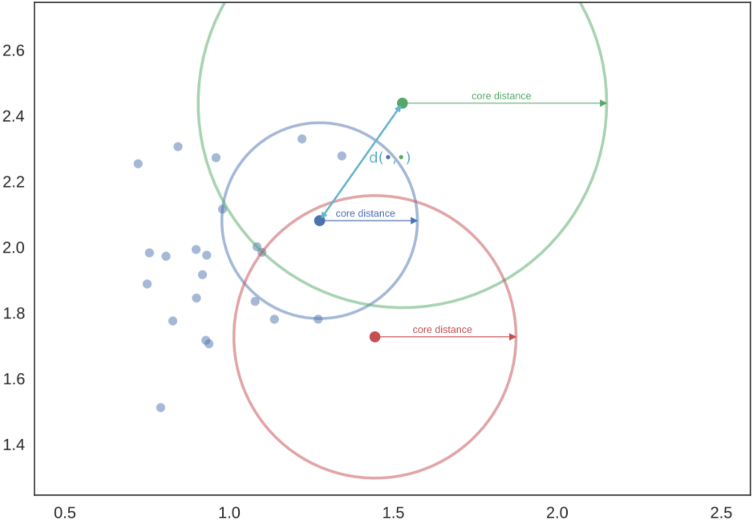
Modified HDBSCAN. Algorithm



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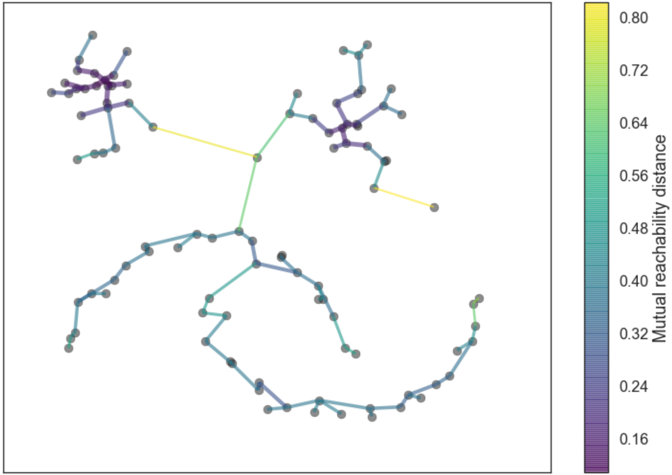
Modified HDBSCAN. Algorithm

Step 3. Construct minimum spanning tree, i.e. tree with the lowest sum of edges weights.



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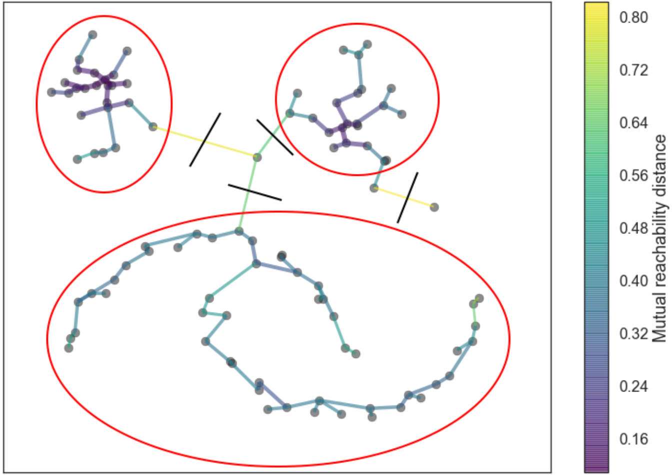
Modified HDBSCAN. Algorithm

Step 4. Iteratively delete edges with the highest weight.



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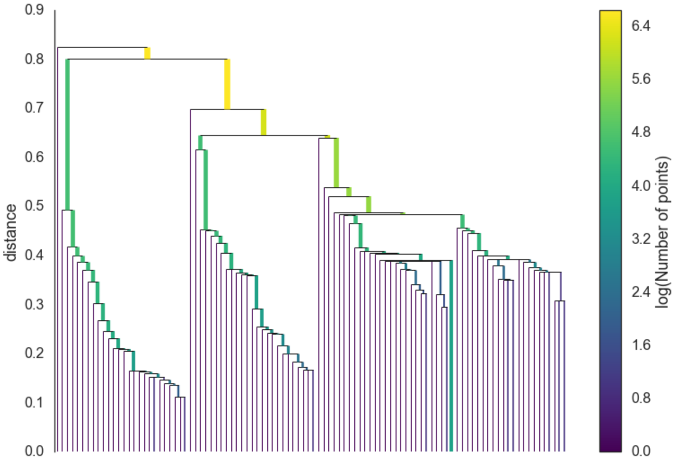
Modified HDBSCAN. Algorithm

Step 5. Choose cut level.



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Modified HDBSCAN for shower extraction. Results.

Modification to original algorithm:

- physically motivated stop criteria;
- modified core distance calculation.

Number of showers in brick	50	100	150	200
Ratio of survived showers	93 %	93 %	91 %	88 %
Ratio of stuck showers	3 %	3 %	3 %	3 %
Ratio of broken showers	1 %	0 %	1 %	2 %
Ratio of lost showers	3 %	4%	5 %	7 %

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Showers separation with MPNN

Graph terminology

- $V = \{v_i\}_{i=0}^{N}$ – set of vertices with:
  - associated features: $x_i \in \mathbb{R}^{D_1}$
  - hidden state: $h_i \in \mathbb{R}^{H_1}$
- $E \subset 2^V \; \& \; \forall \mathrm{e} \in \mathrm{e} \in E \; (|\mathrm{e}| = 2)$ – set of edges with:
  - associated features: $x_{ij} \in \mathbb{R}^{D_1}$
  - hidden state: $h_{ij} \in \mathbb{R}^{H_1}$
- $G(V, E) = \langle V; E \rangle$ – graph;

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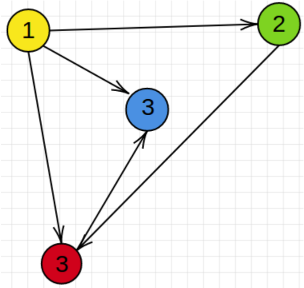
MPNN

MPNN stands for **Message Passing Neural Networks**.

The core idea of MPNN is passing 'messages' from node to node and updating states of nodes accordingly to received 'messages', thus allowing taking into account both structural-wise and node-wise information.

There could be several steps of passing 'messages' and nodes updates. To distinguish them we are going to use upper-score symbol t, $t \in \{1, 2, ..., T\}$



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MPNN(continued)

So, in a nutshell to define MPNN one have to define three operations:

- message passing: $m_{ij}^t = f_{ij}^t(h_i^t, h_j^t, h_{ij}^t)$;
- message aggregation: $M_j^t = g_j^t\left(\{m_{ij}^t\}_i\right)$;
- node update: $h_i^{t+1} = U_i^t(M_j^t, h_i^t)$.

Usually you also want to define readout function to make predictions:

- over single node: $R_i(h_i^T)$;
- or over whole graph: $R_i\left(\{h_i^T\}_i\right)$.

All functions could be handcrafted or parametrized by neural network. In latter case it is possible to learn parameters through backpropagation.

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MPNN for shower separation

To train MPNN for shower splitting I compare two loss functions.

Traditional **siamese loss** or **contrastive loss**:

$$L(x_i, x_j) = (1 - Y)D_W^2(x_i, x_j) + Y \max(0, m - D_W(x_i, x_j))^2$$

$$D_W(x_i, x_j) = ||x_i - x_j||_2$$

Y = 0 when both tracks belong to the same shower and Y = 1 otherwise.

After training this model we can use it to split stuck together showers or as an additional distance for HDBSCAN algorithm.

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MPNN for shower separation(continued)

Batch centered loss:

- For each class robustly find its center: $\mathrm{center}_i = \mathrm{median}(x_i)$
- similarity loss: $L_{similarity} = (\mathrm{center}_i - x_i)^2$
- contrastive loss: $L_{contrast} = \max(0, m - |\mathrm{center}_i - \mathrm{center}_j|)^2$

Advantages in comparison with siamese loss:

- $\sim O(N)$ operations;
- no need for sophisticated sampling strategies;
- more robust to outliers(in theory).

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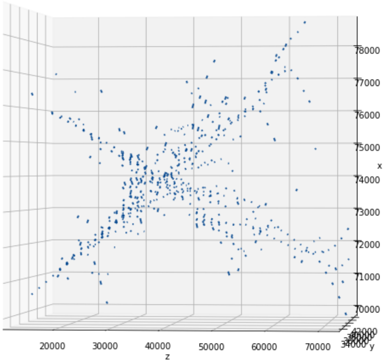
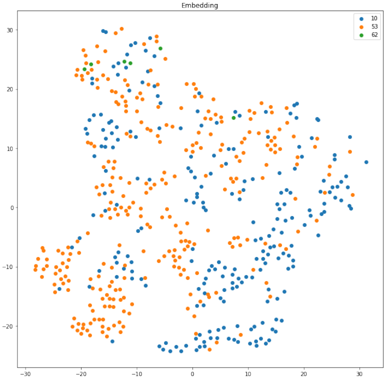
MPNN for shower separation(continued)

Experiments with MPNN still in progress due to computational complexity of MPNNs on big graphs.





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Shower parameters estimation

Parameter estimation with linear models

Features:

- number of selected basetracks;
- spatial parameters of shower, i.e. statistics over $x, y, z, \theta_x, \theta_y$.

For estimation we use Theil-Sen linear estimator which is more robust to outliers than least square estimator.

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Parameter estimation with linear models

Result on test data for different number of showers in brick:

Number of showers in brick	50	100	150	200
$\sigma\left(\frac{\Delta E}{E}\right)$	0.28	0.27	0.28	0.28
MAE(x, y)	0.18 (mm)	0.23 (mm)	0.23(mm)	0.22 (mm)
MAE(z)	1(mm)	1.2(mm)	1 (mm)	1.1 (mm)
MAE(tx, ty)	13(mrad)	14(mrad)	15(mrad)	13(mrad)

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Summary

- works for $\sim 50 - 200$ showers in a brick;
- no a priori information;
- $\sim 90\%$ of showers recovered;

Future plans:

- optimize MPNN for large graphs;
- try unsupervised losses for MPNN;
- generalize HDBSCAN on directed graphs;
- try PointNet/PointNet++(NNs for point cloud segmentation) on this task.

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Backup

Energy-like feature

From Molier's theory of multiple scattering one can derive following probability distributions on track directions and positions:

$$P(z,\theta) = \frac{2\theta}{\langle\theta^2\rangle} \exp\left(-\frac{\theta^2}{\langle\theta^2\rangle}\right), \langle\theta^2\rangle = \theta_s^2 z = \left(\frac{E_s}{\beta cp}\right)^2 \frac{z}{X_0}$$

$$Q(z,\theta_x) = \frac{1}{\sqrt{2\pi}\sigma_{\theta_x}} \exp\left(-\frac{\theta_x^2}{2\sigma_{\theta_x}^2}\right), \sigma_{\theta_x}^2 = \frac{\langle\theta^2\rangle}{2}$$

$$S(z,x) = \frac{1}{\sqrt{2\pi}\sigma_x} \exp\left(-\frac{\theta_x^2}{2\sigma_x^2}\right), \sigma_x^2 = \frac{\theta_s^2 z^3}{6}$$

Using this distributions we can estimate energy($E \approx cp$) for all pairs of tracks and it's likelihood.

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