Energy Reconstruction with CALIFA

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CALIFA Detector @ R³B

CALorimeter for the **I**n **F**light detection of γ-rays and light charged p**A**rticles

Endcap:

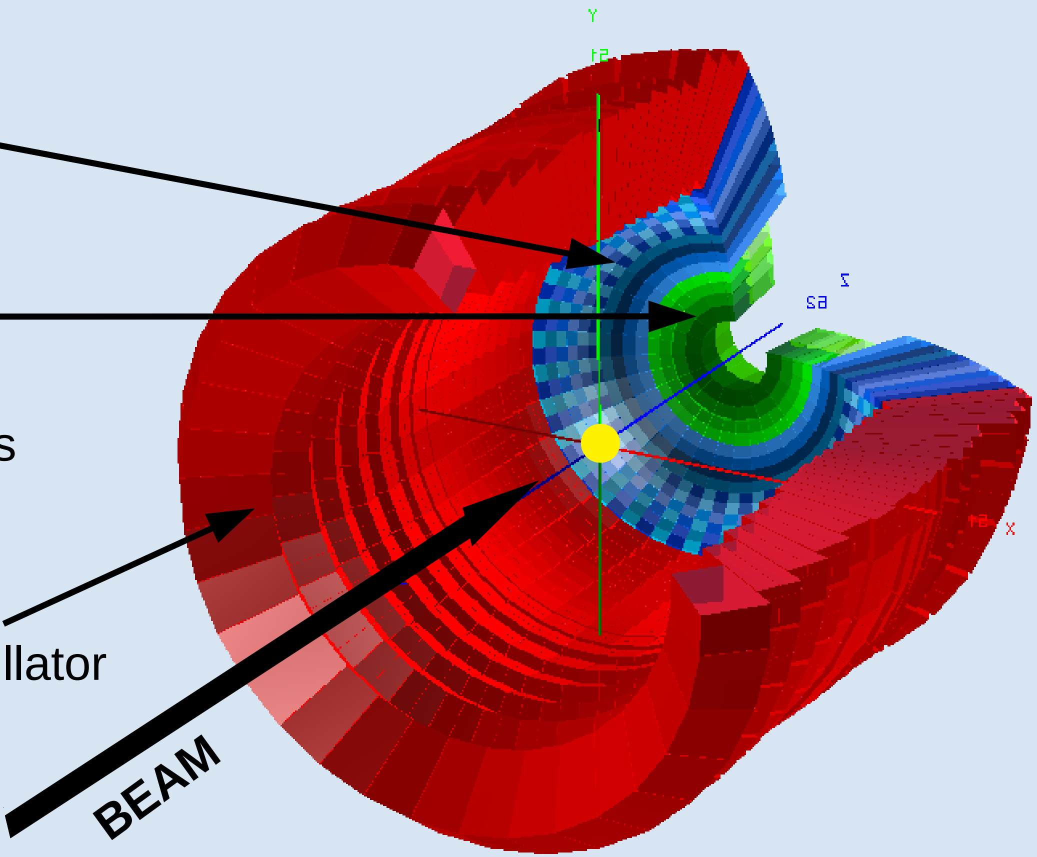
iPhos:

512 CsI(Tl) crystals

CEPA:

96 LaBr3 &

LaCl3 crystals

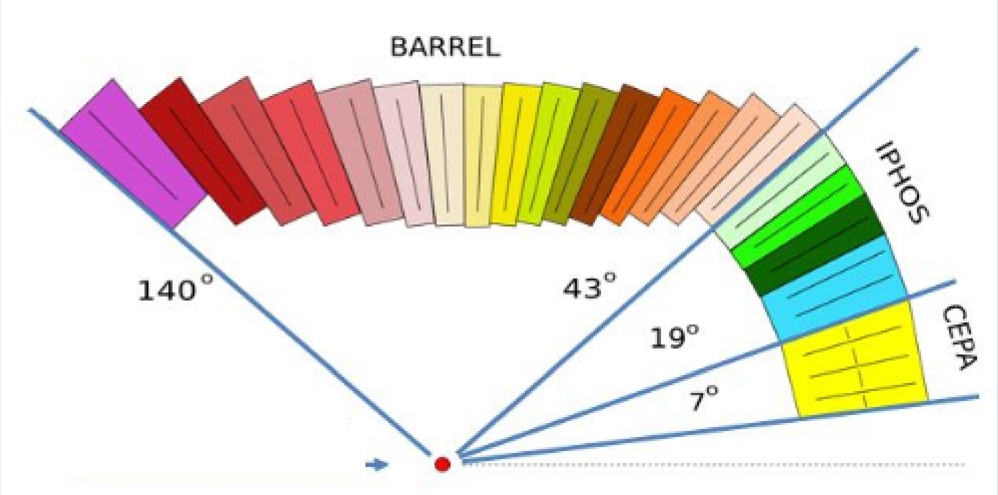


Barrel:
1952 CsI(Tl) scintillator crystals

Over 2500 crystal channels!

Requirements:

- -high dynamic range:
  100 keV γ-rays – 700 AMeV charged particles
- -high efficiency
- -high granularity → Doppler correction
- -particle identification



Observables

Energy

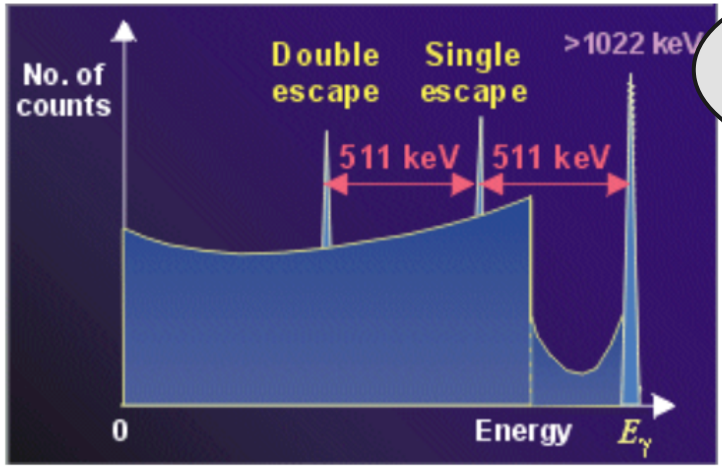
Hit Time

Spatial Position

Correlation with neighboring crystals

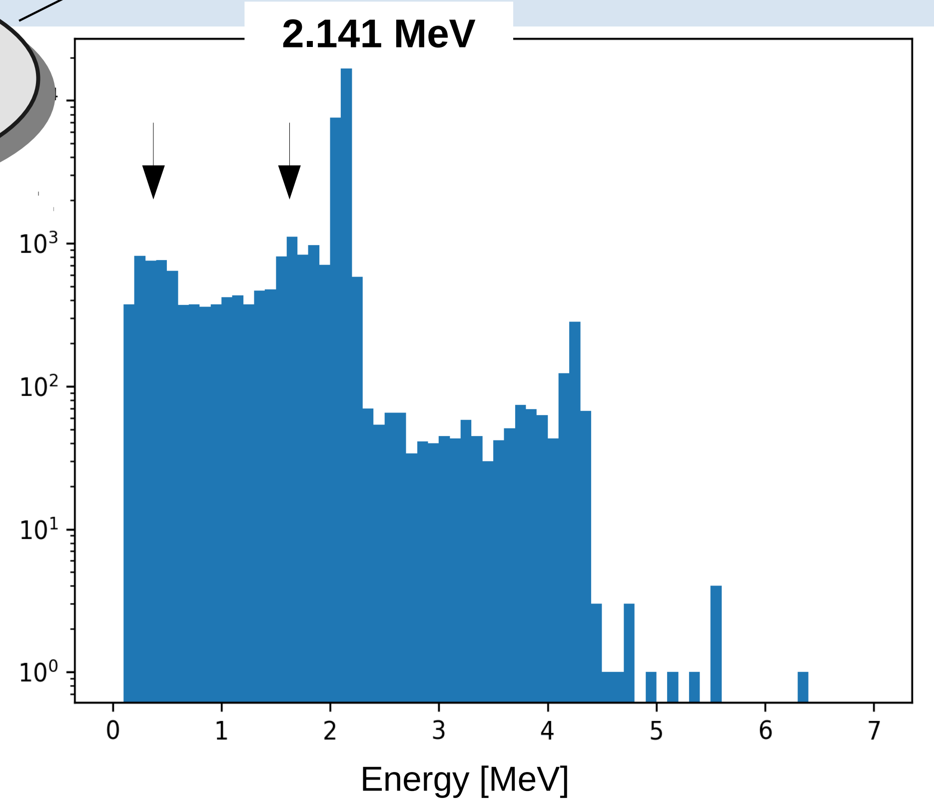
Customized Cluster

In a real detector, if the incident gamma energy is above 1022 keV, pair production events result in the production of two 511 keV annihilation gamma-rays.



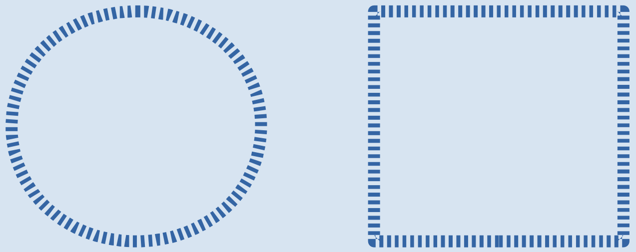
If only one of these gamma-rays escapes while the other is completely absorbed in the detector, 511 keV will be lost from the detector. This results in a separate peak in the spectrum representing Eg-511 keV, called the **single** escape peak.

If both annihilation gamma-rays escape this gives rise to the **double** escape peak at Eg-1022 keV.



Standard Cluster Algorithm

User defines shape and size of cluster:



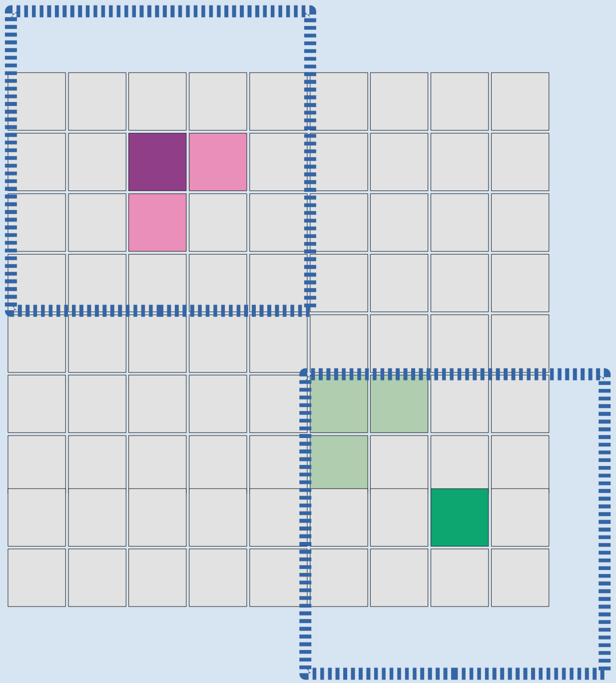
(and set energy threshold for single crystals)

Sort the hit list according to their energy

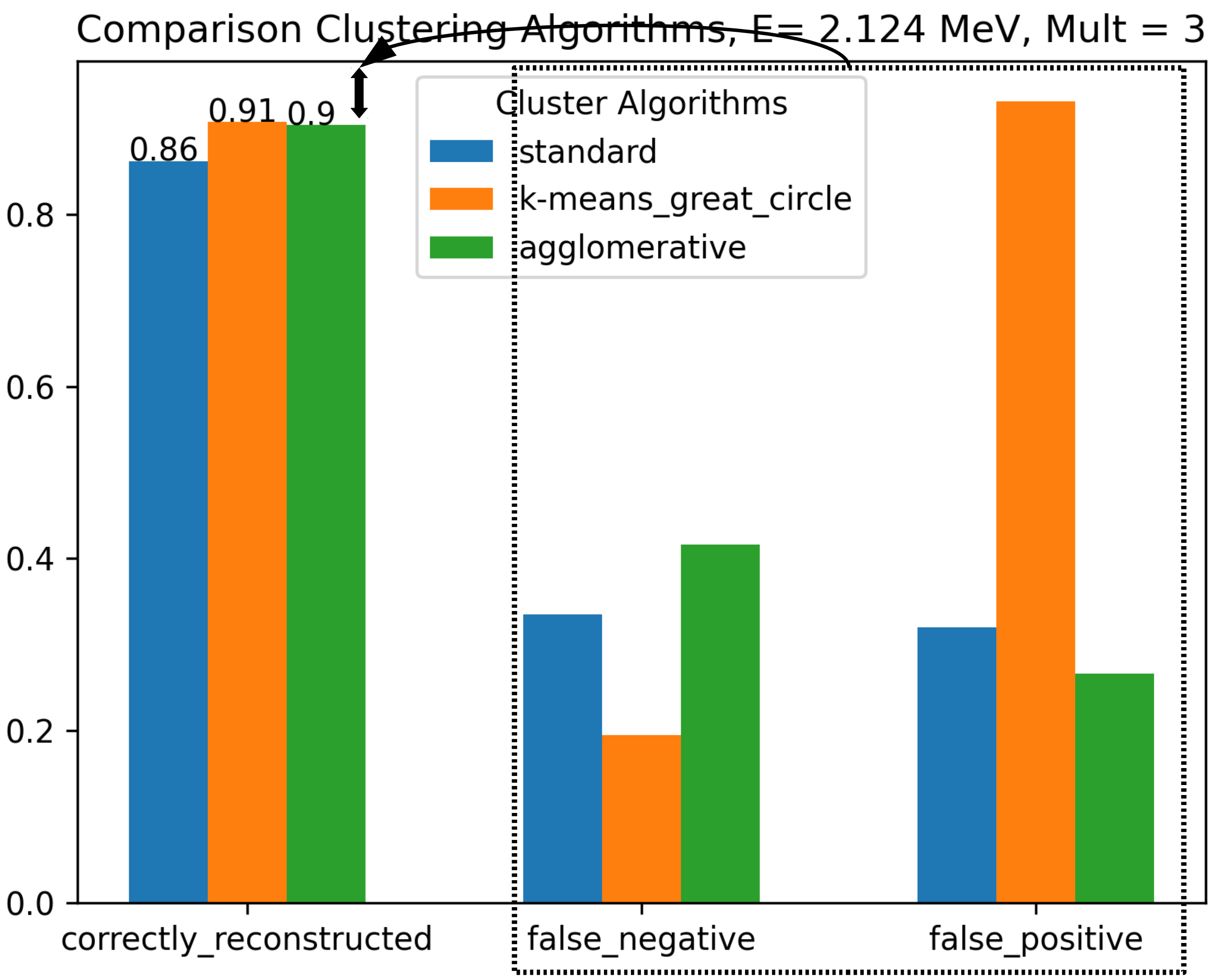
30. MeV
22. MeV
10. MeV
5. MeV
3. MeV
2.5 MeV
0.7 MeV

1. create cluster centered around first hit
2. loop over all hits in list
   → if hit inside cluster add it and remove it from the list

3. Do this procedure until list is empty



Summary Clustering Methods



false_negative:

true cluster	reconstructed cluster
$\begin{pmatrix} 1.2 \\ 0.8 \\ \mathbf{\color{red}{0.124}} \end{pmatrix}$	$\begin{pmatrix} 1.2 \\ 0.8 \\ 0.511 \end{pmatrix}$

$\rightarrow$ false negative $= \frac{0.124}{2.124}$

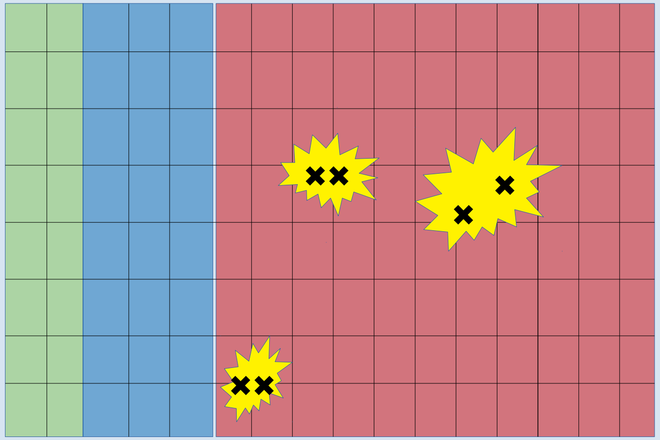
false_positive:

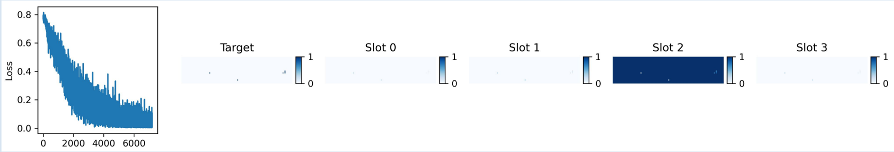
true cluster	reconstructed cluster
$\begin{pmatrix} 1.2 \\ 0.8 \\ 0.124 \end{pmatrix}$	$\begin{pmatrix} 1.2 \\ 0.8 \\ \mathbf{\color{red}{0.511}} \end{pmatrix}$

$\rightarrow$ false positive $= \frac{0.511}{2.124}$

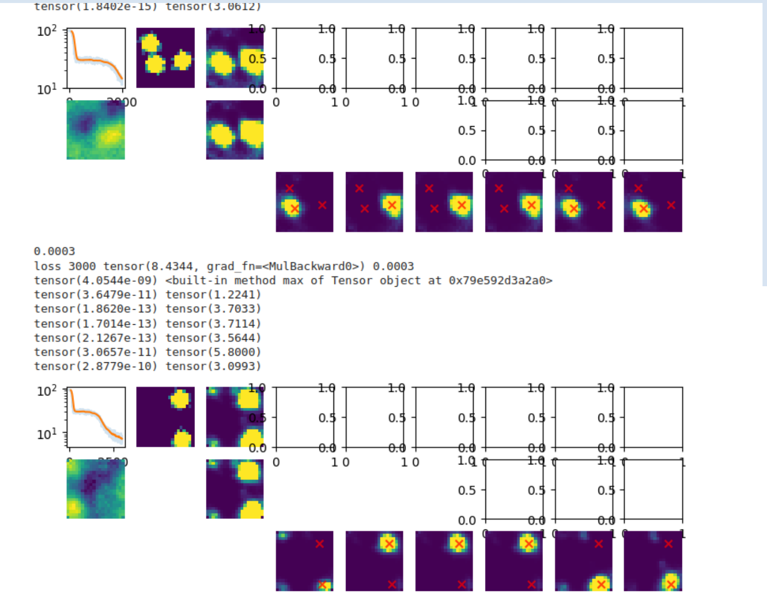
Implementation of Complex ML Models

Invariant Slot Attention:

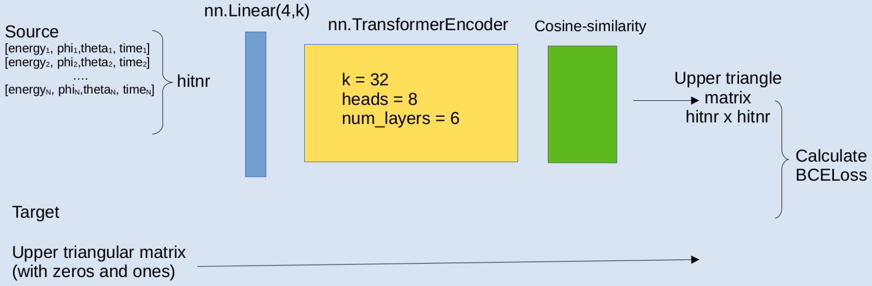


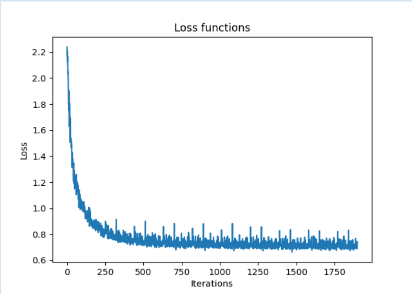


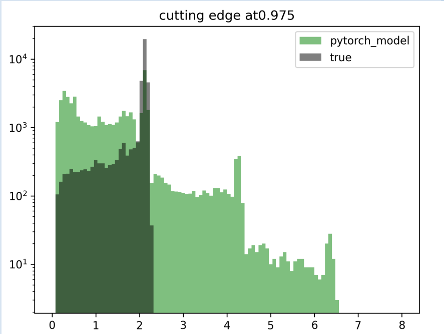
slot_and_tspn_onenotebook from Lukas Heinrich



Transformer Model:







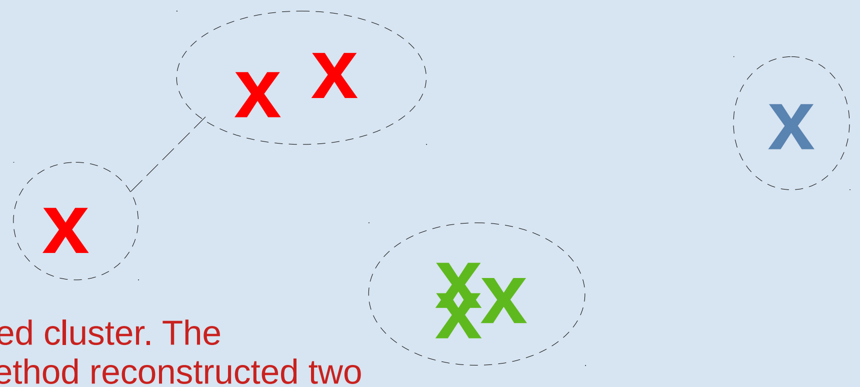
None of the models perfomed well / converged !!!

Next Step:

Agglomerative Model + Basic Feed Forward Model

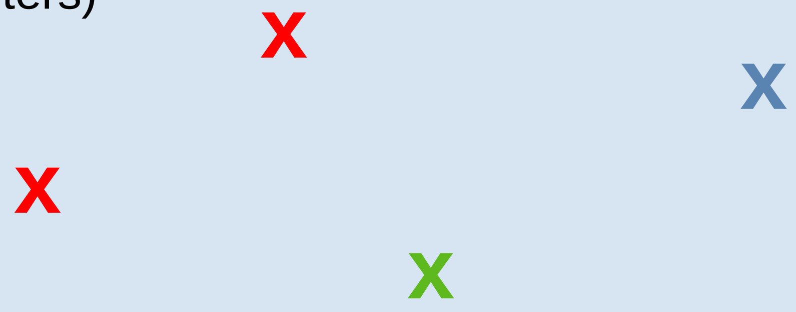
Idea

1. Use first agglomerative method to cluster
2. Select events where we have too many clusters (false negative)



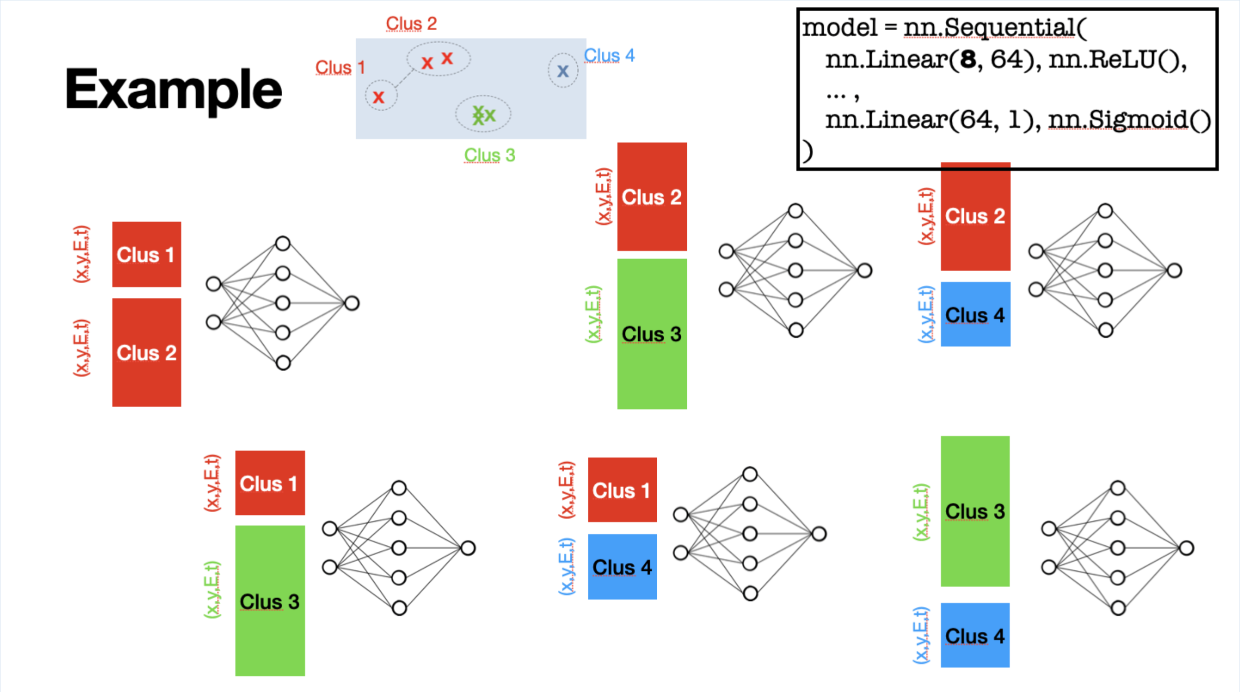
This is one true red cluster. The agglomerative method reconstructed two

3. Feed the clusters to feed forward model (calculating cm of clusters)



Note:
All data you see next is a subset of the whole dataset. It corresponds to events where the agglomerative model has created too many clusters

Tested Feed Forward Models



Basic Scheme:

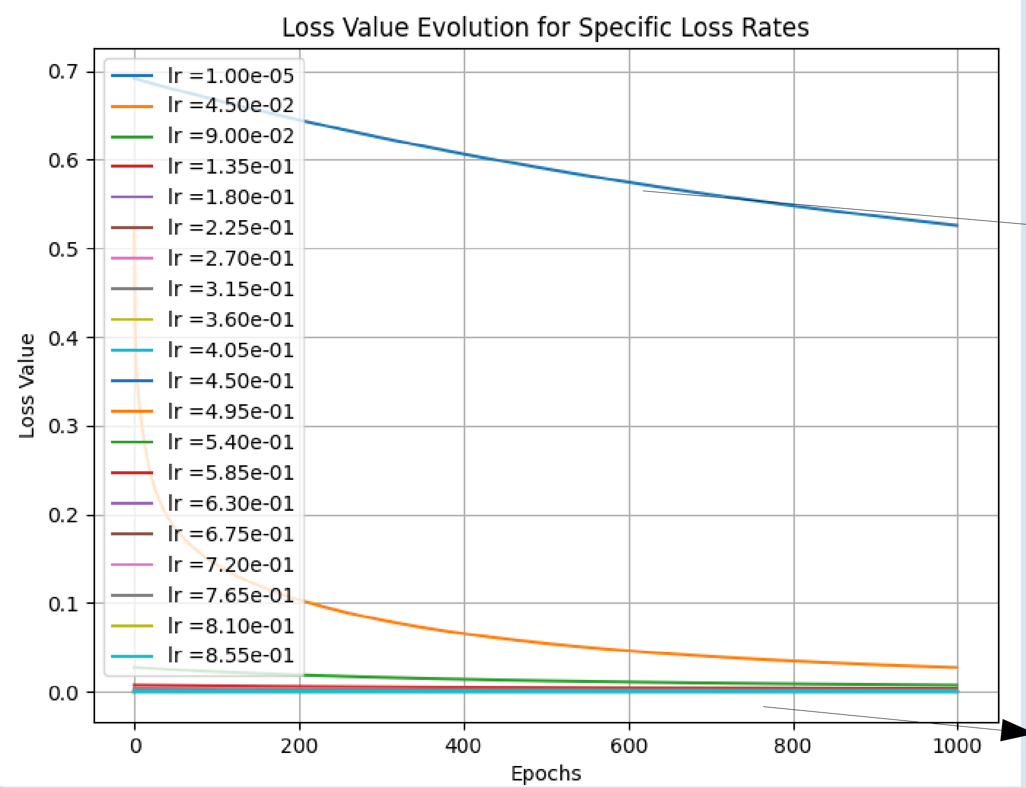
```
Def init :
    self.linear = torch.nn.Linear(8,64)
    self.activation = torch.nn.ReLU()
    self.linear_back = torch.nn.Linear(64,1)

....

Def forward:
    output_tensor = self.linear(output_tensor)
    output_tensor = self.activation(output_tensor)
    output_tensor = self.linear_back(output_tensor)
    output_tensor = torch.sigmoid(output_tensor)
    output_tensor = torch.squeeze(output_tensor)
```

Input to model:
$E_1,\theta_1,\varphi_1,t_1,E_2,\theta_2,\varphi_2,t_2$

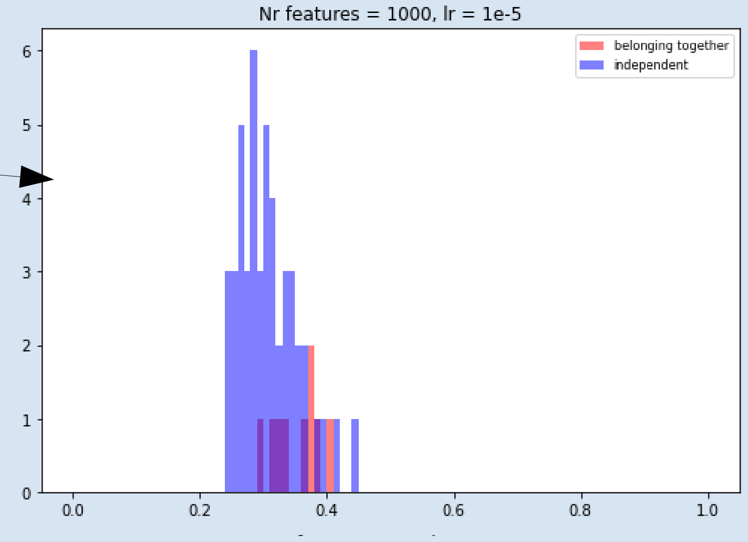
Tuning:

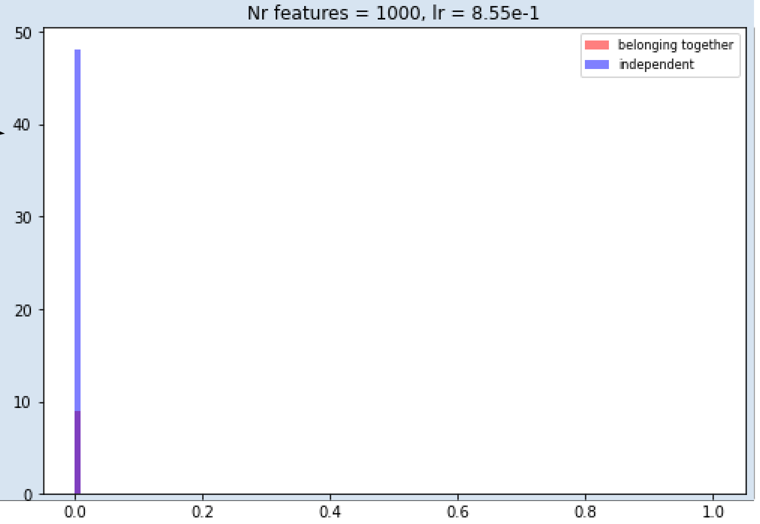
- Lr
- Feature size of hidden layer
- Nr of hidden layers

Tuning the Loss – Learning Rate

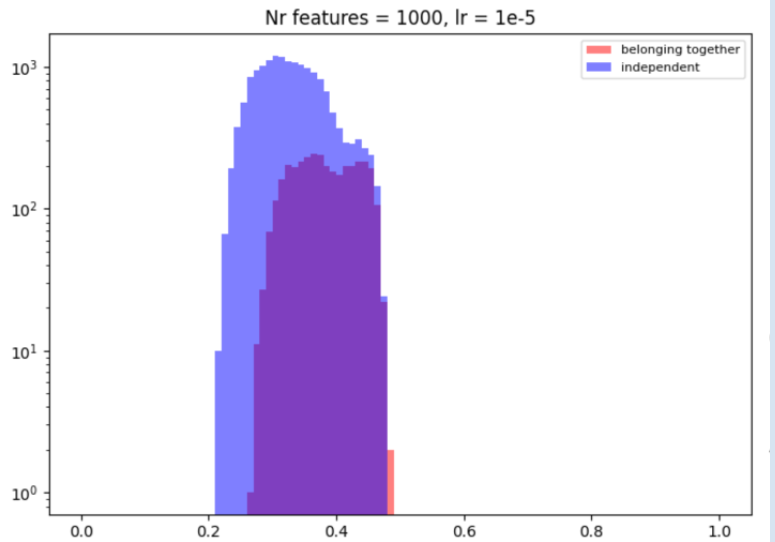


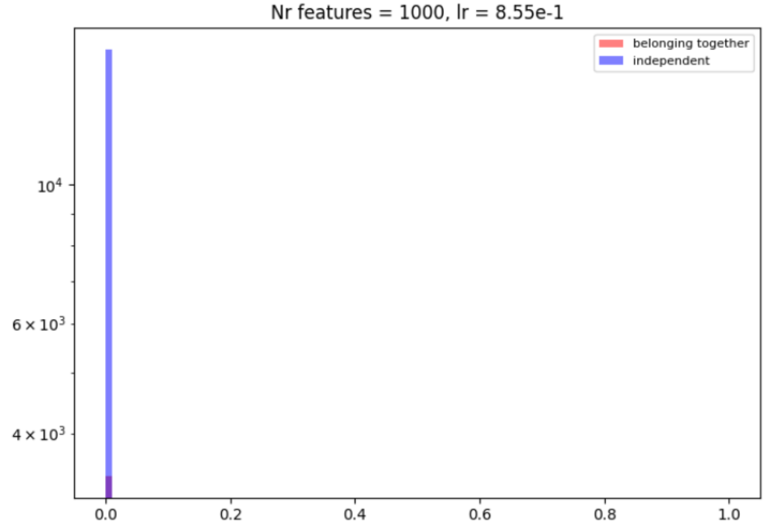
Prediction Distributions





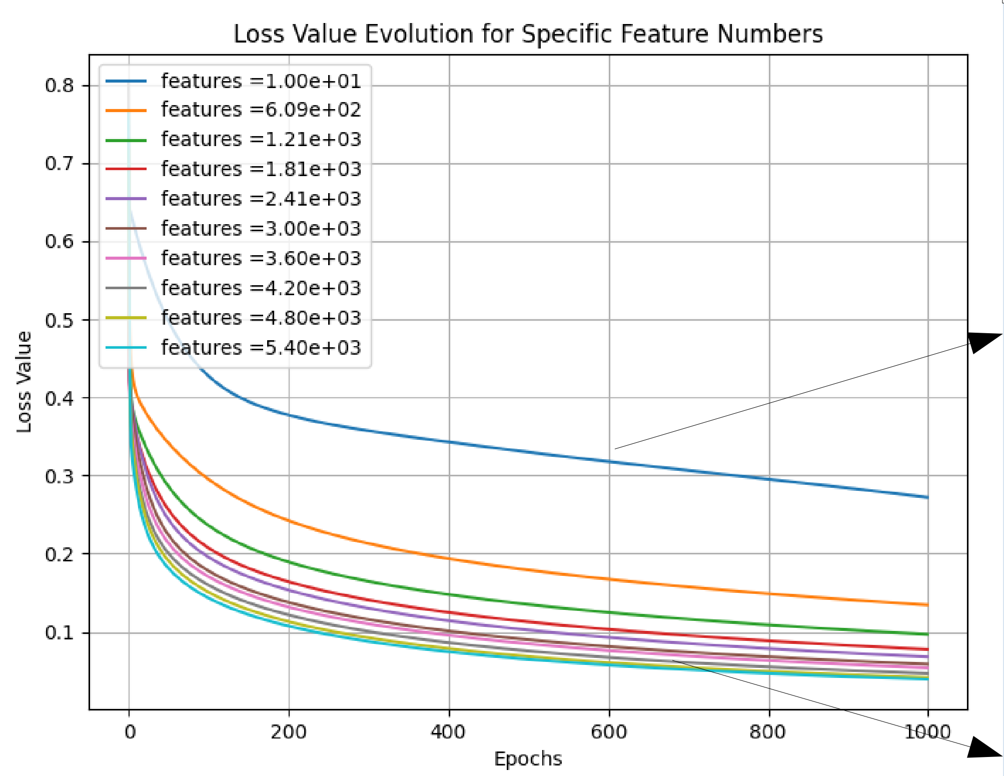
Large data sample



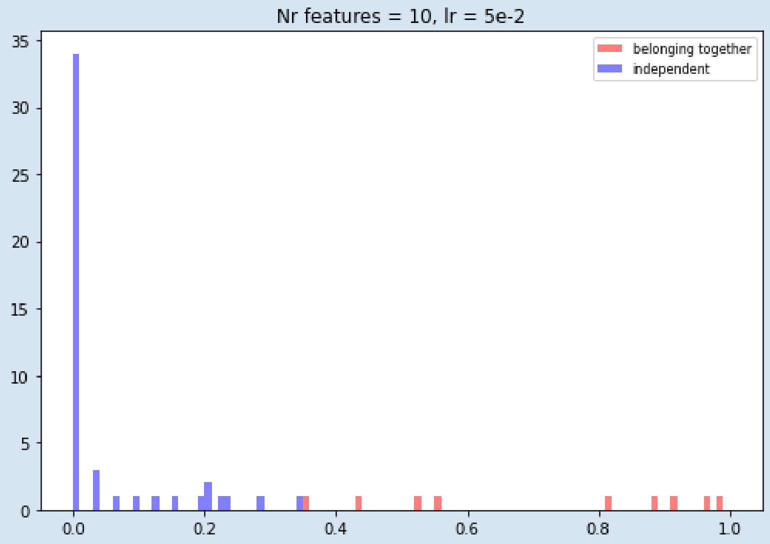


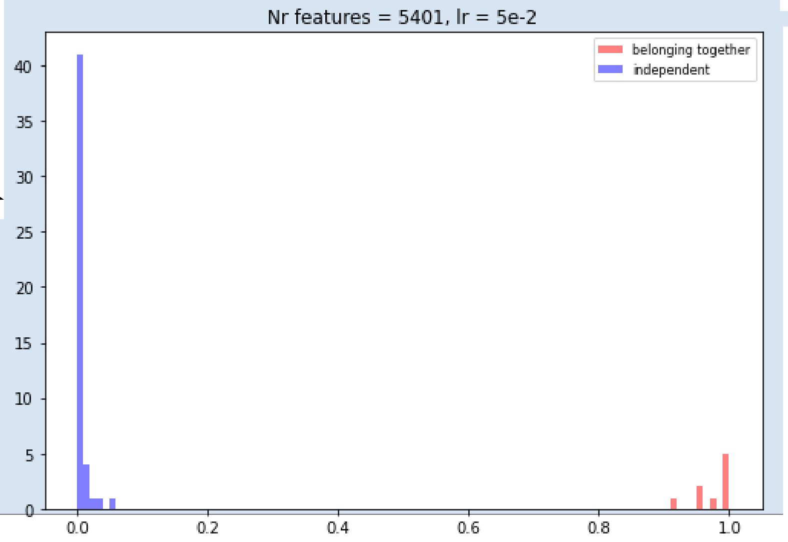
Data size = 10 events
Overfit data to find out if we are in meaningful hyperparameter space

Tuning the Loss – Feature Size

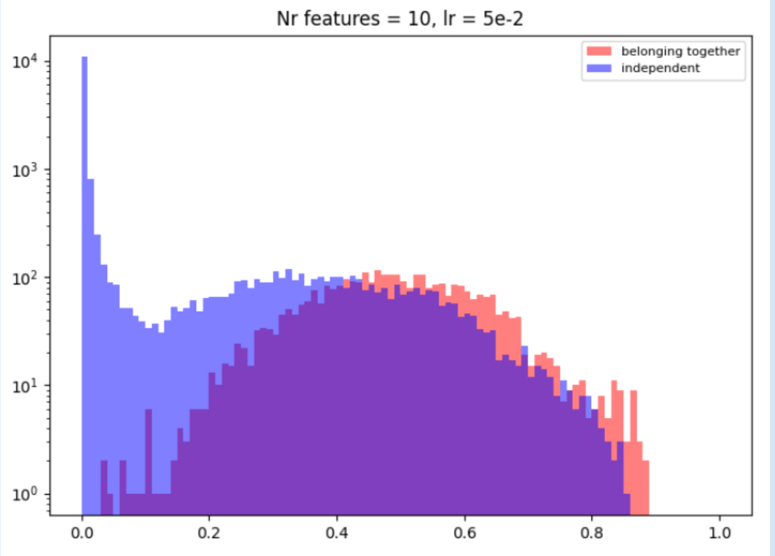


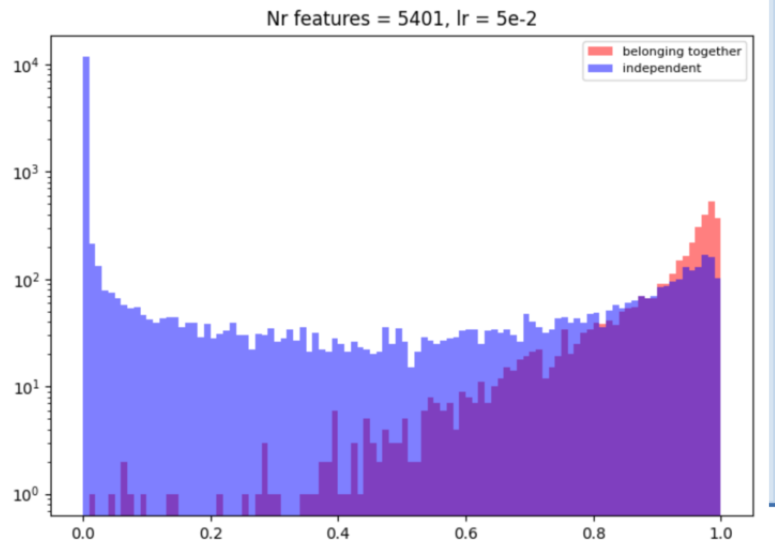
Prediction Distributions





Large data sample

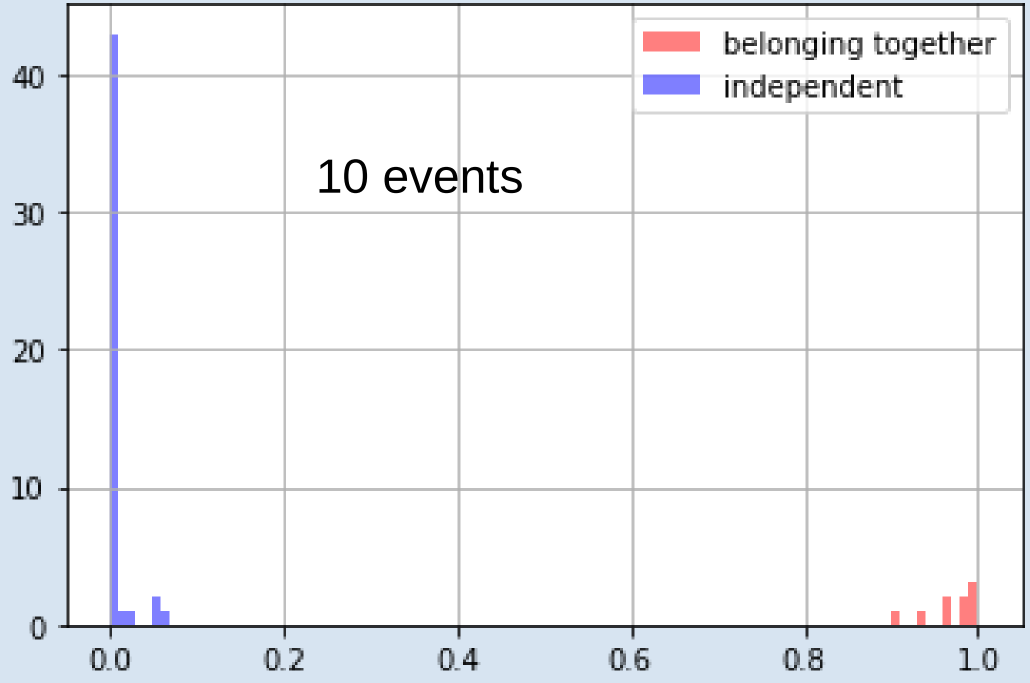


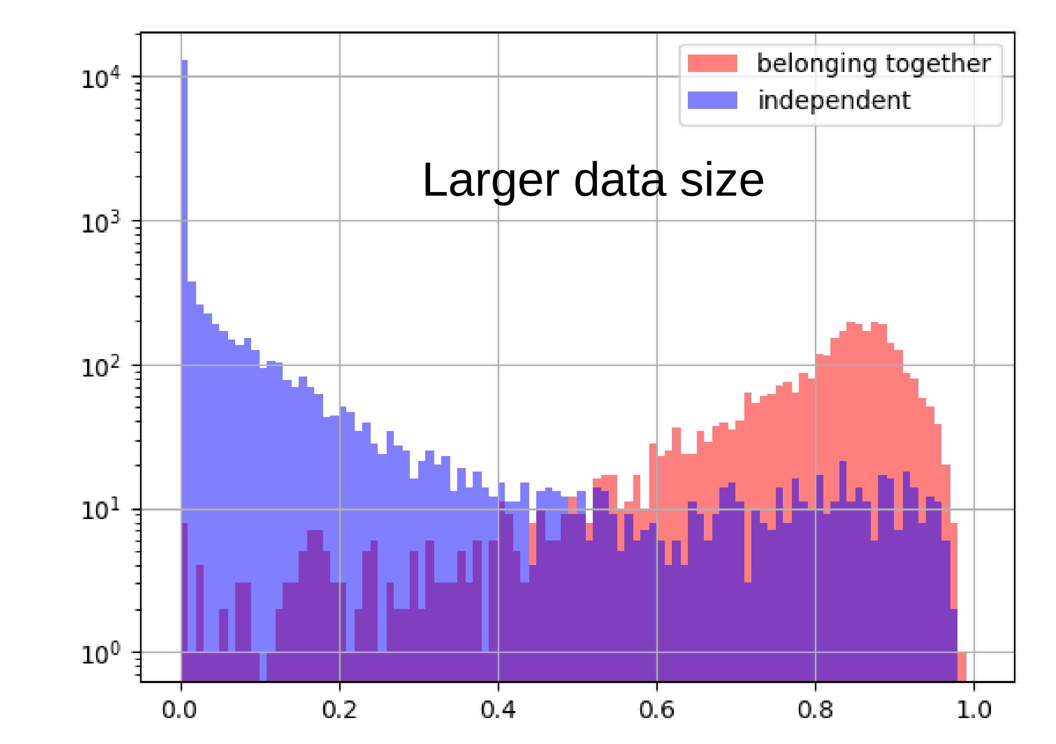


Data size = 10 events
Overfit data to find out if we are in meaningful hyperparameter space

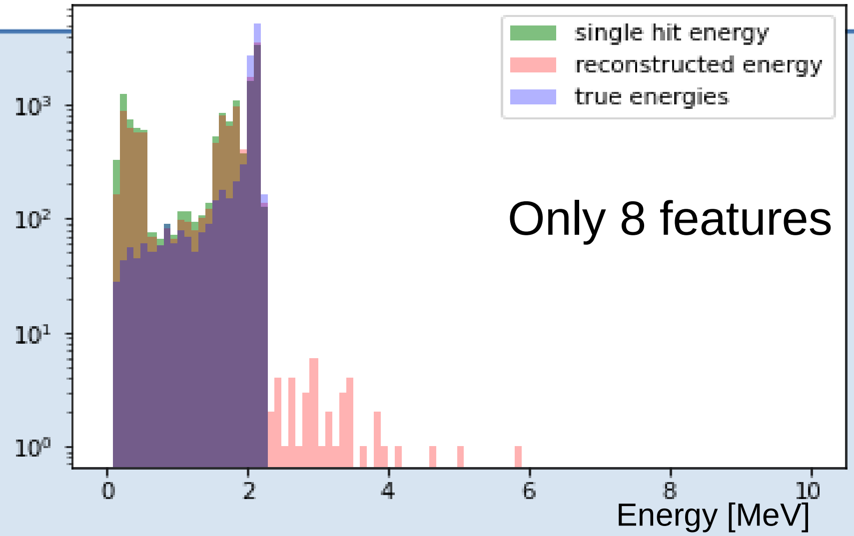
Tuning the Loss – Multiple Layer

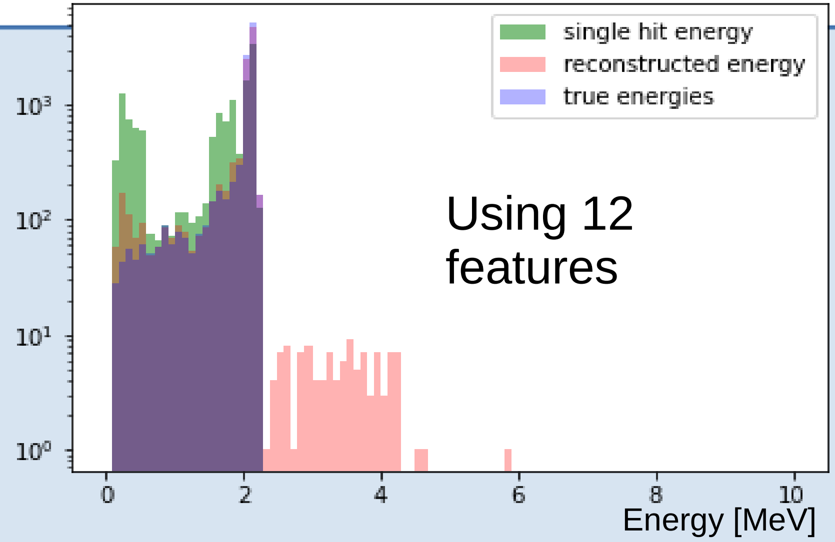
Model:
First layer: 1000 features
Second layer: 100 features
Third layer: 100 features
Lr= 5e-3

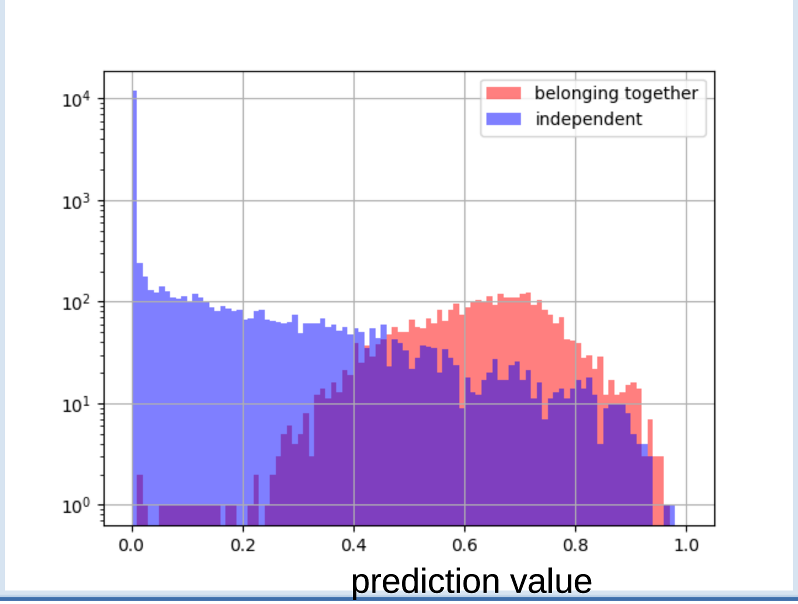


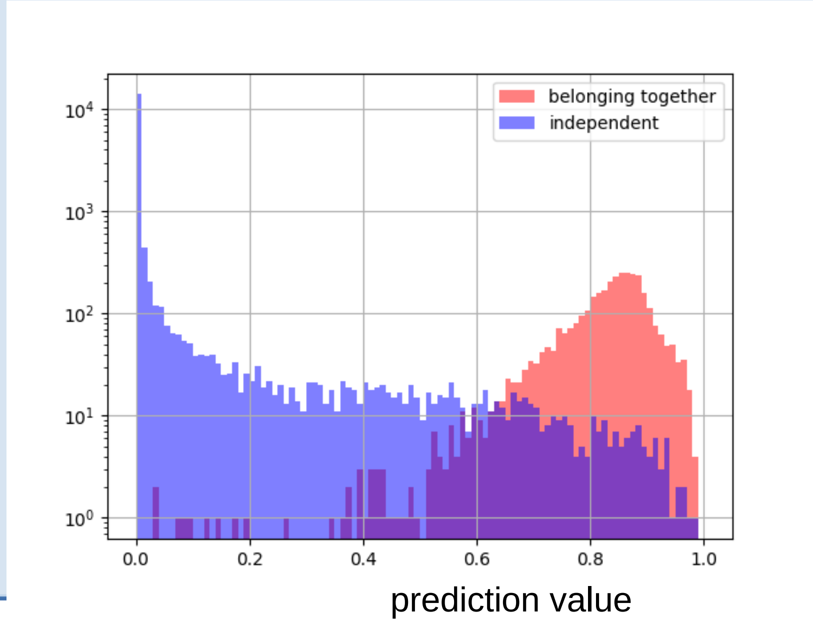


More features: Δt,ΔE,Δφ,Δθ









In both cases same feed forward model !

Summary Agglomerative + Feed Forward

Basic Feed Forward Model implemented
Cluster recognition works quite well when using $\Delta t, \Delta E, \Delta\varphi, \Delta\theta$
Still to do:

- Implement more features → $E1+E2, \varphi1+\varphi2, \ldots$
- Use raw (not preclustered) data and only feed forward model

However:
→ NOT translation invariant (maybe solved with geo. Algebra transformers GATs *)
→ does not focus on the whole event, but only looks at the single hit
→ only tested on training data → overfitting issue…
→ this model only works on simulated data, since for real data we do not have the cluster tags
  → as mentioned, only subset of preclustered dataset used!

Idea from my side:
→ Implement an autoencoder do extract hidden features of cluster recognition
→ implement this features in e.g. agglomerative model to clusterize hits

How to implement this?

*https://github.com/Qualcomm-AI-research/geometric-algebra-transformer

Agenda & Deadlines

Deadline for CALIFA ODSL Project:

→ end of February/beginning of March

→ what should we have at that point of time?

→ How much fine-tuning can be done later on?

→ Intentions to write paper or the like?

*** Latest point of thesis submission : 30.06.2025 (end of contract with TUM) ***

Thank you!

CALIFA @ Technical University of Munich (TUM)

Roman Gernhäuser, Lukas Ponnath, Philipp Klenze, Tobias Jenegger

Backup

Invariant Slot Attention Model – also with time info

→ Dimension of mask: → same as before! 10 x 3 x 27 x 112

→ Dimension of evt_histogram_array : 10 x **2** x 27 x 112

Lr = 5e-5

#observables:
time & energy

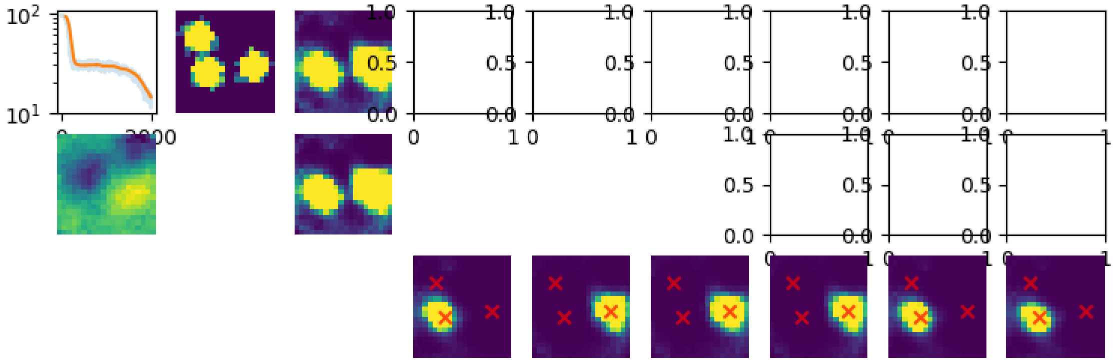
```
self.gru = torch.nn.GRUCell(self.query_dim, self.query_dim)

kwargs = {'out_channels': hidden_dim,'kernel_size': 5, 'padding':2 }
#cnn_layers = [torch.nn.Conv2d(1,**kwargs)] old cnn, with one input channel, energy
cnn_layers = [torch.nn.Conv2d(2,**kwargs)] #now also with time info

for i in range(num_conv_layers-1):
```

Loss function does not converge!

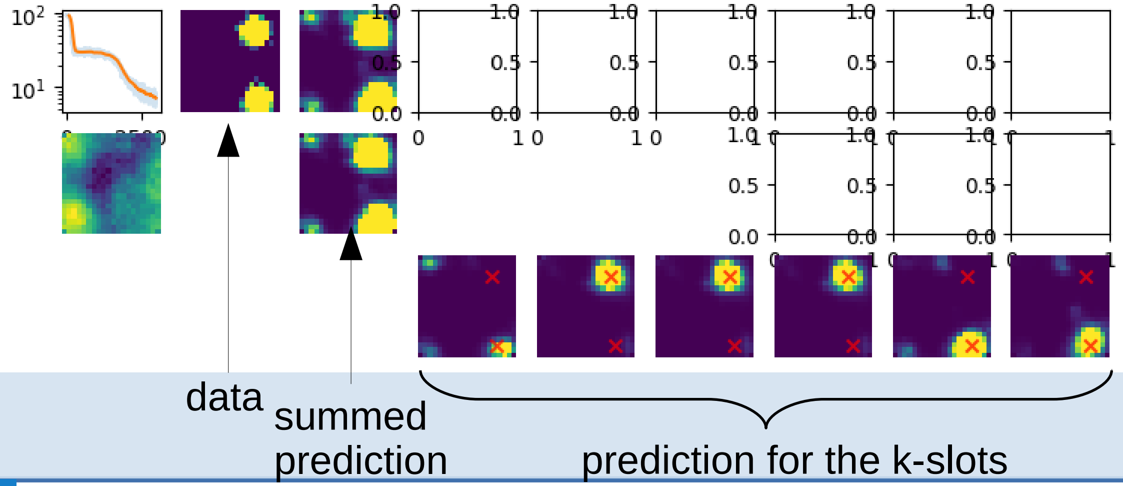
slot_and_tspn_onenotebook from Lukas Heinrich

https://gist.github.com/lukasheinrich/31d06bc4918e52d7ae3663a197b90d71

```
tensor(1.8402e-15) tensor(3.0612)
```

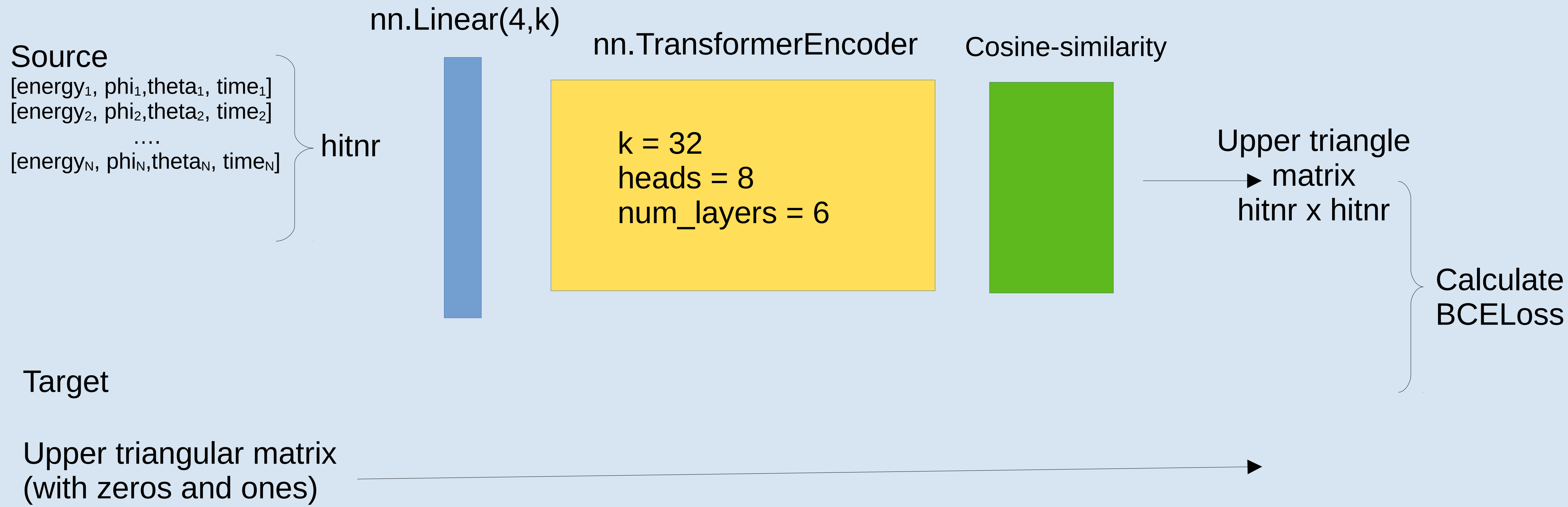


```
0.0003
loss 3000 tensor(8.4344, grad_fn=<MulBackward0>) 0.0003
tensor(4.0544e-09) <built-in method max of Tensor object at 0x79e592d3a2a0>
tensor(3.6479e-11) tensor(1.2241)
tensor(1.8620e-13) tensor(3.7033)
tensor(1.7014e-13) tensor(3.7114)
tensor(2.1267e-13) tensor(3.5644)
tensor(3.0657e-11) tensor(5.8000)
tensor(2.8779e-10) tensor(3.0993)
```



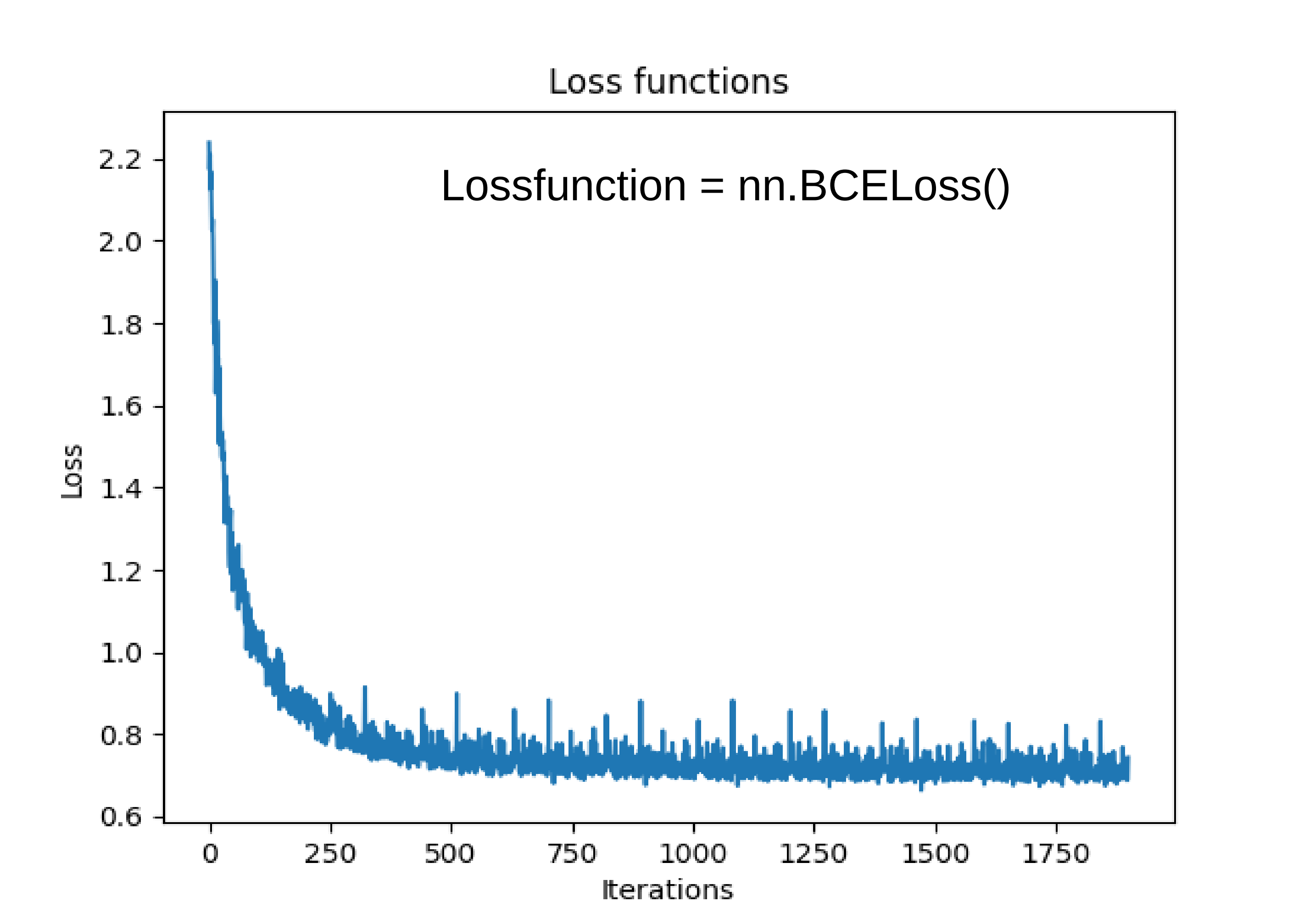

```python
class AttModel(torch.nn.Module):
    def __init__(self):
        super().__init__()
        self.latent_dim = 32

        # self.encoder = TSPNEncoder(n_slots = 6)
        # self.encoder = SlotAttentionEncoder(n_slots = 6)
        self.encoder = AddNoiseEncoder(n_slots = 6)
        self.decoder = torch.nn.Sequential(
            torch.nn.Linear(self.latent_dim,128),
            torch.nn.ReLU(),
            torch.nn.Linear(128,256),
            torch.nn.ReLU(),
            torch.nn.Linear(256,NBINS*NBINS),
            torch.nn.Unflatten(-1,(NBINS,NBINS))
        )


    def forward(self, data):
        Nbatch, *_ = data.shape
        positions,queries = self.encoder(data)
        decoded = self.decoder(positions).exp()/2.
        reco = decoded.sum(dim = 1)
        return reco,queries,decoded
```

Transformer model



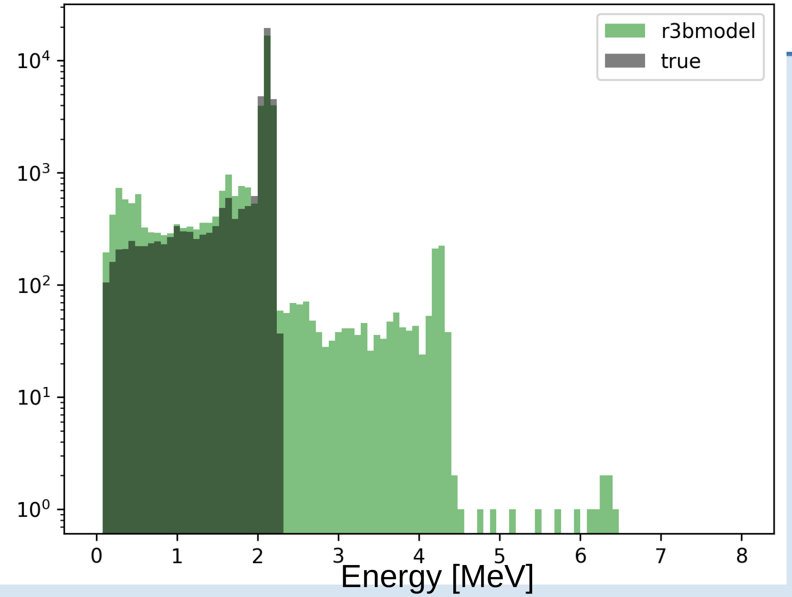
Transformer model – further parameters

Batchsize = 64
Feature number = 32
n_epochs = 10
Loss_rate = 2e-4
Loss function = nn.BCELoss()



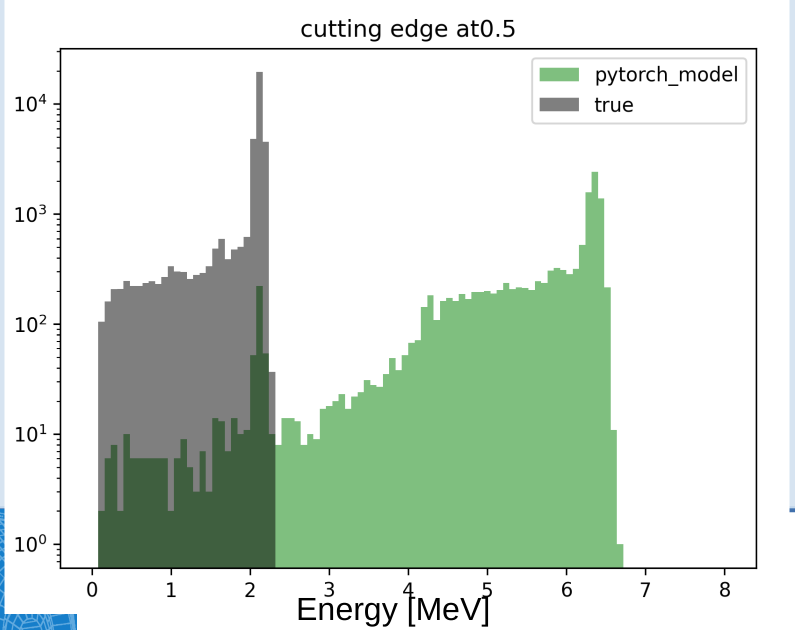
How do the energy spectra look like?

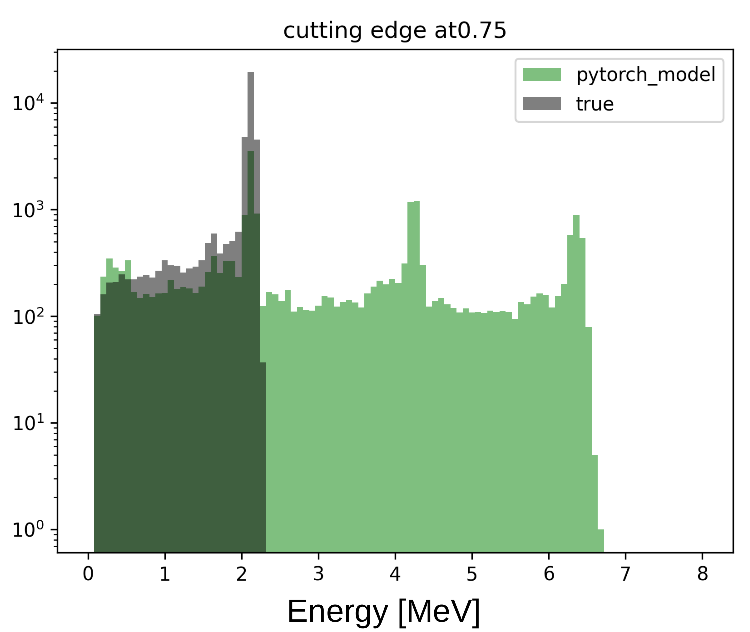
Standard Cluster vs True Clusters

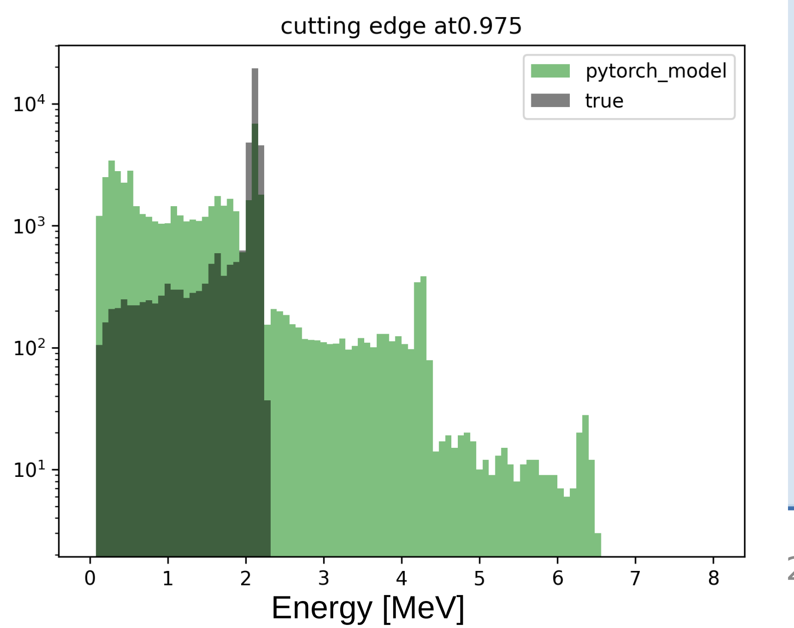


How to clusterize hits from output of transformer model:

1) Take the upper triangular matrix tri[hitnr x hitnr]
2) set “merge cut”. If tri[i,j] > “merge_cut” → hits belong to same cluster
3) do this for all combinations and merge them appropriately







Why energy spectra so bad while loss function seems to decrease ?

Most entries in model output tensor ~0.5. This diminishes the loss BCELoss function!

How to improve?

- Include some cut condition in the forward part of the transformer model

```
#out_ret_val = torch.where(ret_val > 0.7, torch.FloatTensor(1,requires_grad=True), torch.FloatTensor(0,requires_grad=True))
```

→ discontinuity of loss function → no learning!

- Use linear net instead of cosine similarity

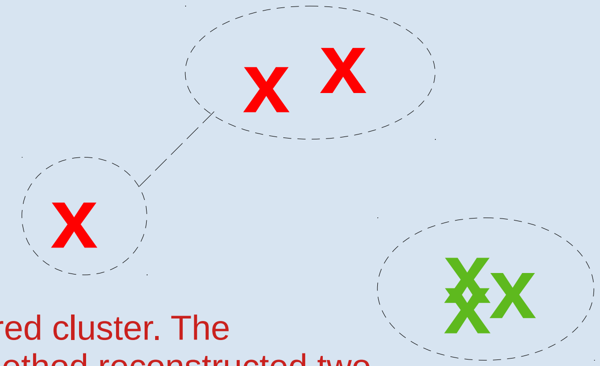
```
output_tensor = torch.cat([tensor_i.expand(-1, -1, expansion_factor, -1), tensor_j.expand(-1, expansion_factor, -1, -1)], dim=-1)
#small net:
net = nn.Sequential(
        nn.Linear(64,8),
        nn.ReLU(),
        nn.Linear(8,1),
        nn.Sigmoid()
        )
res = net(output_tensor)
temp_res = torch.squeeze(res)
upper_tri_mask = torch.triu(torch.ones((temp_res.shape[1],temp_res.shape[1])),diagonal=1).bool() #out[1] is max hit number in batch
result = temp_res[:,upper_tri_mask]
```

No improvements!

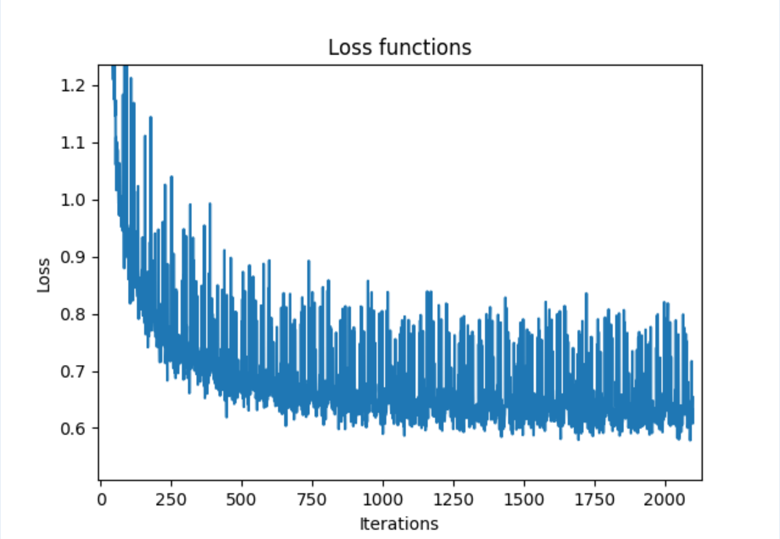
Agglomerative Model + Transformer Model

Idea:

1. Use first agglomerative method to cluster
2. Select events where we have too many clusters (false negative)



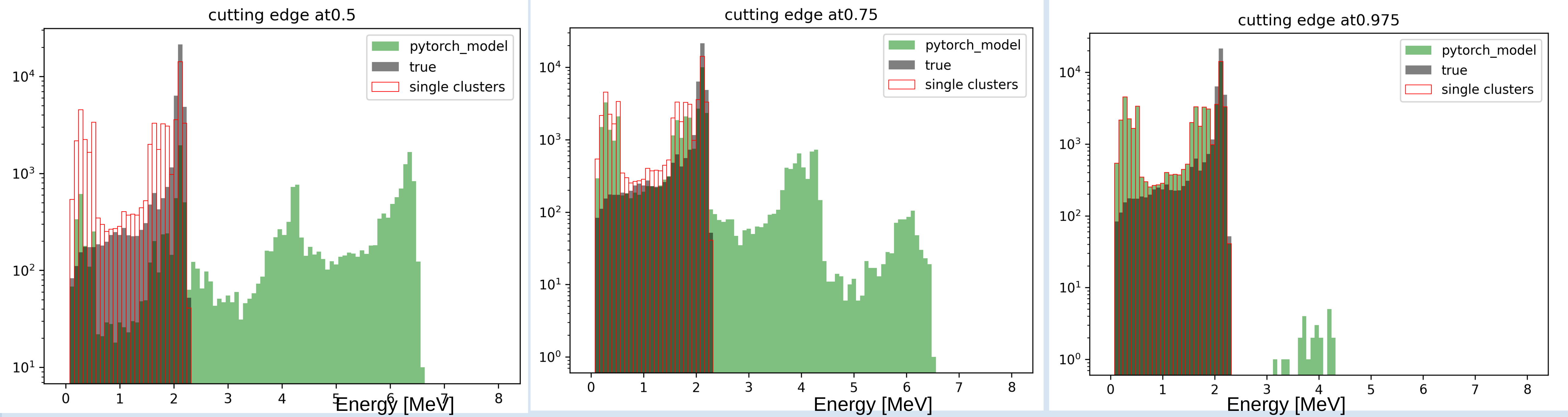
This is one true red cluster. The agglomerative method reconstructed two



3. Feed the clusters to the transformer model (calculating cm of clusters)

Transformer Model

Reconstruction with transformer model (after application of agglomerative model)



Cutting edge: model give output in range [0,1]. Cutting edge is threshold:
If cutting edge > pairwise cluster output → clusters do not belong together
If cutting edge < pairwise cluster output → clusters belong together

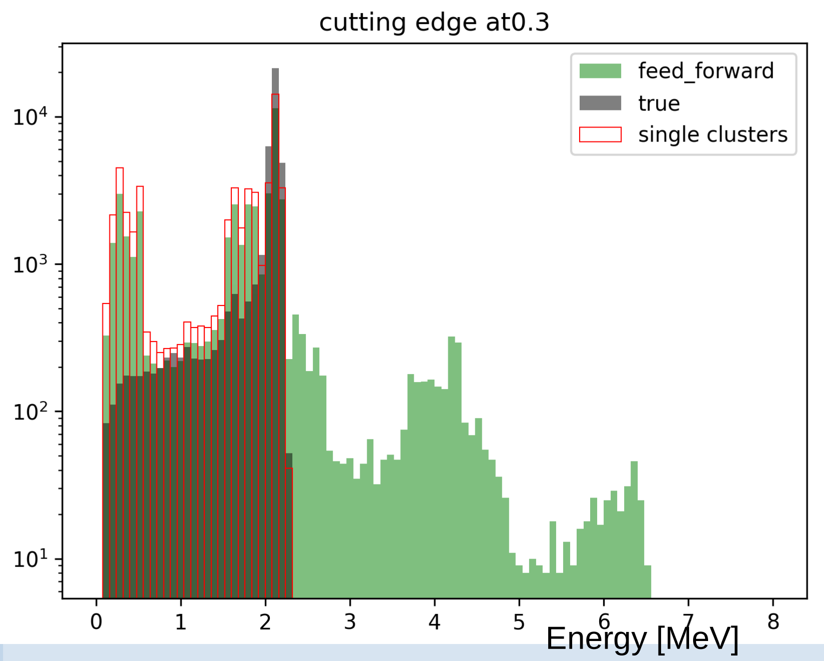
No improvement in reconstruction,
High cutting edge → = single clusters
Low cutting edge → too many clusters are merged

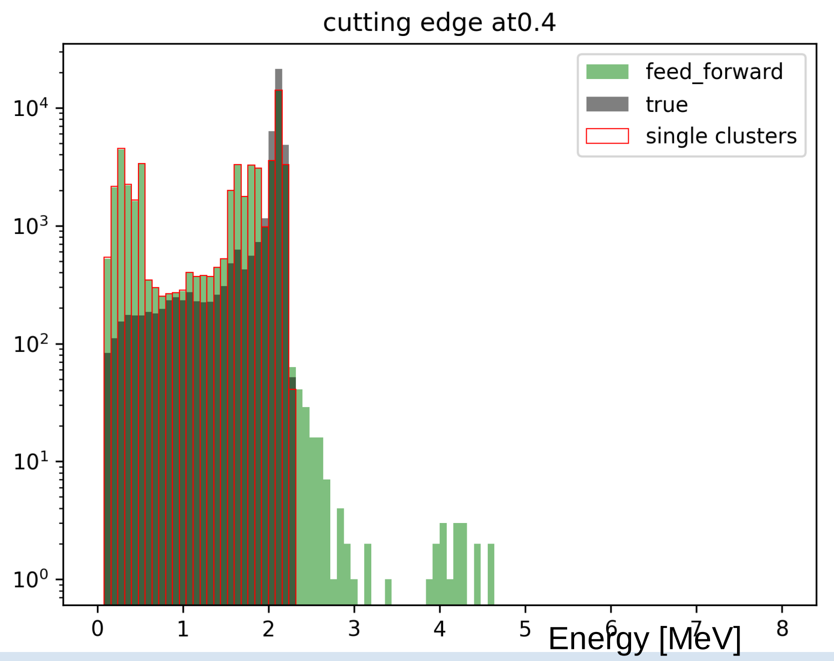
Single Feed Forward NN

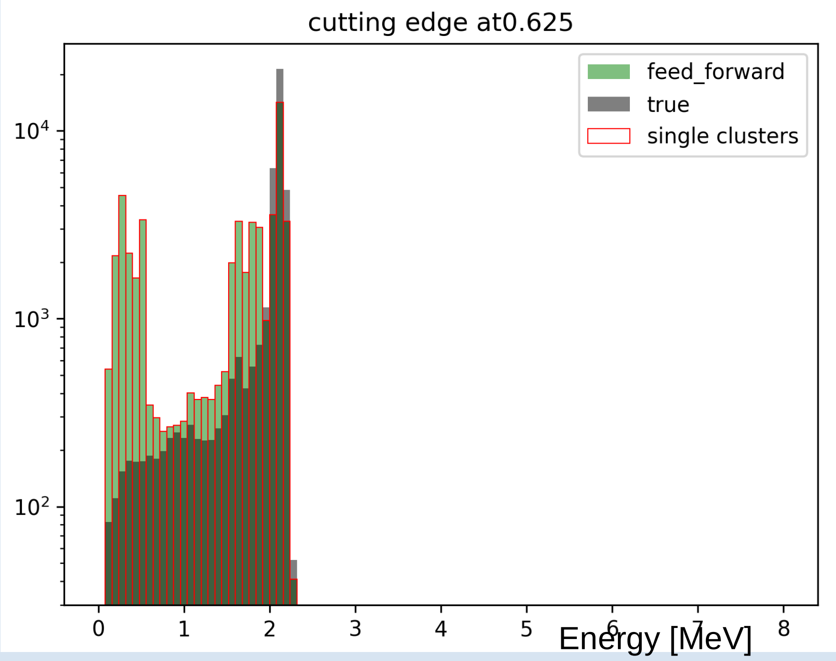
Since transformer method not successful, start with basic model:

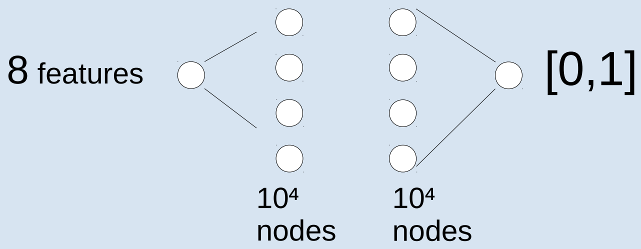
```
Def init :
        self.linear = torch.nn.Linear(8,64)
        self.activation = torch.nn.ReLU()
        self.linear_back = torch.nn.Linear(64,1)

….

Def forward:
        output_tensor = self.linear(output_tensor)
        output_tensor = self.activation(output_tensor)
        output_tensor = self.linear_back(output_tensor)
        output_tensor = torch.sigmoid(output_tensor)
        output_tensor = torch.squeeze(output_tensor)
```

Reconstruction with feed forward (after application of agglomerative model)







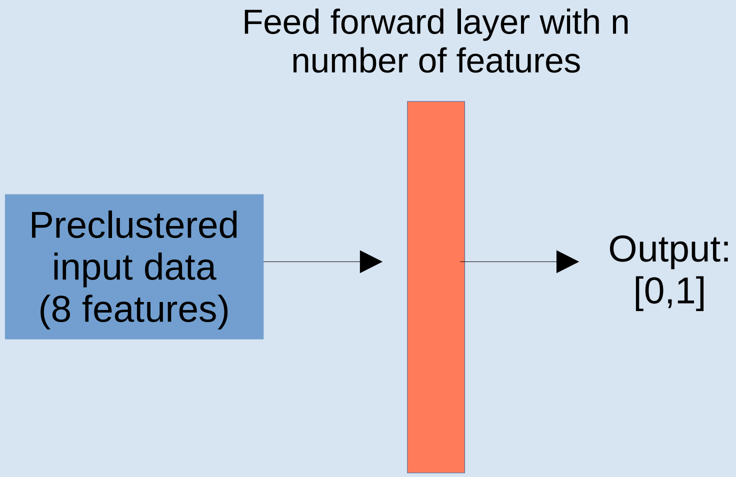


0: indep. hits
1: belonging together

No improvement in reconstruction!

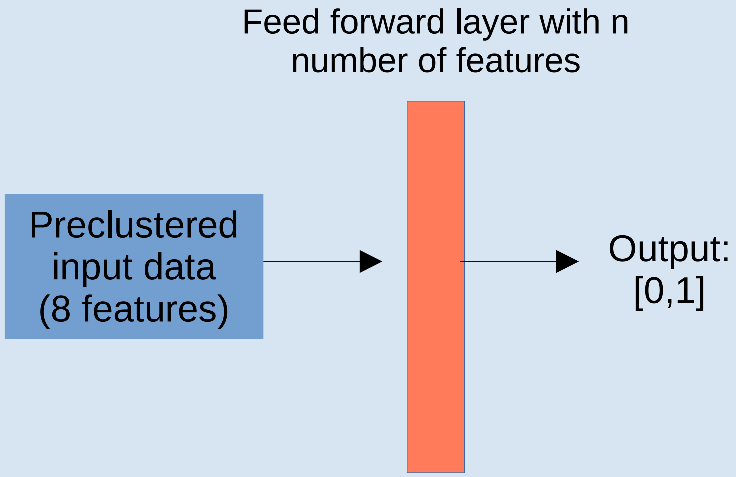
Reconstruction with feed forward (after application of agglomerative model)

Feature Size vs Loss Rate for Single Feed Forward Model:



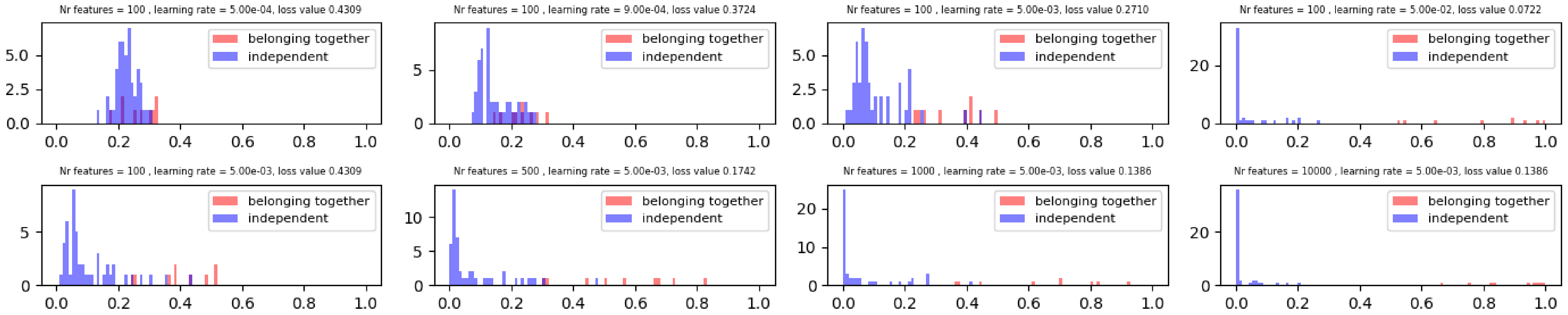
Large feature size → low loss value!

Learning Rate vs Loss Rate for Single Feed Forward Model:



High learning rate → low loss value!

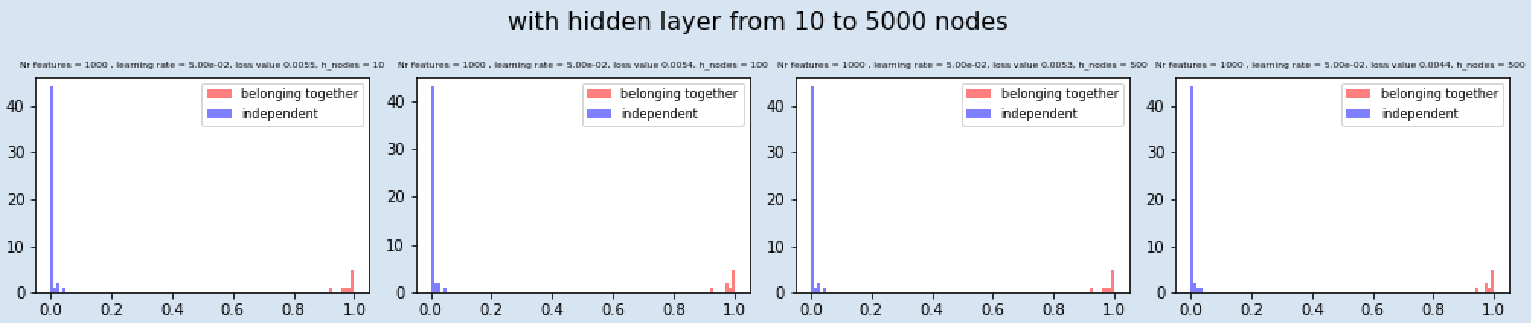
Prediction value distribution

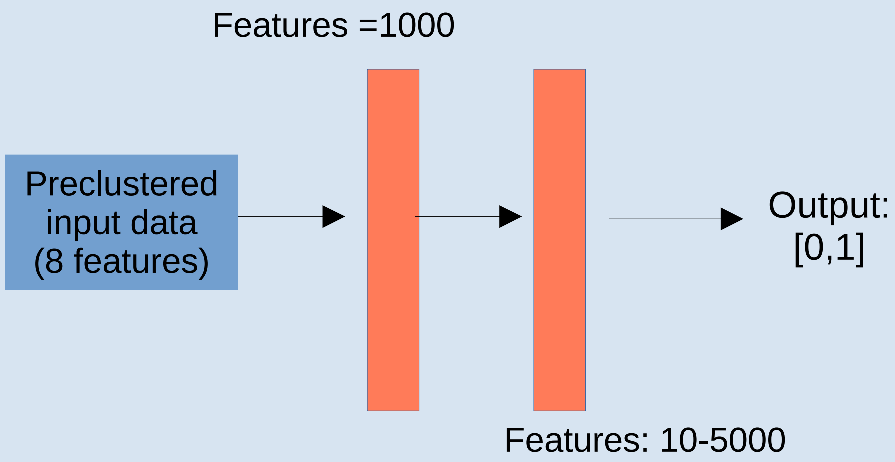


Note: here I used only 10 events! Models should be over-determined….

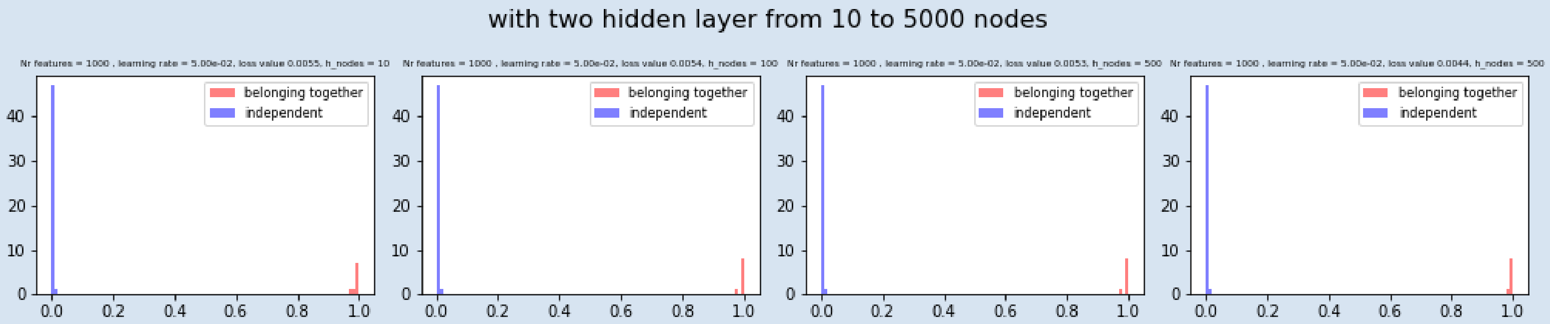
Using more hidden layers….

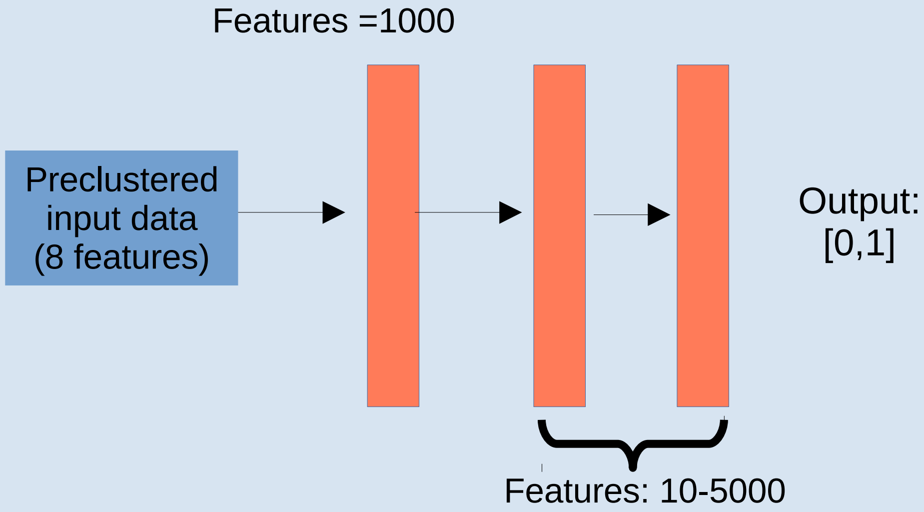
One hidden layer:





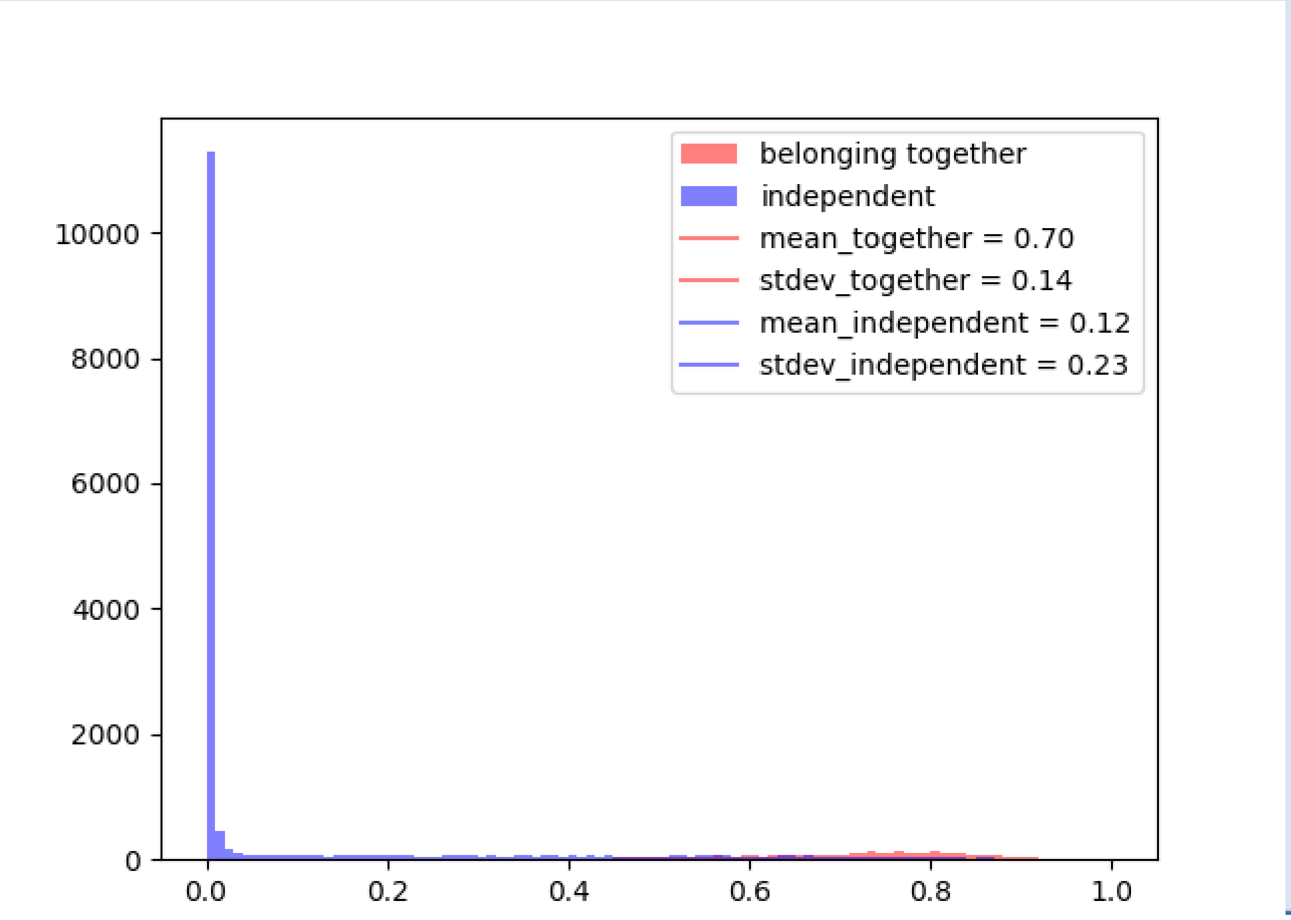
Two hidden layers:





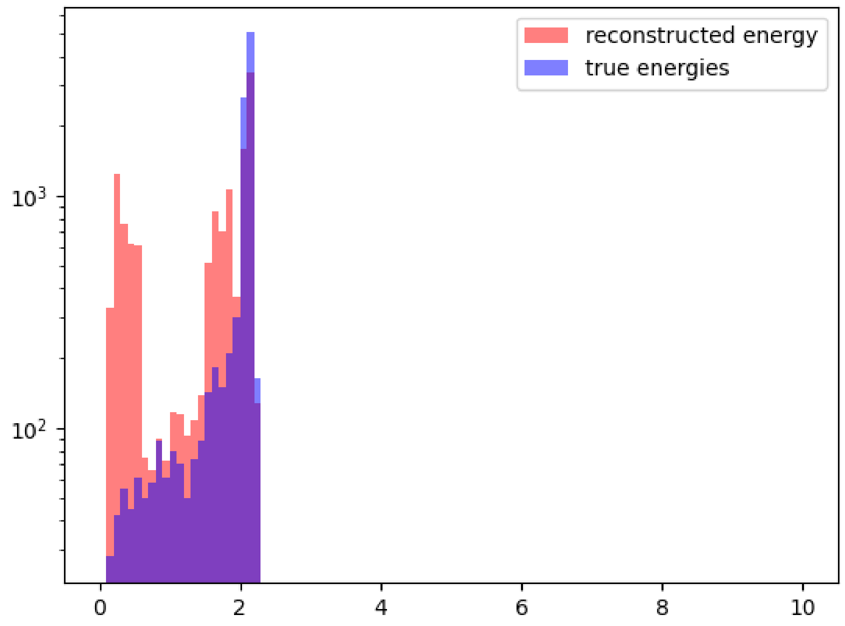
Applying Feed forward with two hidden layer on larger data...

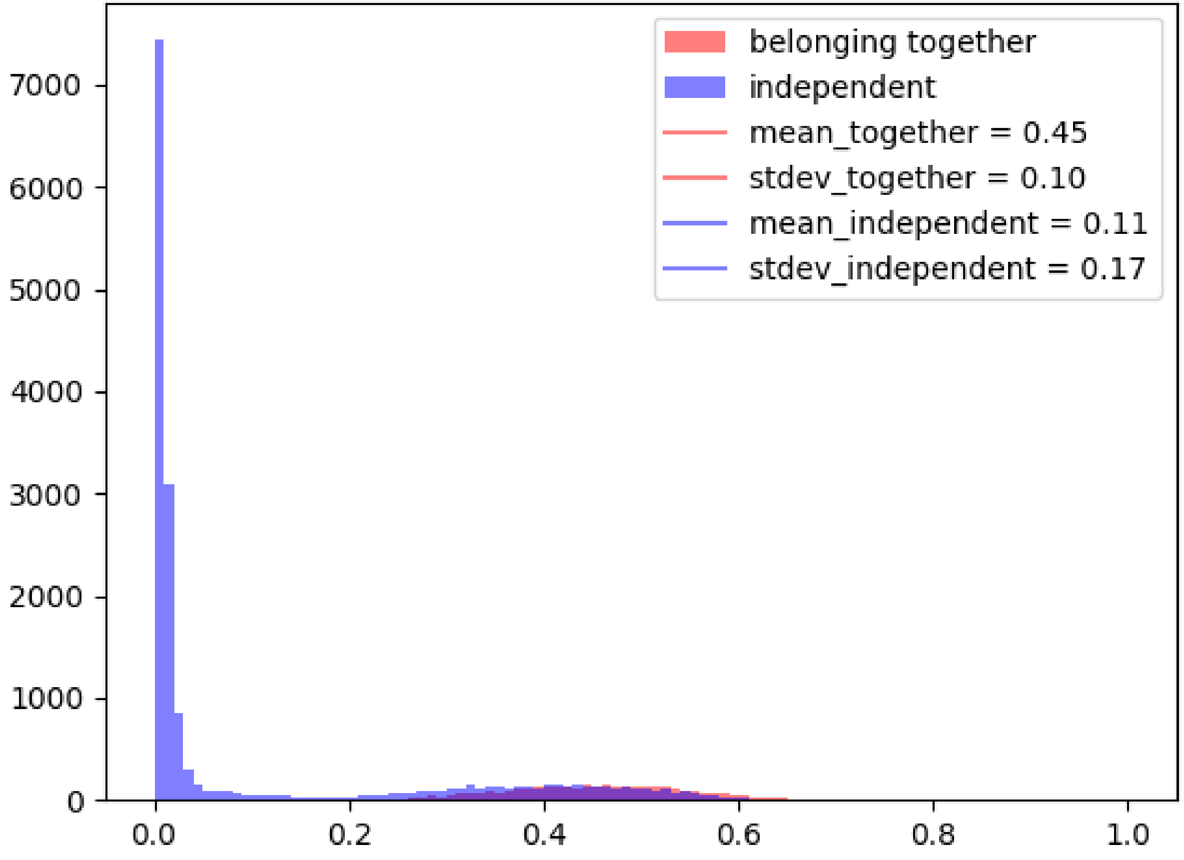
Model:
First layer: 1000 features
Second layer: 100 features
Third layer: 100 features
Lr= 5e-2



Using lower learning rate...

Model:
First layer: 1000 features
Second layer: 100 features
Third layer: 100 features
Lr= 5e-3

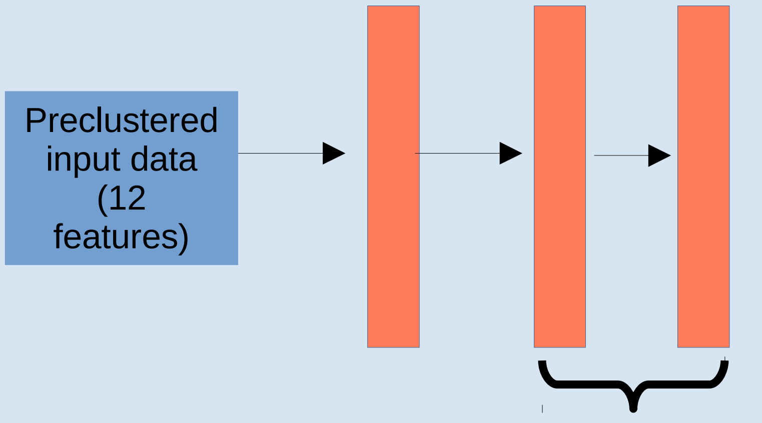




Using more features: delta_E, delta_theta, delta_phi, delta_t

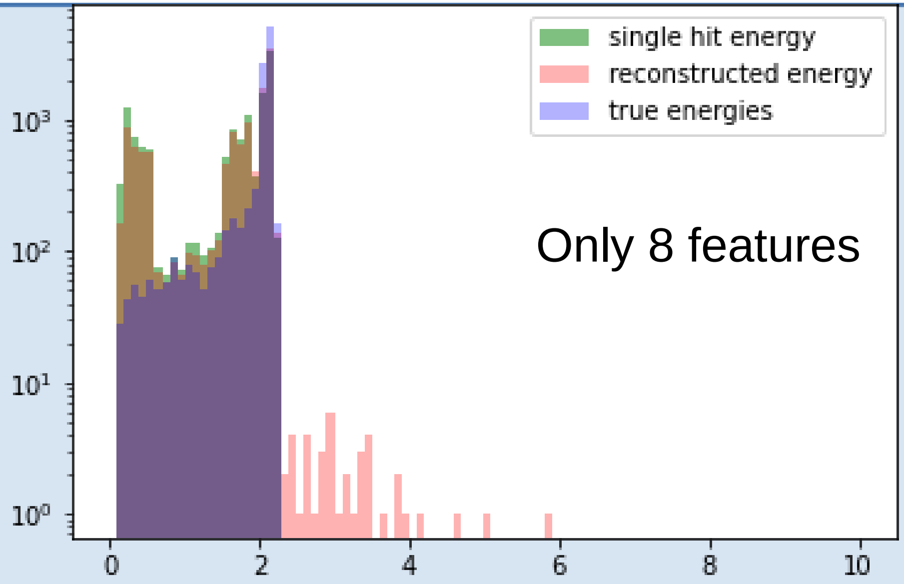
Input features: 12 = (8+4)

Features =1000



Output:
[0,1]

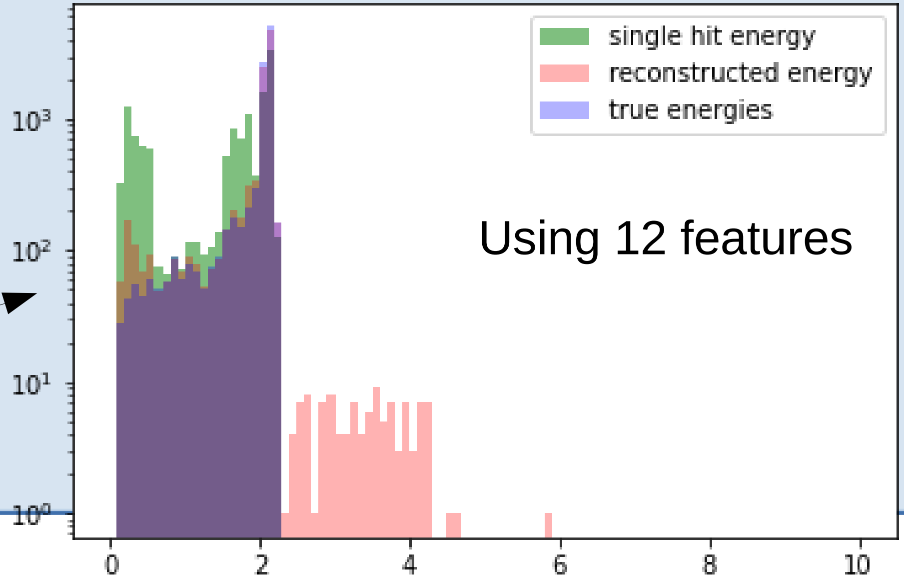
Combine if output > 0.75



Lr = 5e-3

Bigger data sample used here

Epochs = 10000

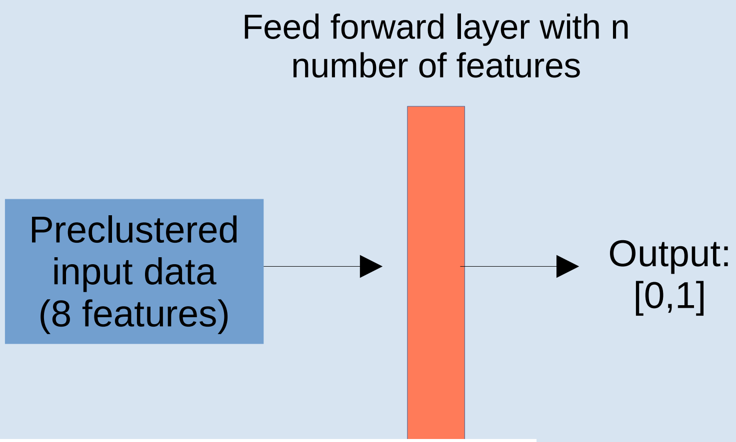


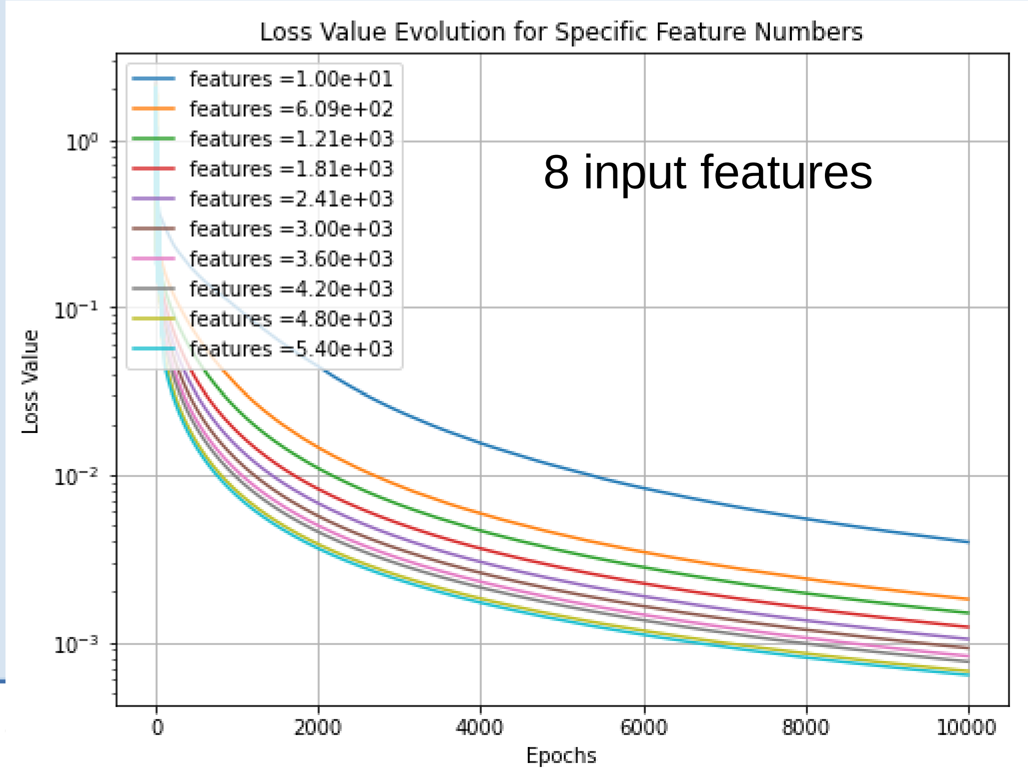
This is good!

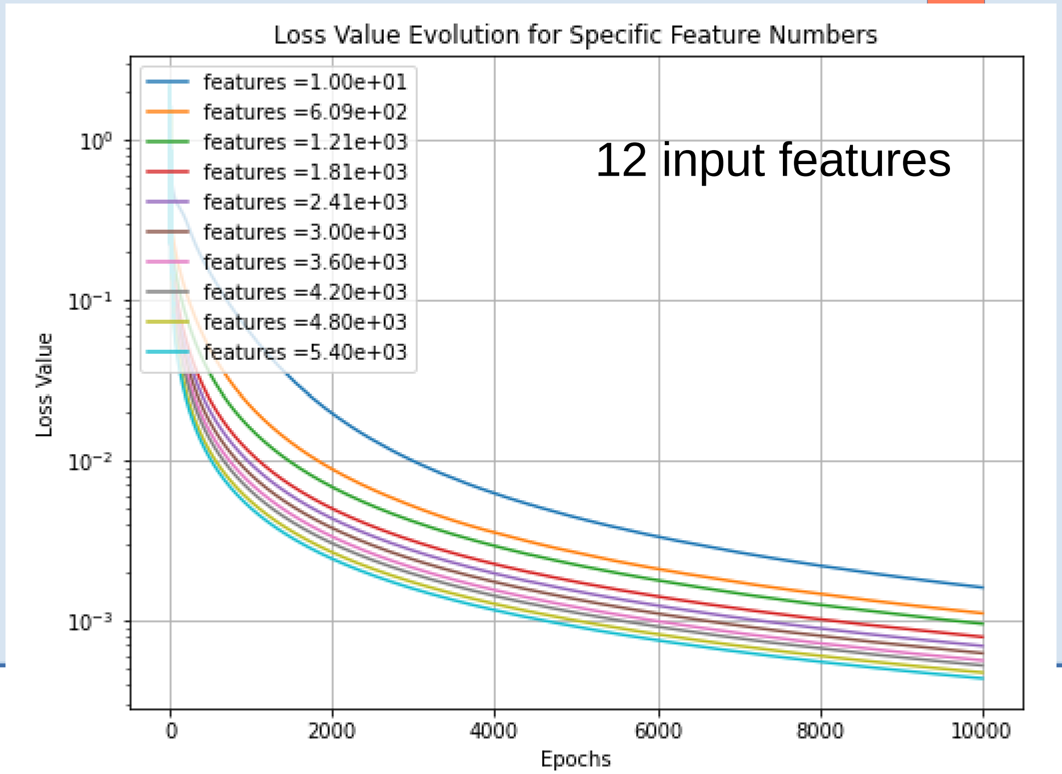
But be aware: it’s training data,…
I have to provide validation data

Loss: 8 vs 12 features

Here I use simple feed forward model, small data sample (10events)







Summary Feed Forward Model

Pros:

→ simple model, easy to deploy

Cons:

→ does not reconstruct well the clusters
→ NOT translation invariant
→ does not focus on the whole event, but only looks at the single hit combinations per time

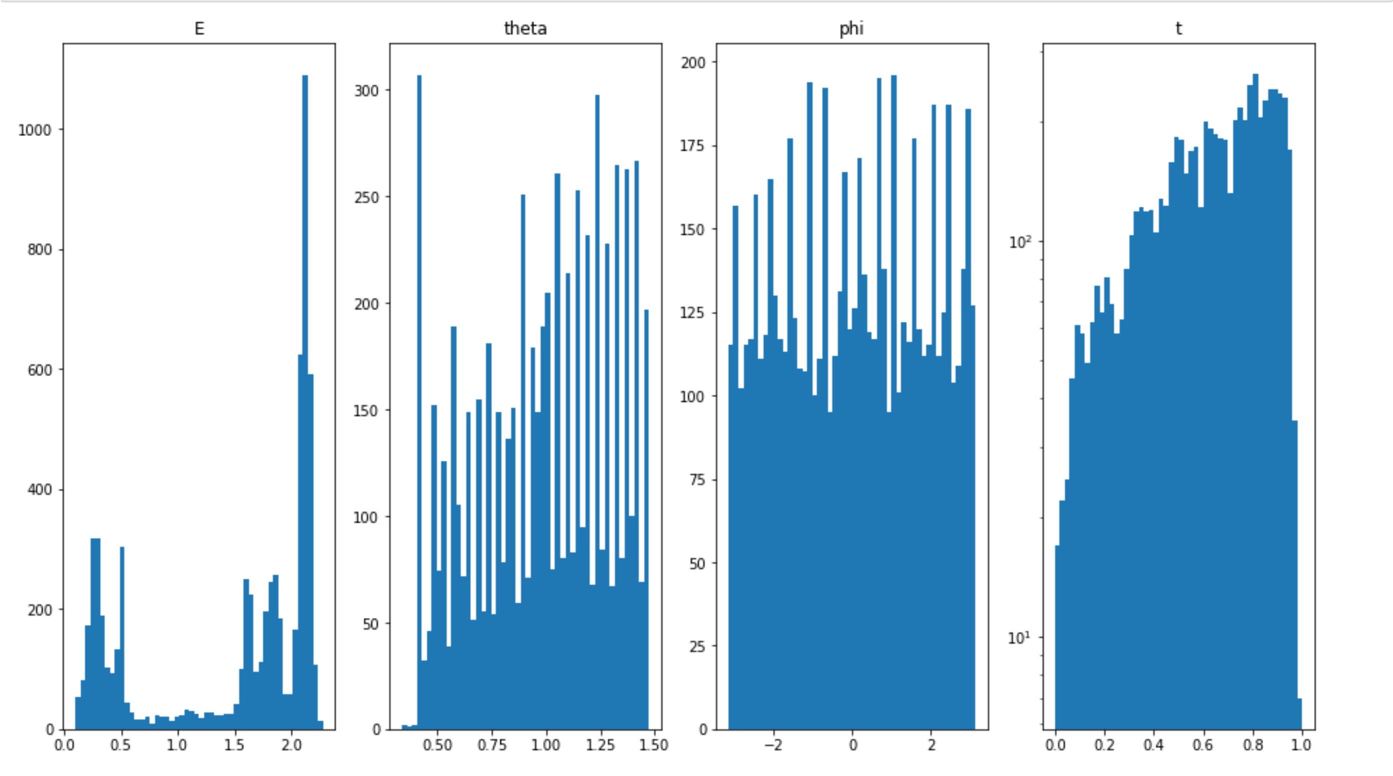
Idea from my side:

→ Implement an autoencoder do extract hidden features of cluster recognition
→ implement this features in e.g. agglomerative model to clusterize hits

How to implement this?

How data looks like we give to the feed forward NN

We applied agglomerative cluster
What you see here is already clustered data
BUT all events where you have too many clusters



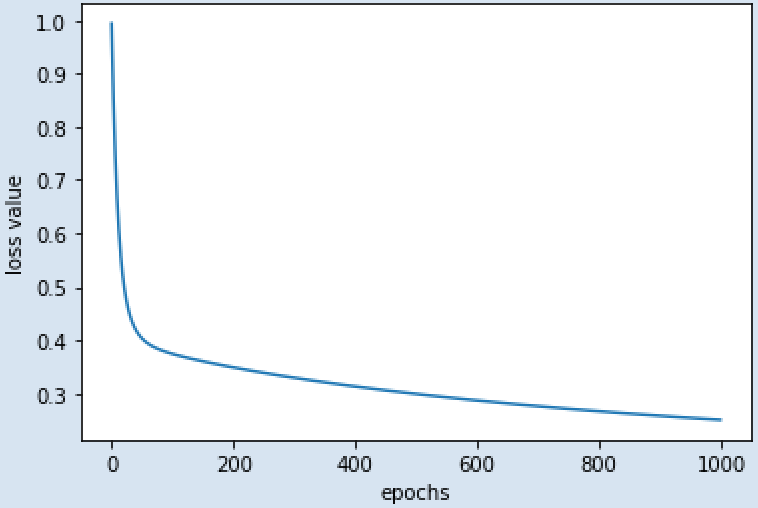
Agglomerative clustering has also drawbacks:
Clustering is done using E,theta,phi,time where the time is taken as radius

→ time starts from 0 up to…
→ for time ~0 everything is clustered togeter!

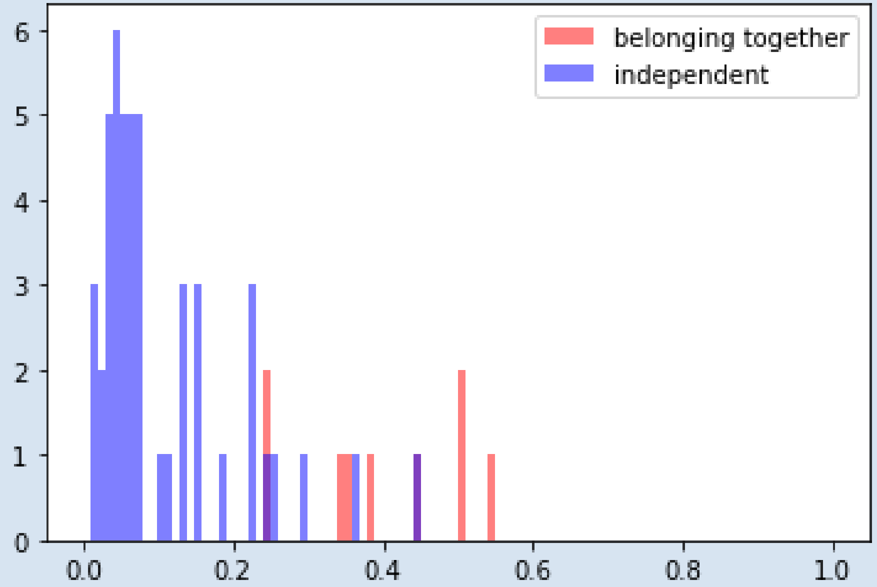
Selecting only 10 events (with 3 sub-events)

[0.	1.128016	0.913283	-2.69977	0.27121927]
[1.	0.952915	0.519144	0.878809	0.95261156]
[1.	0.434082	0.56767	-2.311936	0.93668561]
[2.	2.209619	1.105468	2.333682	0.52416023]
[3.	1.71197	1.189179	1.119164	0.78435412]
[3.	0.461599	0.777167	-0.144536	0.75403444]
[4.	2.029792	1.287946	1.30295	0.]
[5.	0.756178	1.33176	-2.309371	0.68407621]
[6.	2.1872	0.476108	2.85122	0.8842718]
[7.	1.921325	1.287711	-2.407052	1.]
[7.	0.24677	0.972258	1.512456	0.95922116]
[8.	2.12424	1.190137	0.532672	0.63181968]
[9.	2.165567	0.780356	1.333373	0.52338727]
[10.	1.927867	0.979187	-1.390222	0.83159162]
[10.	0.155214	1.058012	-2.217043	0.81032574]
[11.	2.17151	0.581699	-0.050691	0.75626808]
[12.	2.145626	0.444849	1.000789	0.69102447]
[13.	2.124236	0.907799	1.22338	0.93919196]
[14.	1.594131	0.931724	-0.470997	0.35572331]
[14.	0.518059	0.958237	1.420141	0.31123073]
[15.	1.55693	0.851083	-1.916148	0.3734817]
[15.	0.206072	1.377727	0.637334	0.43616126]
[16.	1.702479	1.014433	2.493843	0.51384286]
[17.	1.654359	1.057384	1.224166	0.95706616]
[18.	1.647063	1.212656	-0.142311	0.9388571]
[18.	0.479129	1.147077	2.998456	0.88034231]
[19.	0.887473	0.777098	-2.89615	0.68520254]
[20.	2.10968	0.773892	1.628614	0.85522686]
[21.	1.16823	1.331397	-1.120366	0.96468413]
[21.	0.287956	1.237488	-2.217654	0.97093477]
[22.	2.154496	0.828804	-0.161298	0.79557305]
[23.	1.302665	0.712428	-0.693234	0.61380342]
[24.	1.599256	0.952238	-2.448033	0.93131397]
[24.	0.505705	1.100893	-2.893951	0.92312015]
[25.	2.141112	0.839635	0.501495	0.51226942]
[26.	2.075262	1.398027	1.62944	0.71680964]
[27.	2.107771	1.101413	-2.803576	0.52078744]
[28.	2.133439	1.160672	0.212617	0.49220052]
[29.	0.432454	1.237877	-2.503905	0.94673509]

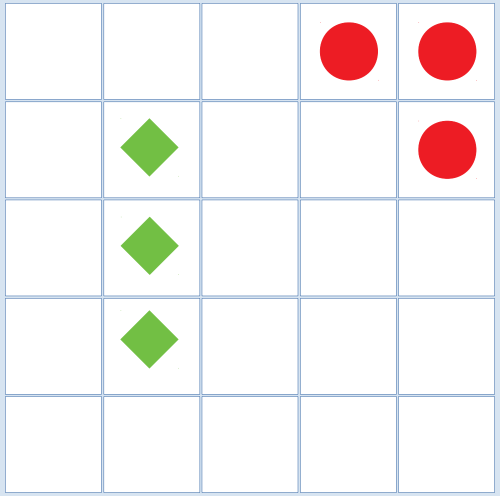
Lr = 9e-4
torch.nn.Linear(8,1000)



Prediction value distribution



i,i+1,i+2 belong together, in sets of 3



Small grid (10x10)
Two (true clusters), with sparse data
Gaussian energy distribution of cluster hits

With machine learning tools we should get at least as good as with the standard clustering (even without considering time information)!