Machine Learning for HGCal

ID and Clustering using graphs and CNN based deep learning

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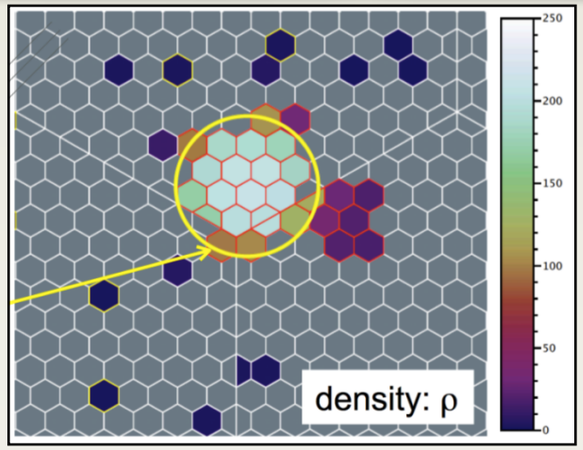
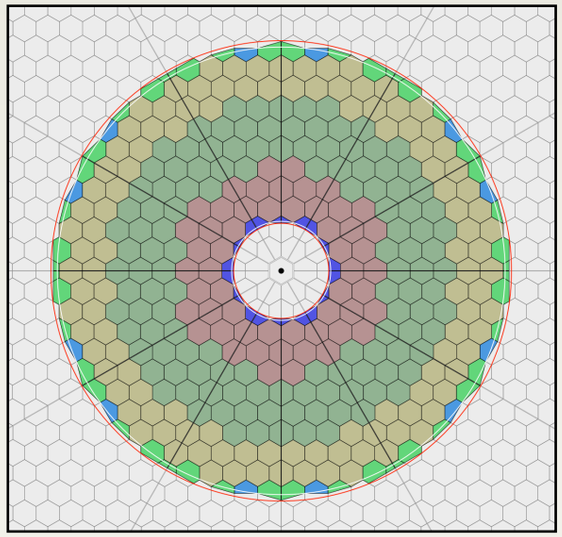
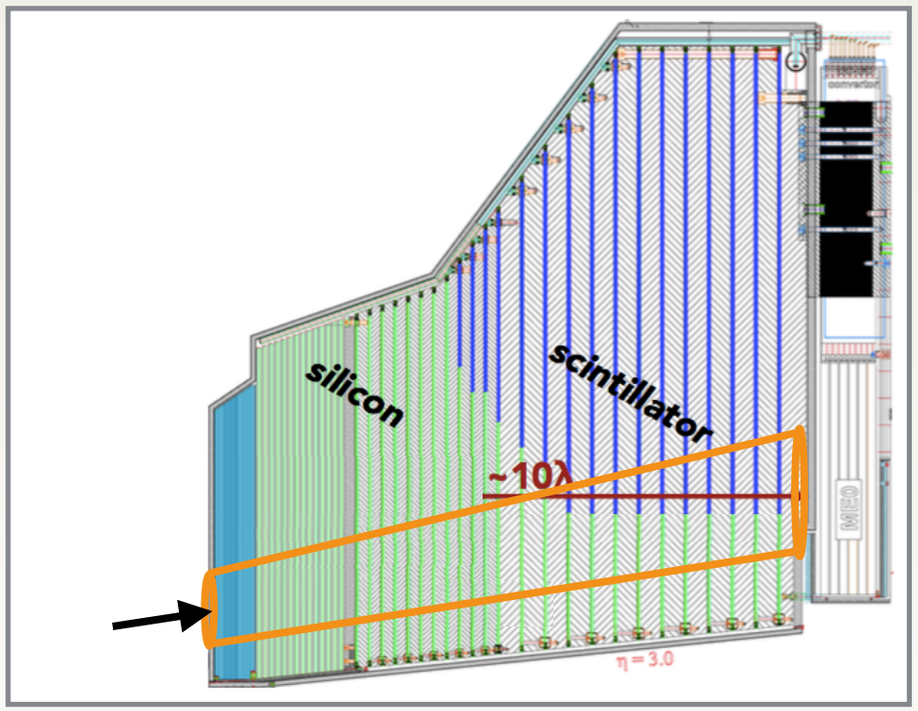
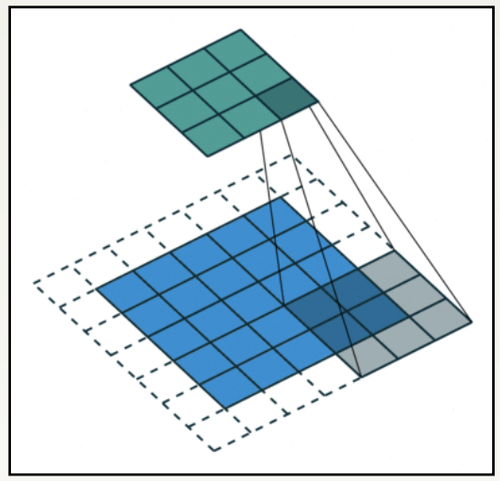
HGCal and Neural Networks (reminder)







- Sensors hexagonal
- Sensor size/area changes with layers
- Sensor size/area changes within one layer



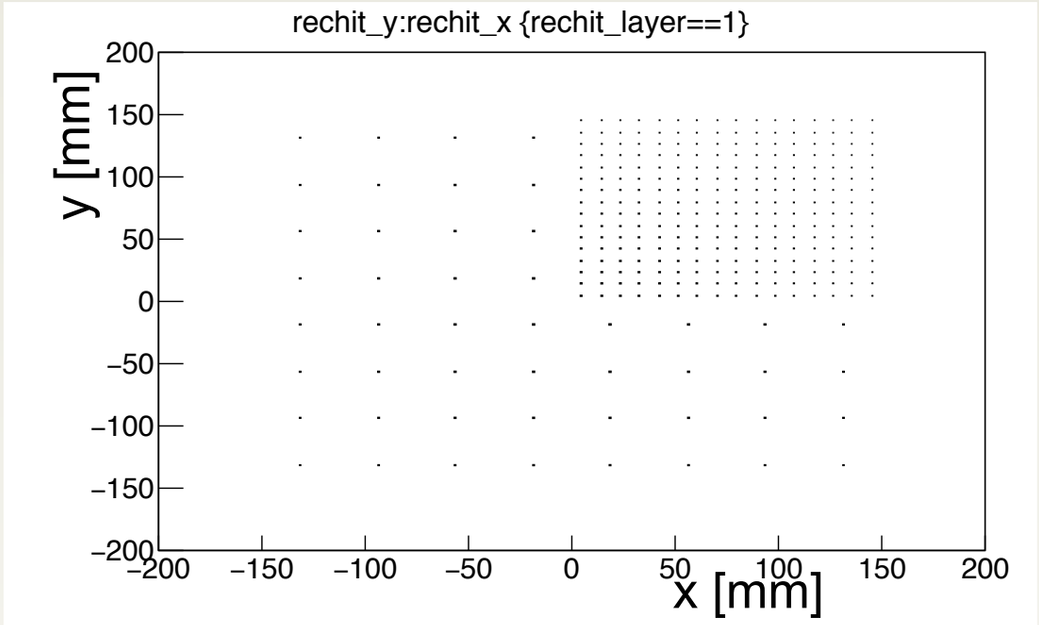
- Convolutional networks (as used in TDR): Uniform pixel size in all dimensions
  - works but not natural to the problem and creates overhead

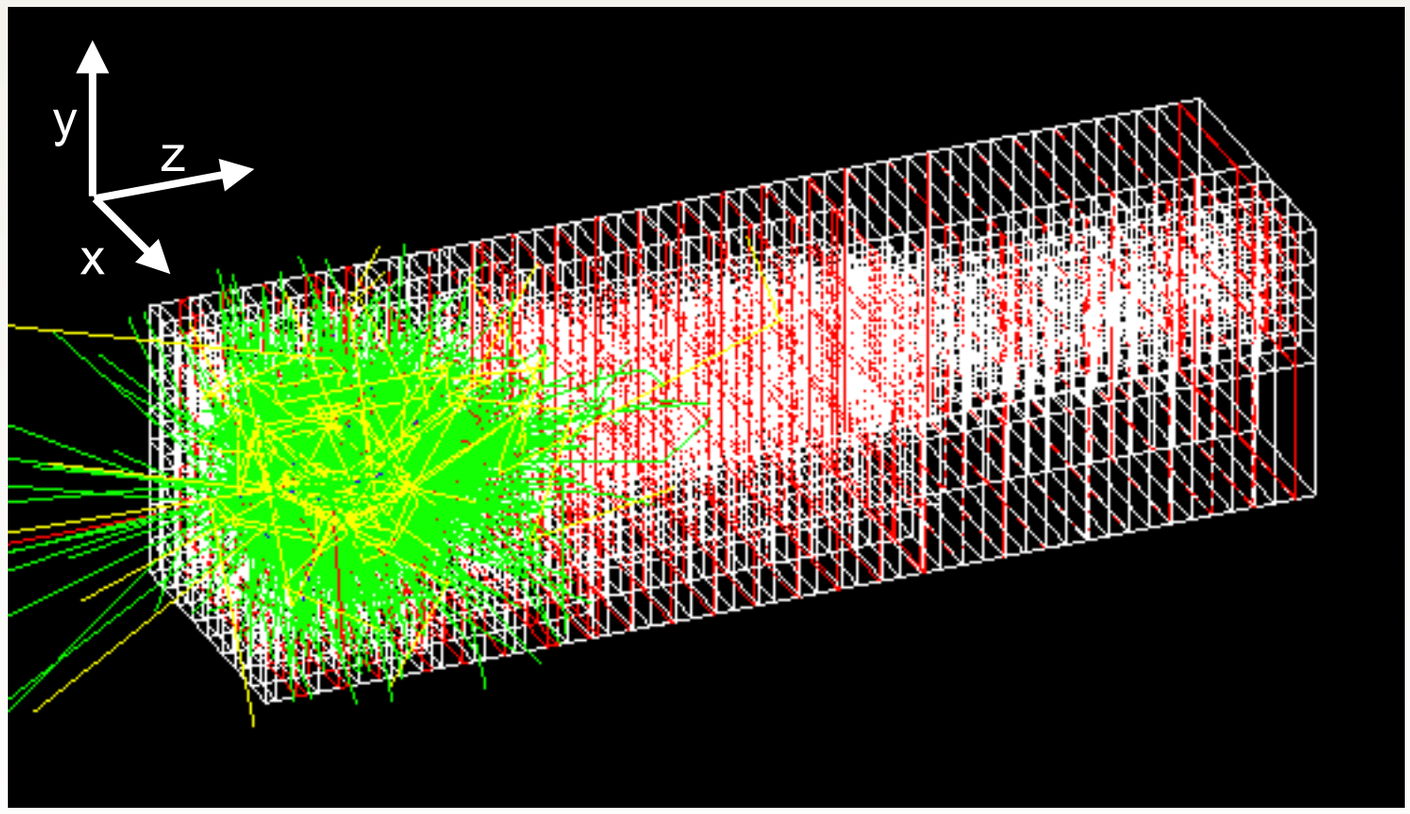
➡Try to use networks not based on a fixed grid

Dataset

- Simple calorimeter simulation
  - Not using HGCal simulation
    - Fast generation of samples and simple to change geometry
    - Direct output in right format (otherwise 3-4 steps)
  - Full Geant4 simulation
  - Tungsten, about 11 λ_0 in z, 30 cm x 30 cm in (x,y)
  - Non homogenous geometry
    - Sensor sizes from about 1 cm^2 to 15x15 cm^2
    - Sizes change within the layer
  - Particles with energies 1-100 GeV
    - 5 cm x 5 cm window around (x,y)=(0,0)
    - Different granular parts are hit
    - Shot from distance of 2 m
    - Total size: 1M events
    - (more details later)

➡Resembles properties of HGCal that pose challenges to ML approaches





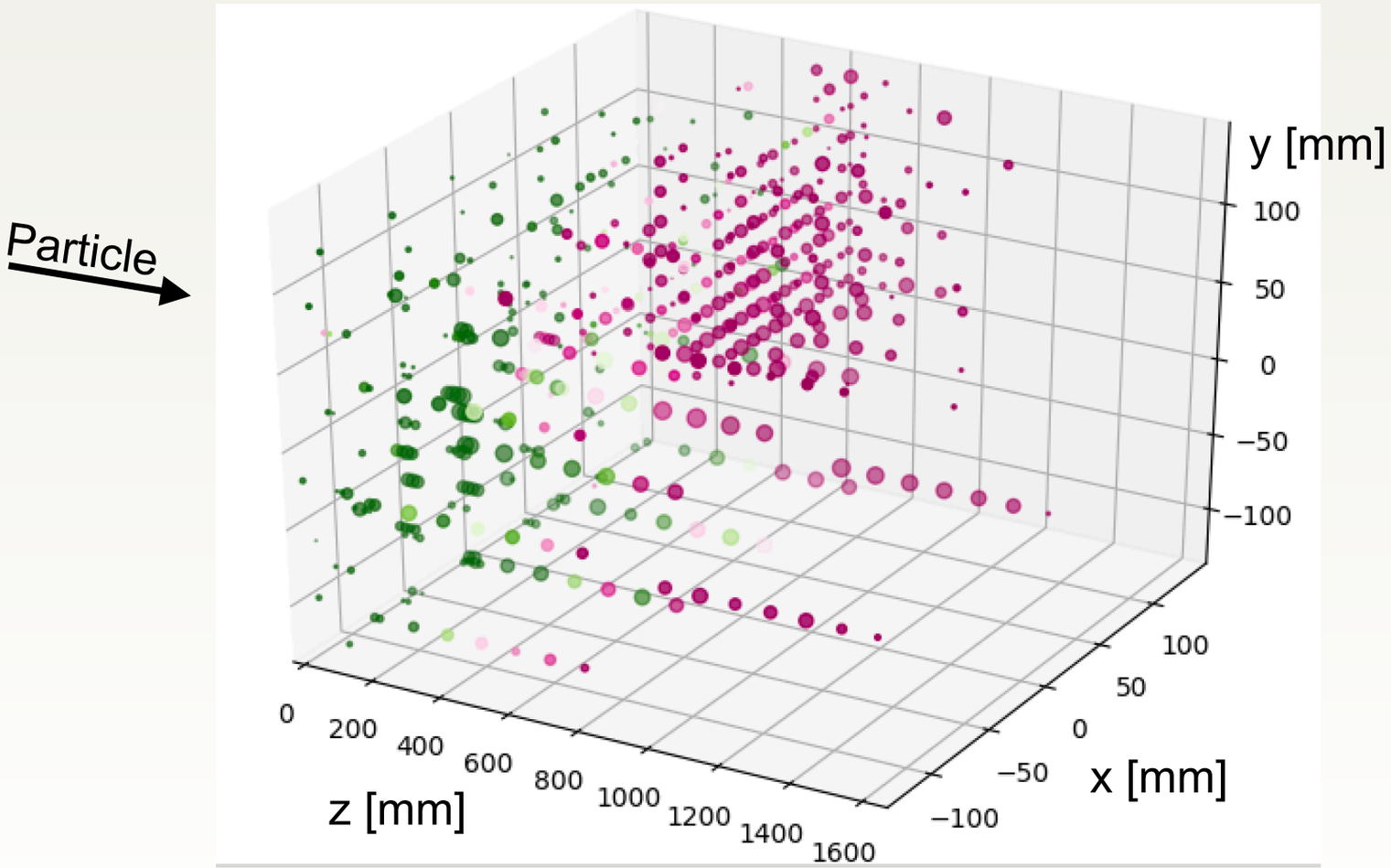
Clustering

- Clustering

  Two showers at in any sample

  Both charged pions

  Dataset: linear combination of showers of both particles



Clustering - Notation

Ground truth shower fractions:

- Matrix of shape [N, 2] donated by **T** (for target)

$$T = \begin{bmatrix} t_1 & t_2 & \dots & t_N \end{bmatrix}$$

- Where t_i is a 2D vector, fractions of of two showers of ith sensor

Predicted shower fractions

- Matrix of shape [N, 2] donated by **P** (for prediction)

$$P = [p_1 \quad p_2 \quad \dots \quad p_N]$$

- Where p_i is a 2D vector, fractions of of two showers of ith sensor

Energy deposited on sensors

- ND vector denoted by **e**

$$e = [e_1 \quad e_2 \quad \dots \quad e_N]$$

- Where e_i is a scalar representing energy deposited on ith sensor

Clustering - Loss function

Loss functions (12)

$$L(\boldsymbol{P}, \boldsymbol{T}, \boldsymbol{e}) = \frac{1}{\hat{E}} \sum_{s=1}^{N} \|(\boldsymbol{p_s} - \boldsymbol{t_s}) * f(e_s)\|_2$$

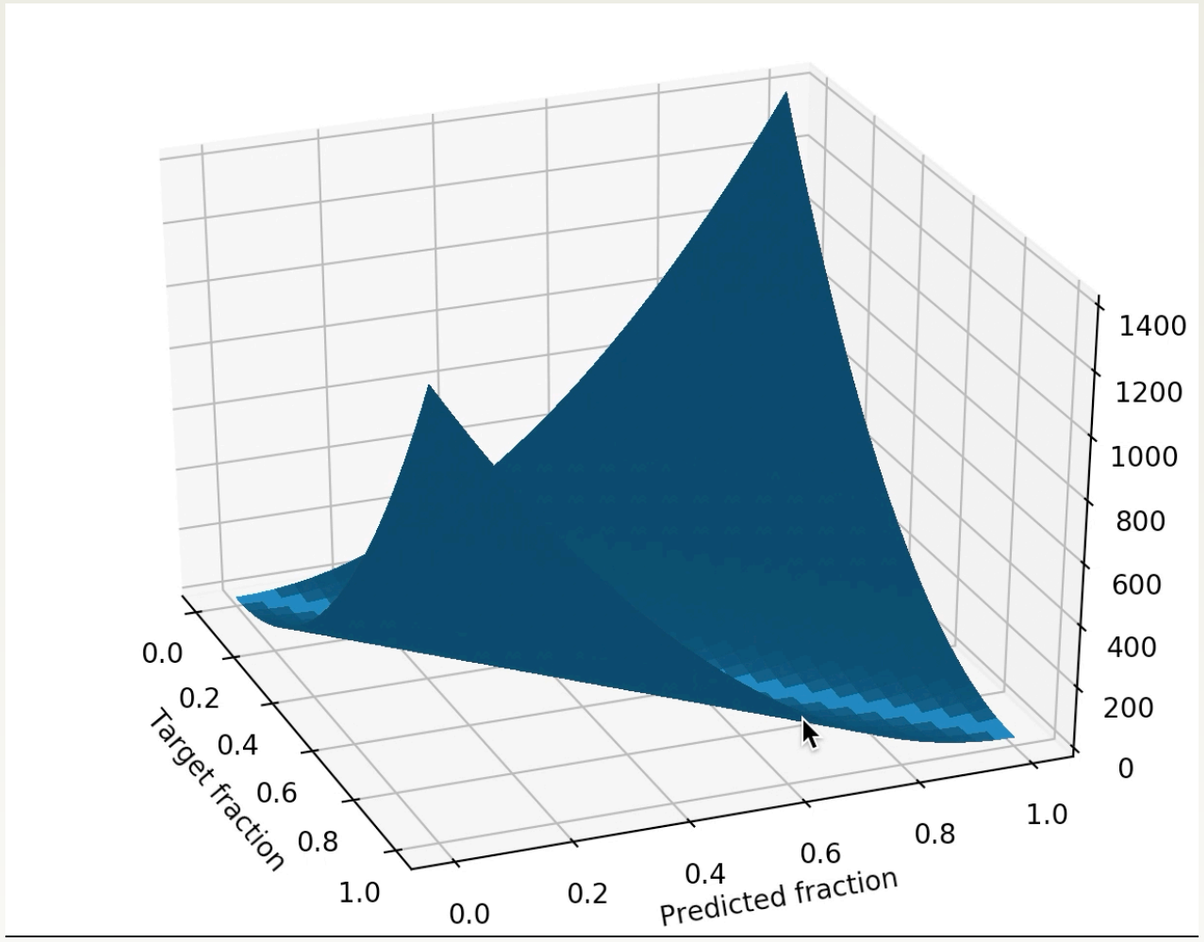
$$\hat{E} = \sum_{s=1}^{N} f(e_s)$$

Tried different

$f(e_s) = \sqrt{e_s}$ (Works best)

$f(e_s) = e_s$

$f(e_s) = ln(e_s + 1)$



$\|(p_s - t_s) * f(e_s)\|_2$

Clustering - Min loss function

Same solution if columns are swapped

$$\boldsymbol{P}' = 1 - \boldsymbol{P}$$

Since:

$$p_{s1} + p_{s2} = 1$$

We could, in theory, use more forgiving loss function:

$$L_{min} = min(L(\boldsymbol{P}, \boldsymbol{T}, \boldsymbol{e}), L(1 - \boldsymbol{P}, \boldsymbol{T}, \boldsymbol{e}))$$

Doesn't help for training

- Showers are well defined (first by x, then by y)

However, can use it for analysis

Swap the predicted or ground truth showers if

$$argmin(L(\boldsymbol{P}, \boldsymbol{T}, \boldsymbol{e}), L(1 - \boldsymbol{P}, \boldsymbol{T}, \boldsymbol{e})) = 2$$

Clustering - Binning

CNN based method

Input is tensor of dimensions [8, 8, 25, 64] (obtained by histogram based binning, scatter op)

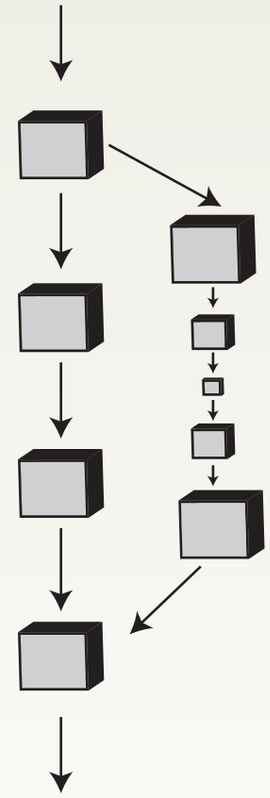
Multiple layers of 3D convolutions

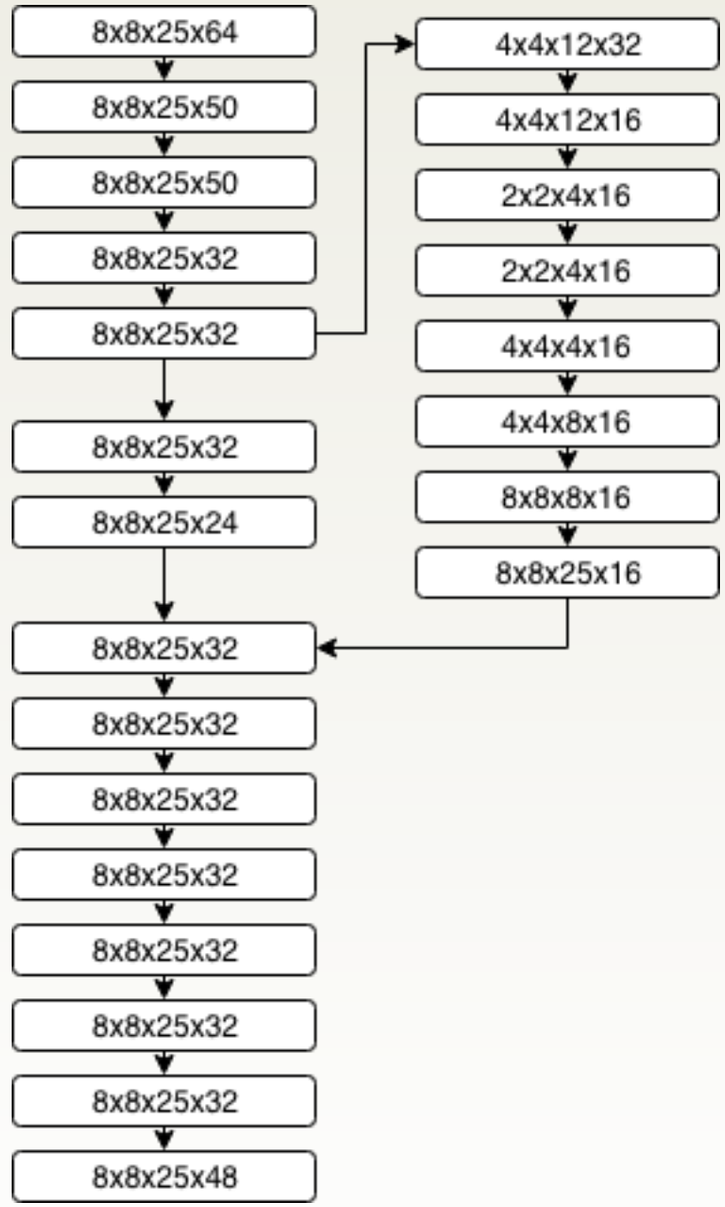
Combined with enc-dec network

- For better receptive field

Unbinned at the end (gather op)

~100k parameters





Graph convolution

Vertex = all sensors

Find k nearest neighbours for each vertex (in euclidean space)

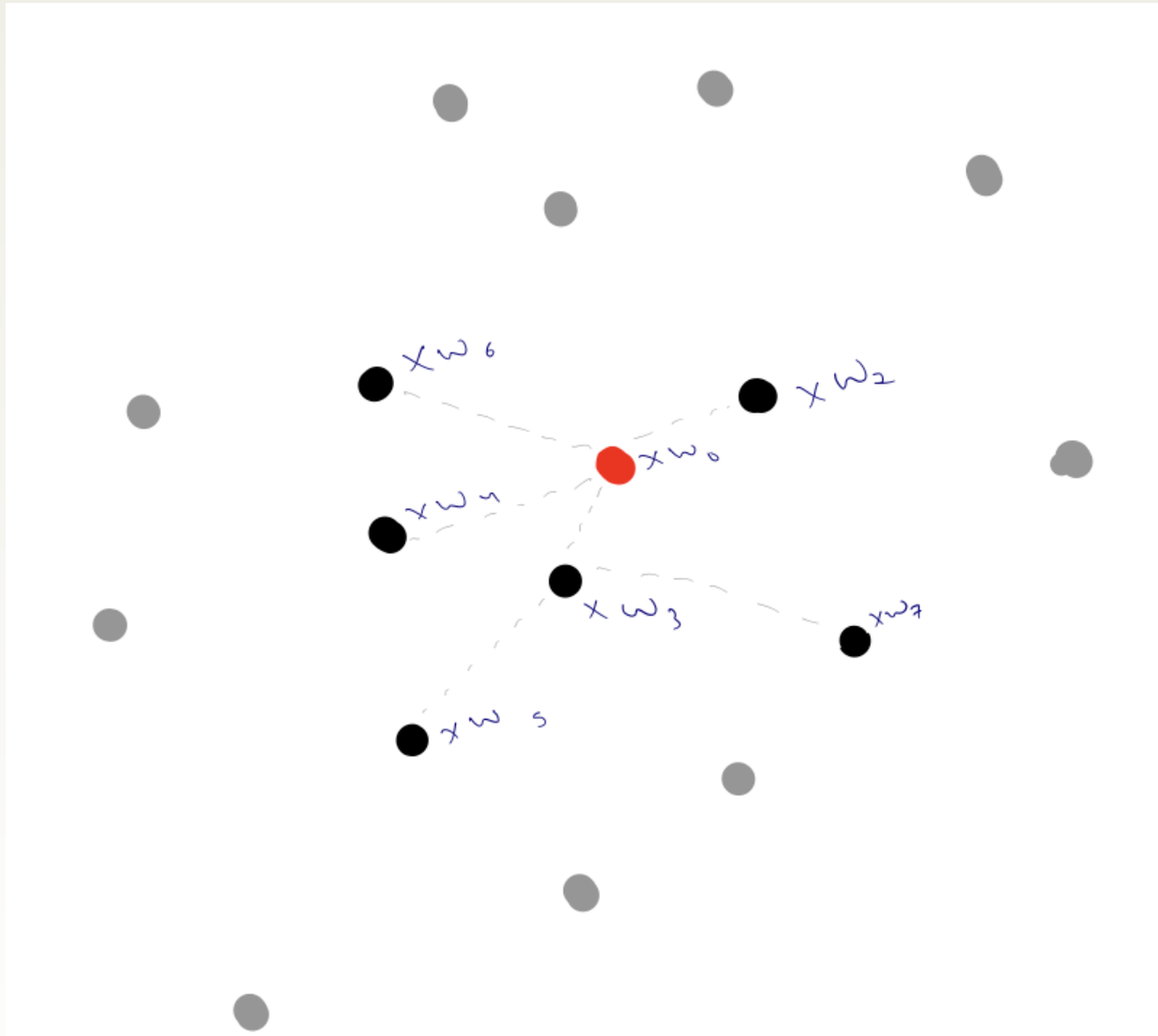
Apply conv filters on selected neighbours for each of the vertex

Propagate the result as in CNNs

5 layers of graph convolution

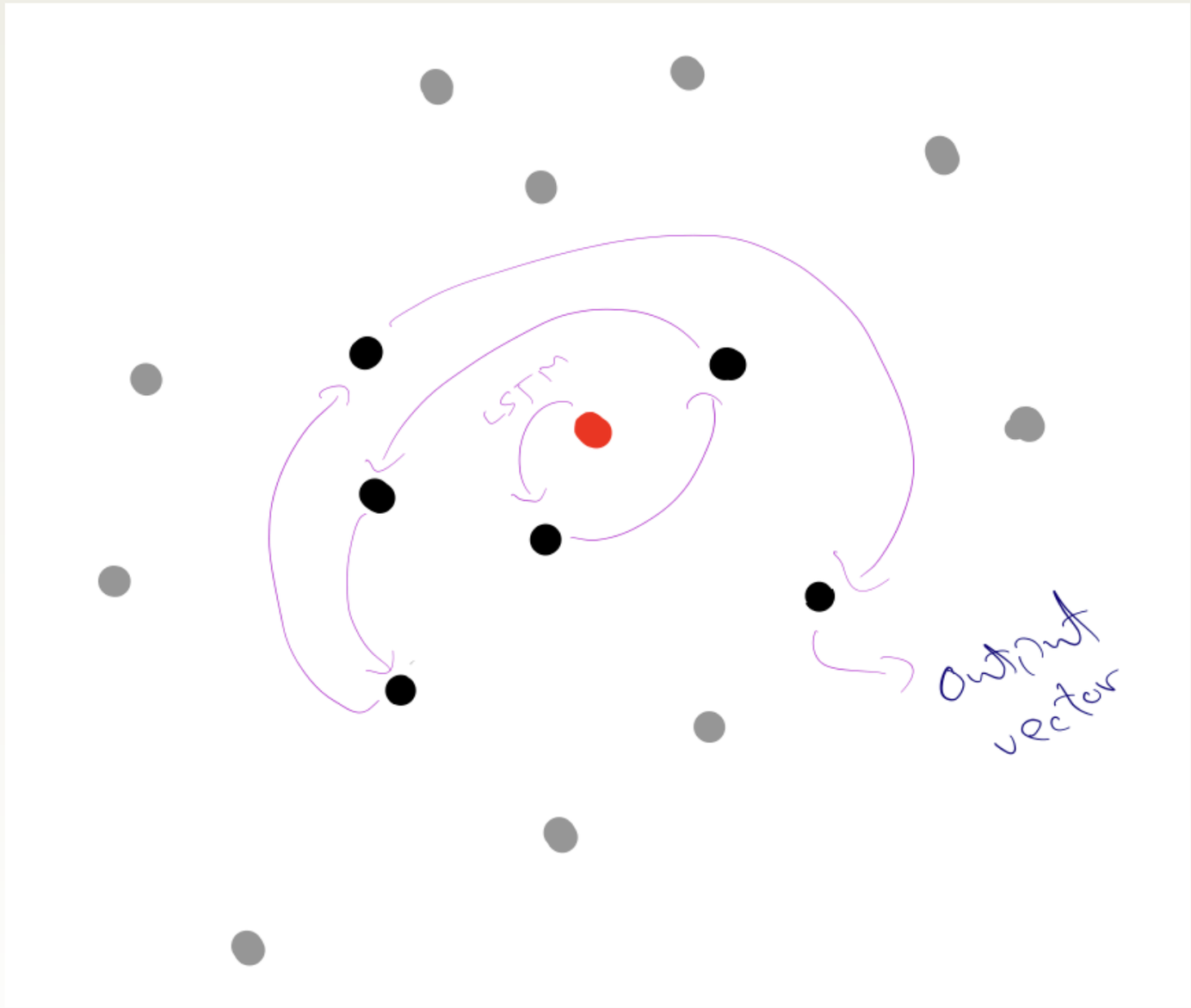
18 neighbours in each of the layers

$$o = \sum_{i=0}^{N} c_i * w_i$$



Graph neural network, LSTM aggregation

- Find k nearest neighbours for each vertex
- Use LSTM to aggregate the result to produce output
- Propagate the result as in graph convolution
- 7 layers of the network
- Each layer works aggregates on 18 neighbours



Graph neural network - Dynamic space

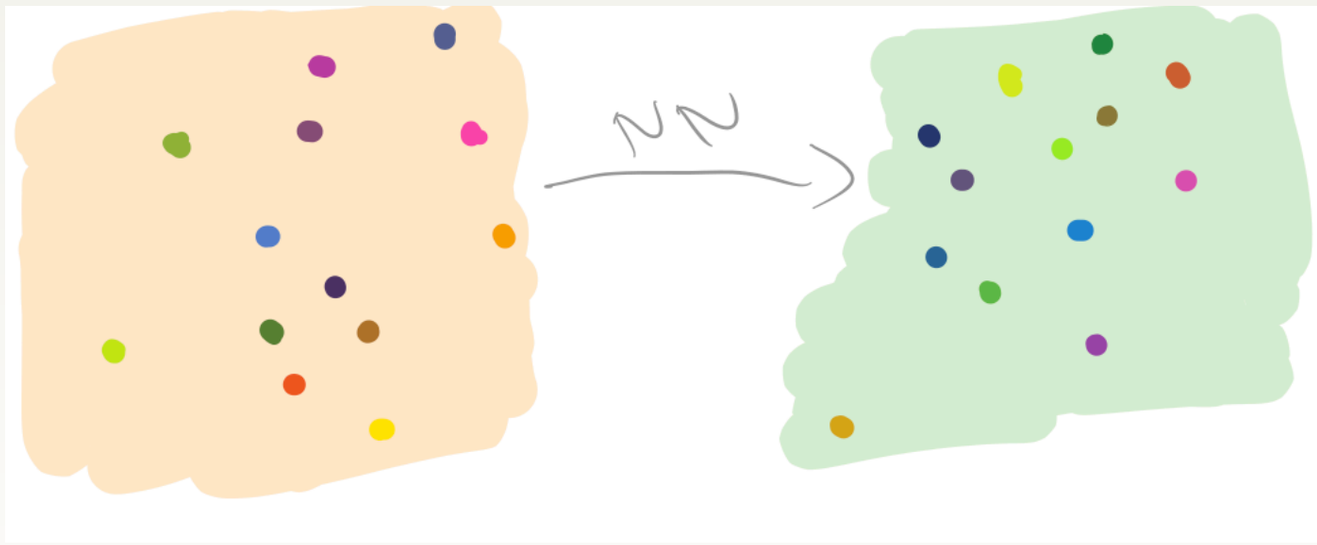
Transform features to another space

$$S' := NN(S)$$

Find nearest neighbours in new space **S'**

Aggregate the nearest neighbours using different methods

- Can be LSTM
- Can be simple filter sum



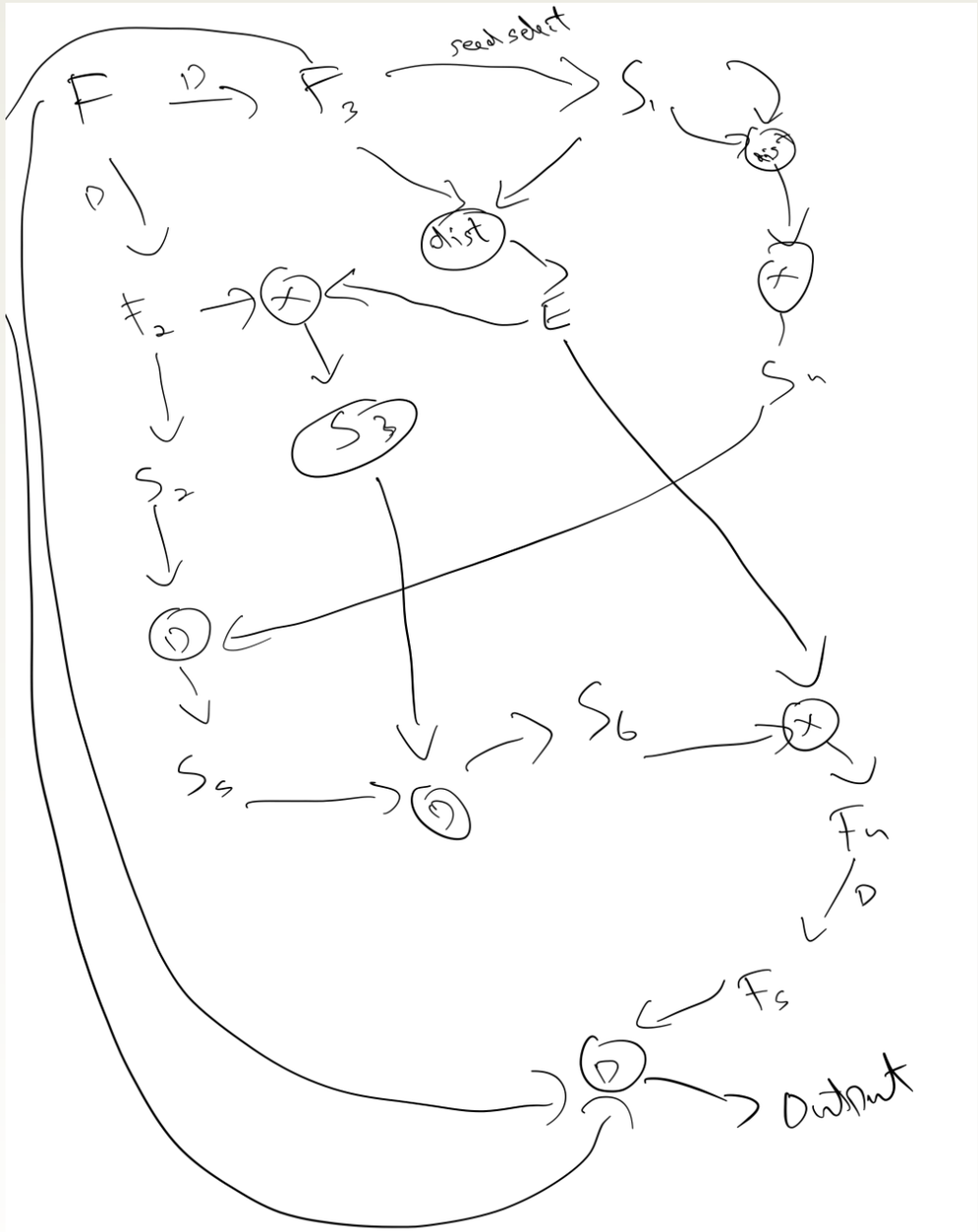
Reference: Wang, Y., Sun, Y., Liu, Z., Sarma, S.E., Bronstein, M.M., Solomon, J.M.: Dynamic Graph CNN for Learning on Point Clouds. ArXiv e-prints (our network is very similar to this)

Graph neural network - Seed based

Each shower has a seed

Define seed as rechit with highest energy (or vertex in terms of graphs)

Complex network



Graph neural network - Seed based

Basic idea: propagate information through seeds

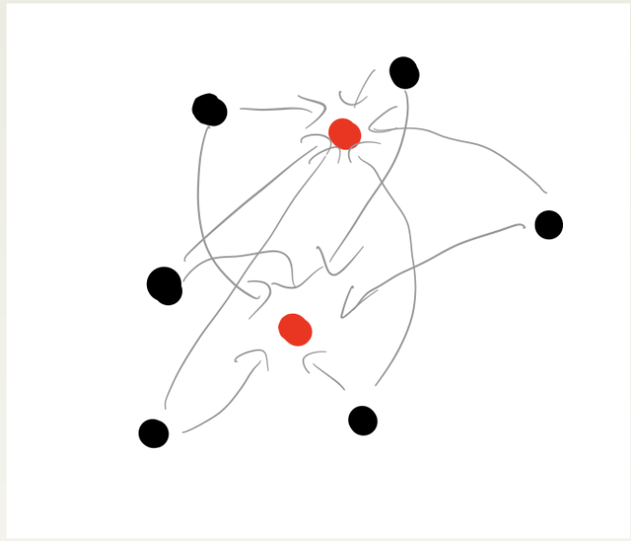
$$v'_s = NN_S(v)$$

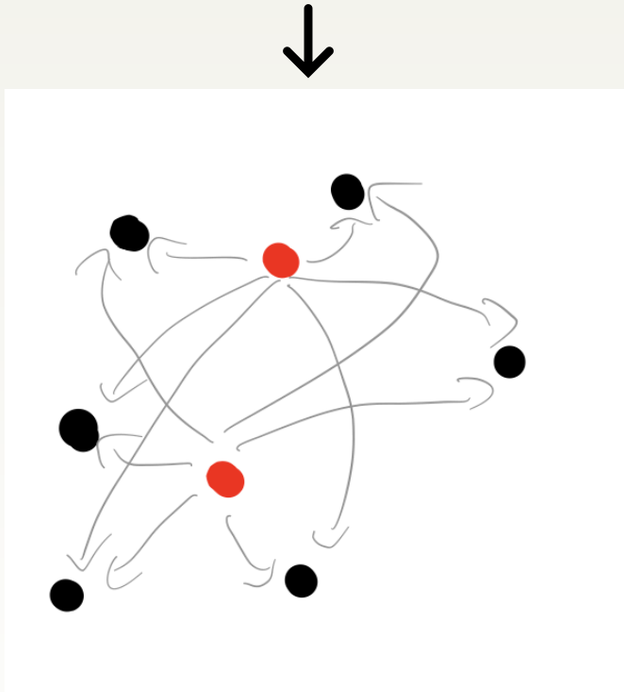
$$v' = NN_F(v)$$

$$e = NN[L_2(v'_s, v_s^{seed}), v'_s - v_s^{seed'}]$$

$$v^{seed''} = NN_c[e \,.\, v', e_s \,.\, v^{seed'}, v^{seed'}]$$

$$v'' = NN_o[v, e \,.\, v^{seed''}]$$





8 layers of previous network

Number of parameters = ~100k

(Another variation: include one random seed in addition)

Results

Test shower:

- Randomly select one of the showers, compute its response

Noise shower

- Shower overlapping with the test shower

$$r_q = \frac{\sum_{s=1}^{N} p_{sq} * e_s}{\sum_{s=1}^{N} t_{sq} * e_s} \qquad q \in \{1,2\}$$

If you test N showers, store N responses in N-d vector **r’**

Results

Mean: (standard statistic)

$$m = \frac{1}{N}\sum_{i}^{N} r'_i$$

Variance: (Standard statistic)

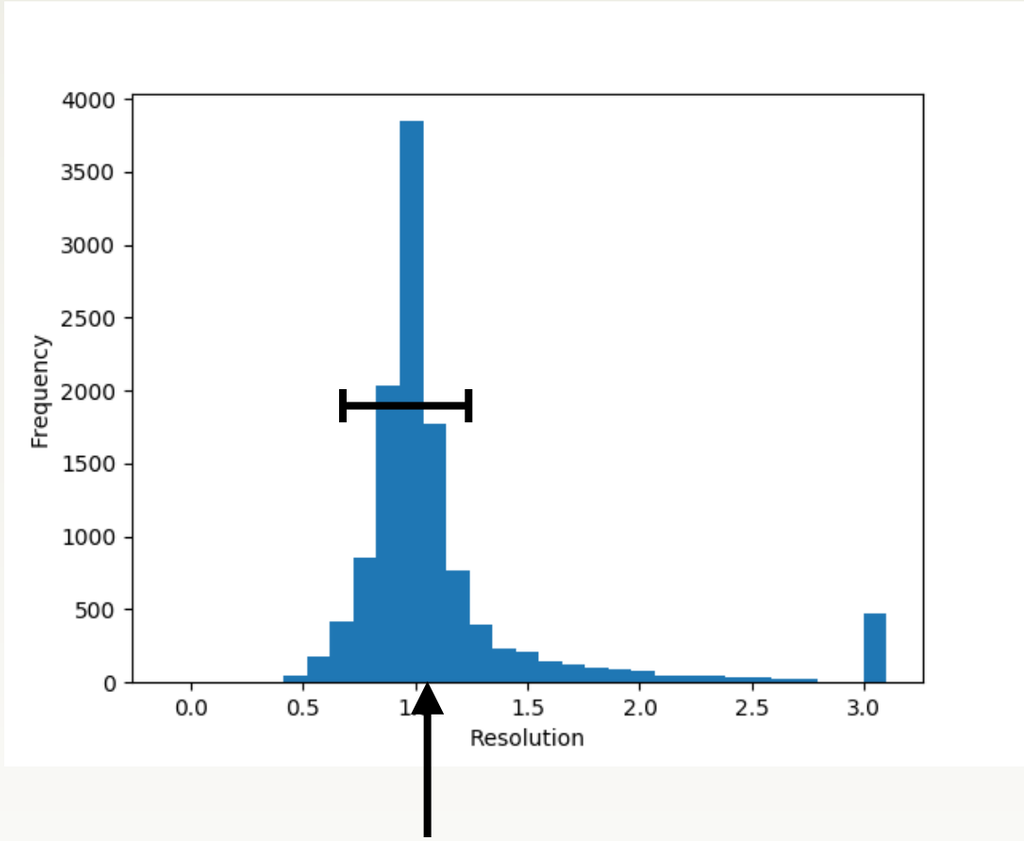
$$v = \frac{1}{N}\sum_{i}^{N} (r'_i - m)^2$$

Variance from 1:

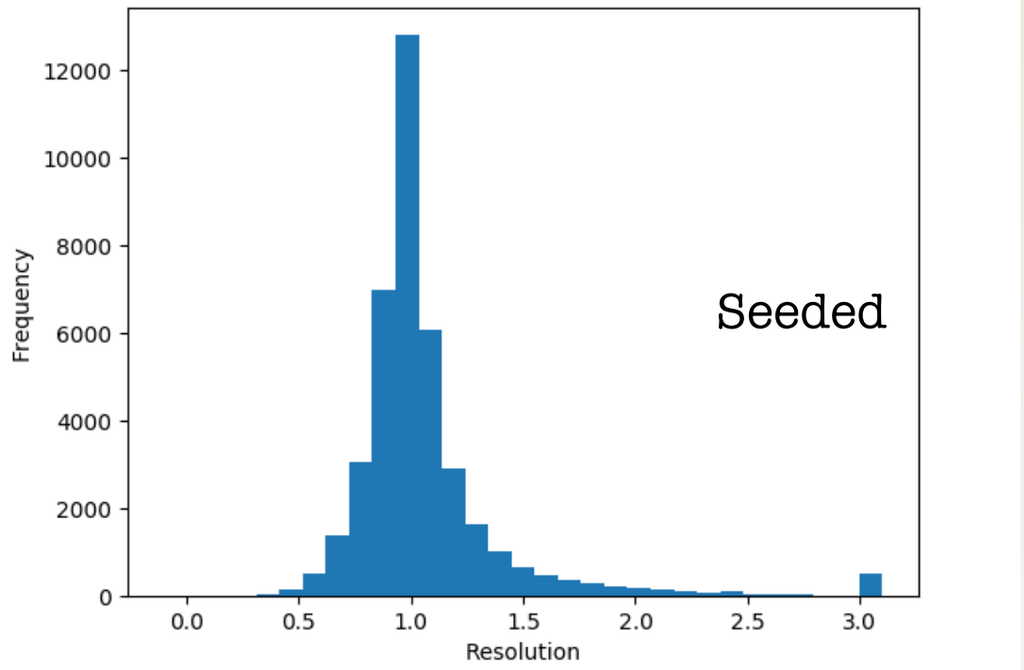
$$v' = \frac{1}{N}\sum_{i}^{N} (r'_i - 1)^2$$

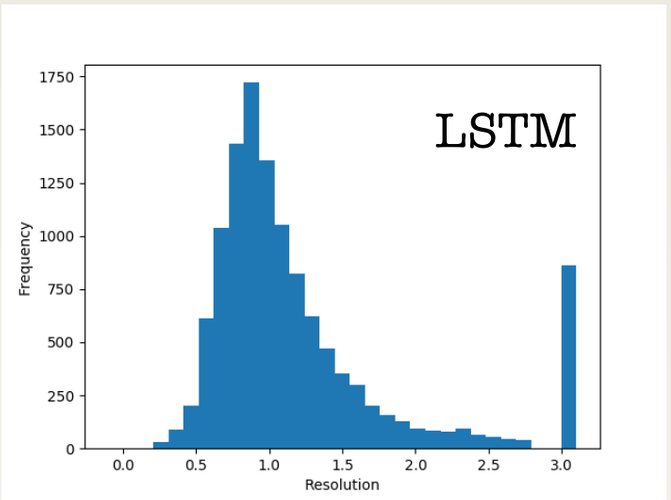
Missed showers fraction:

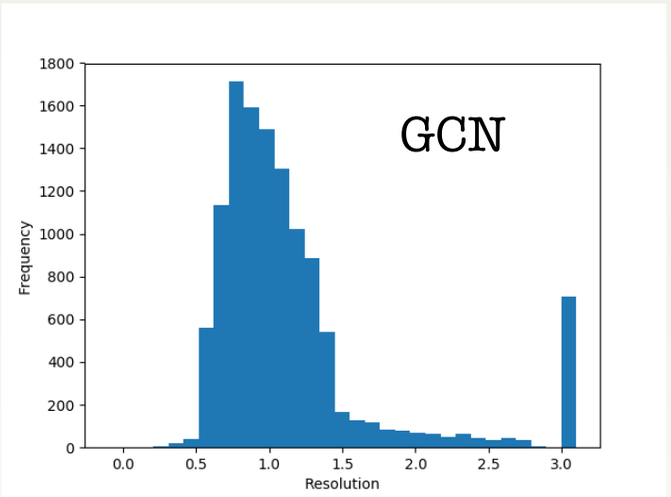
$$q = \frac{|\{r'_i > 1.3\} \cup \{r'_i < 0.7\}|}{|\{\boldsymbol{r}'\}|}$$

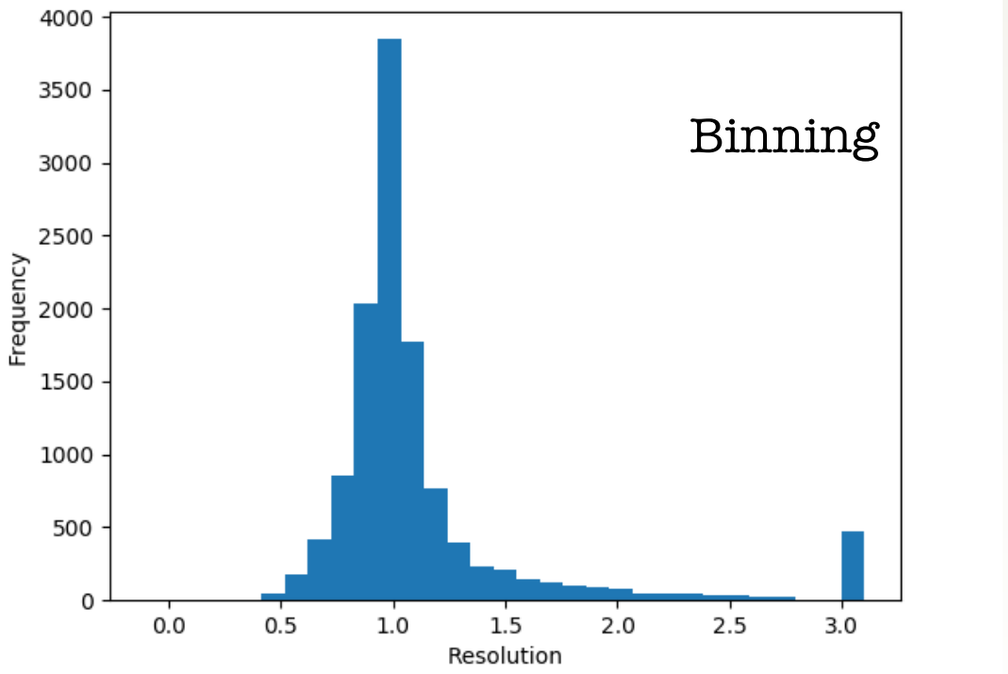


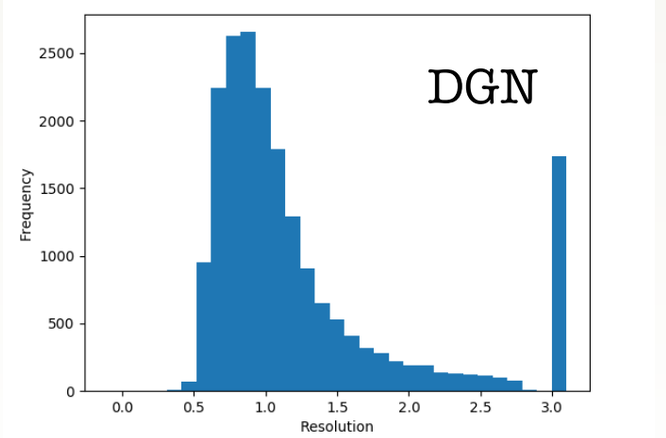
Response histograms



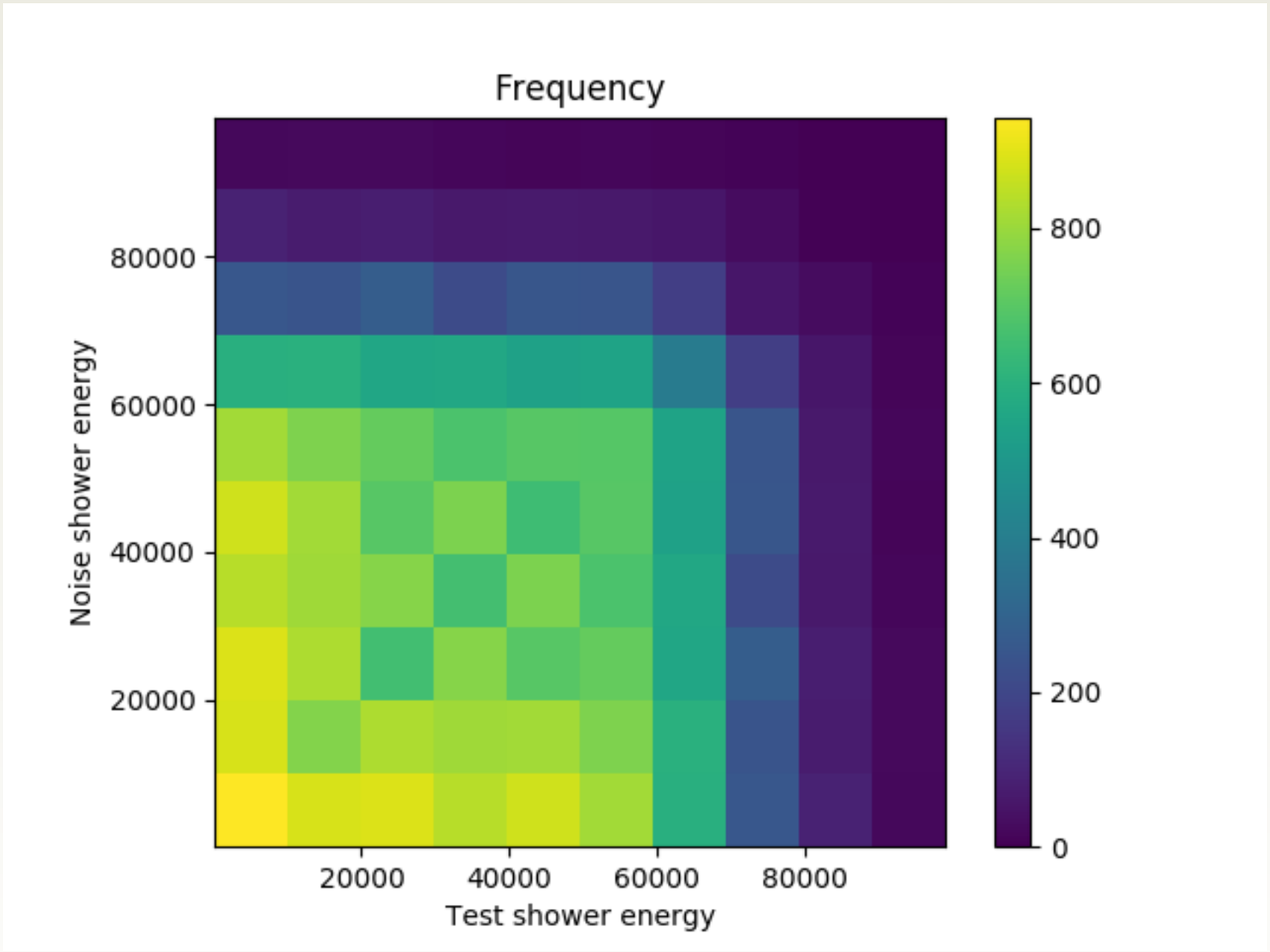




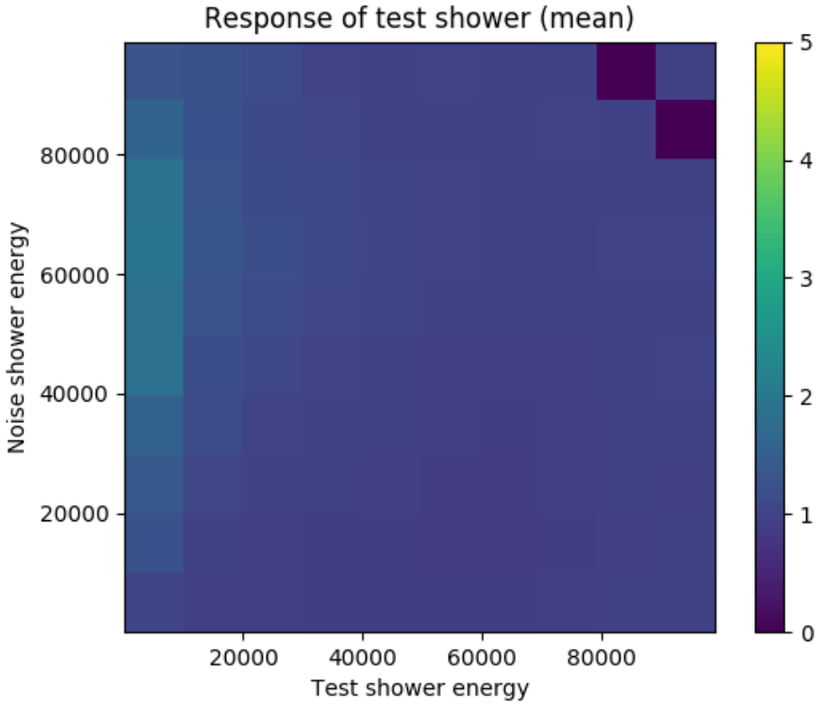




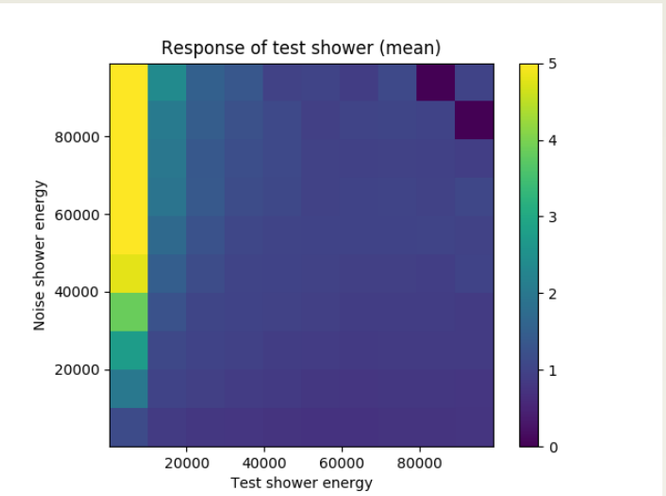
Frequency distribution



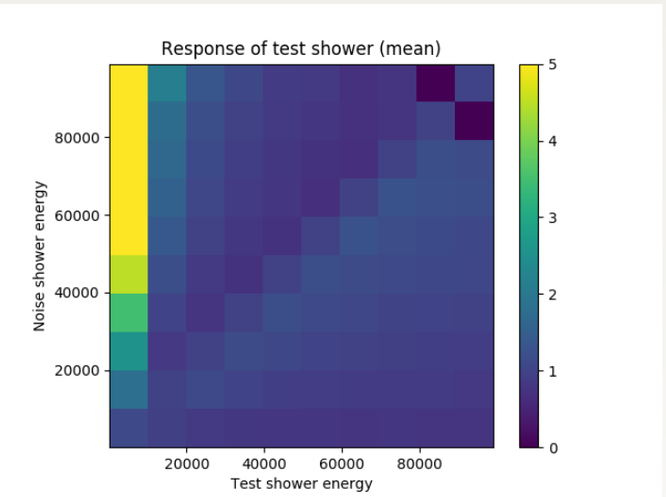
Response (mean)



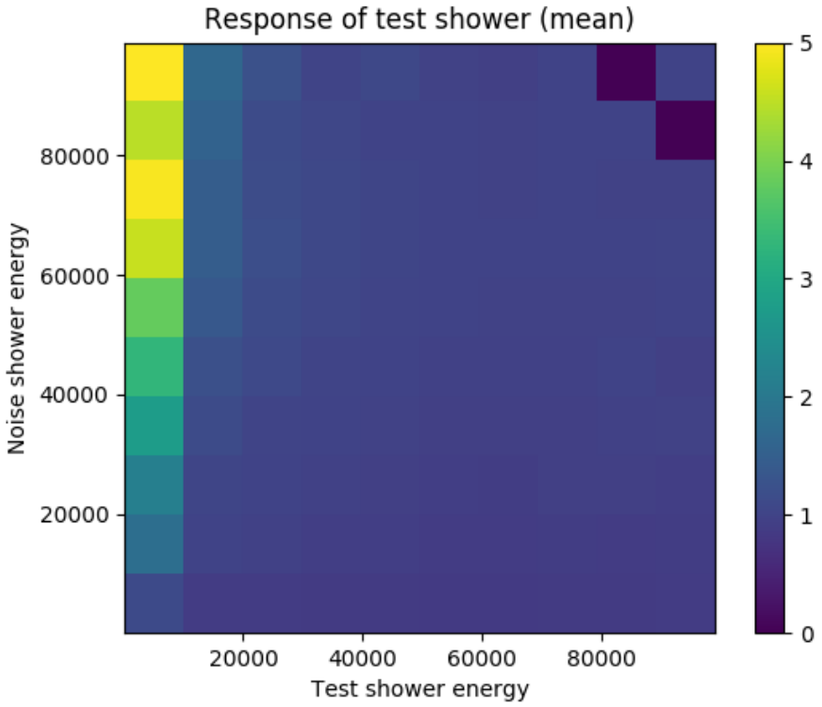
Seeded



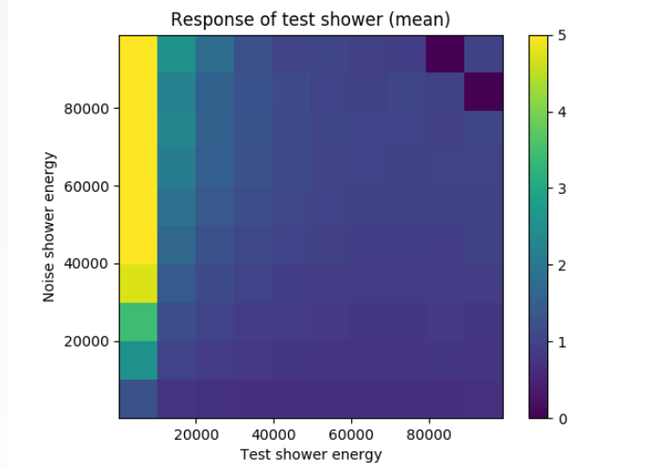
LSTM



GCN

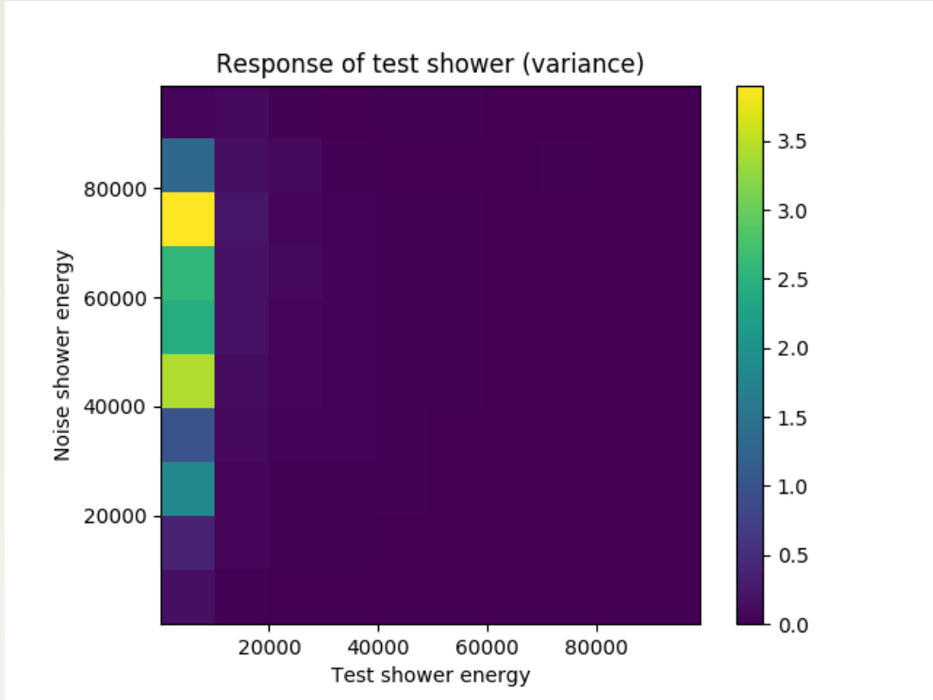


Binning

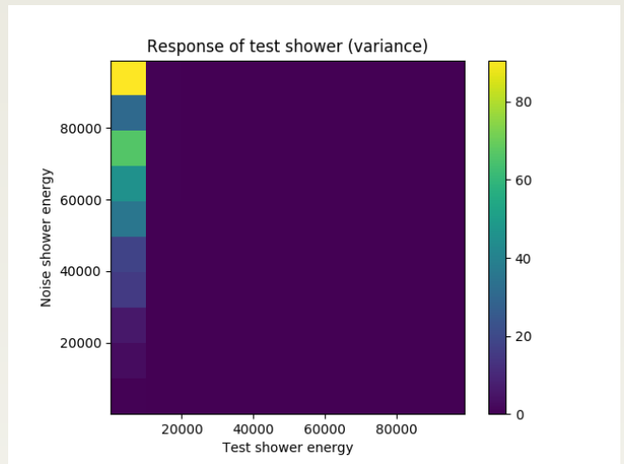


DGN

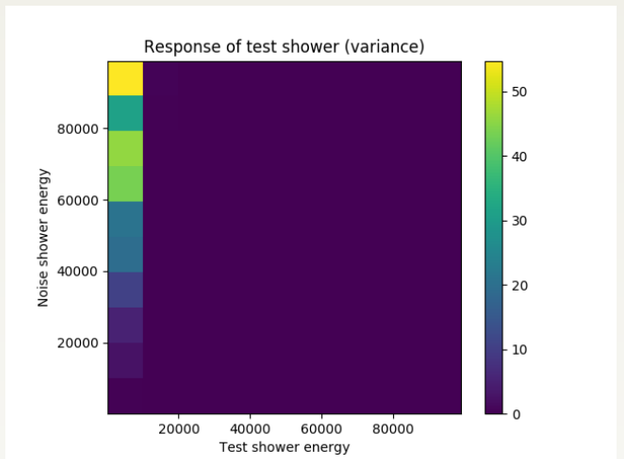
Response (variance)



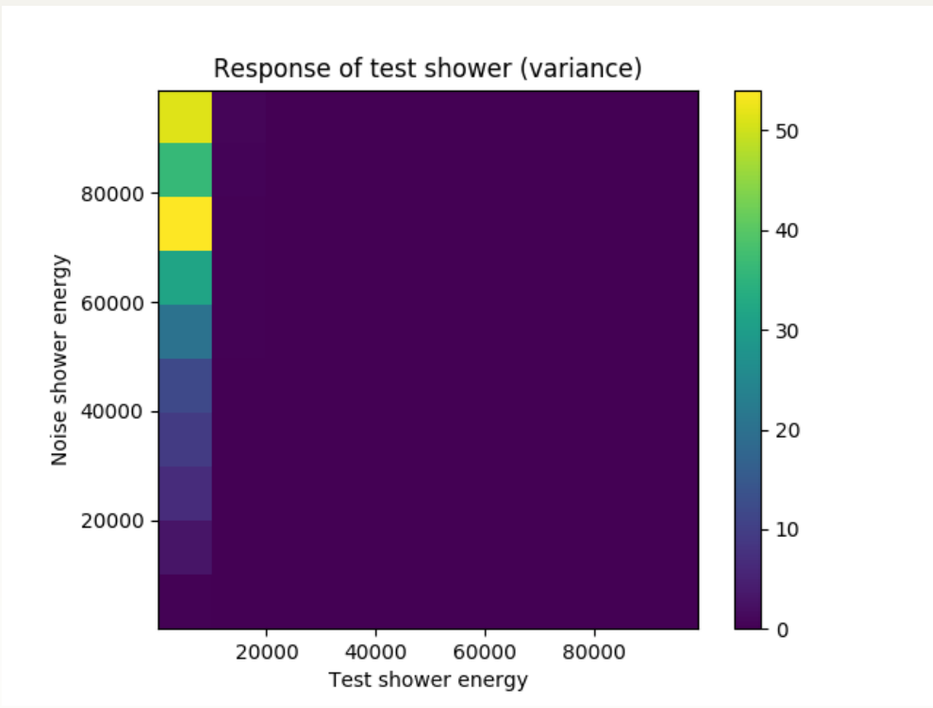
Seeded



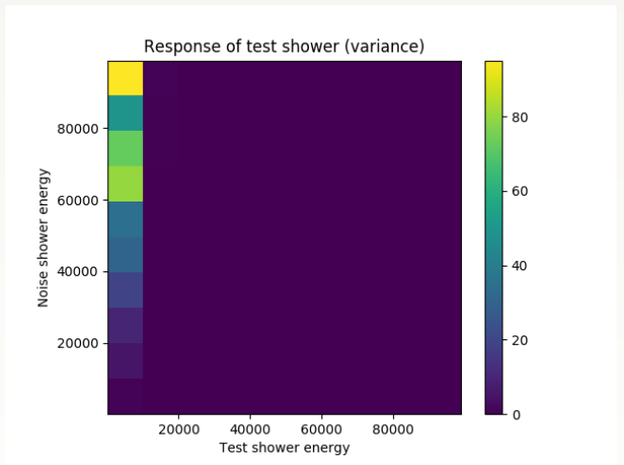
LSTM



GCN

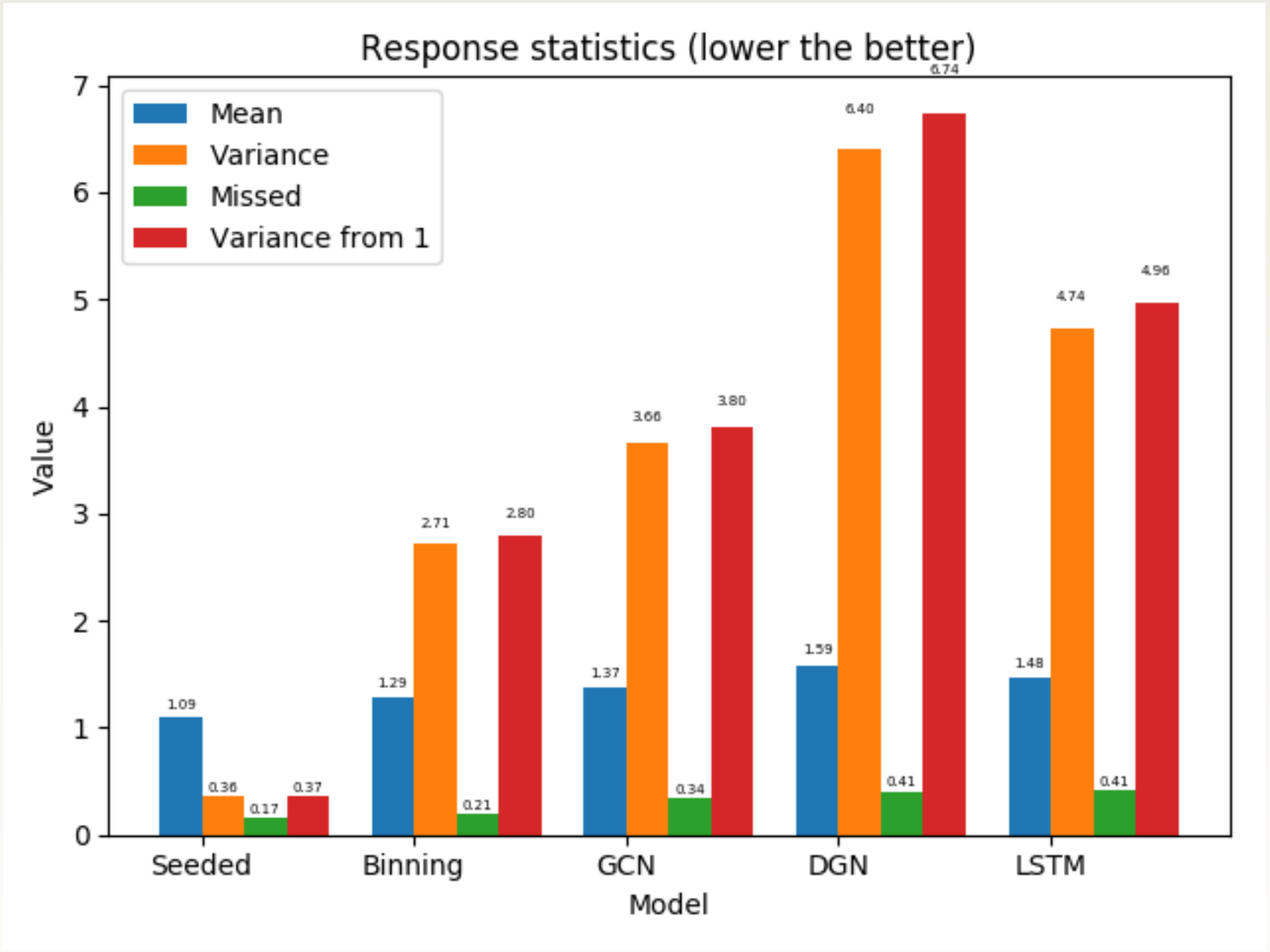


Binning

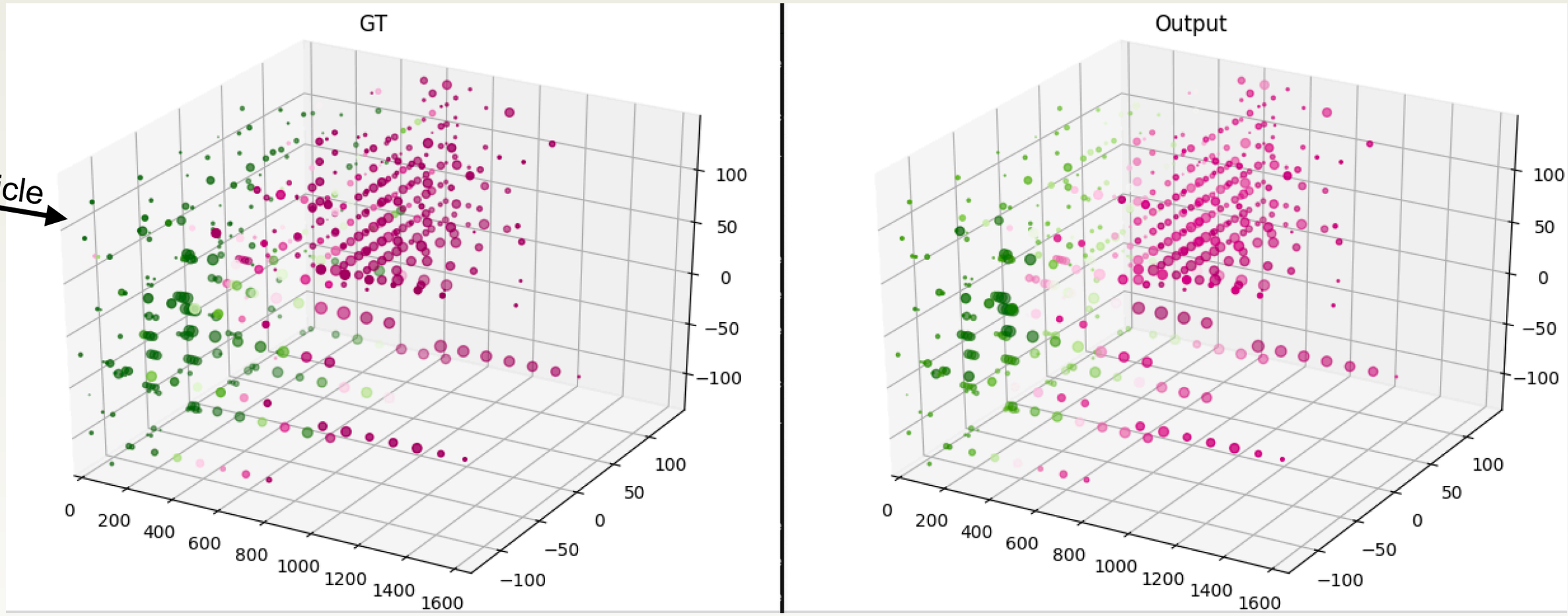


DGN

Results - Summarized



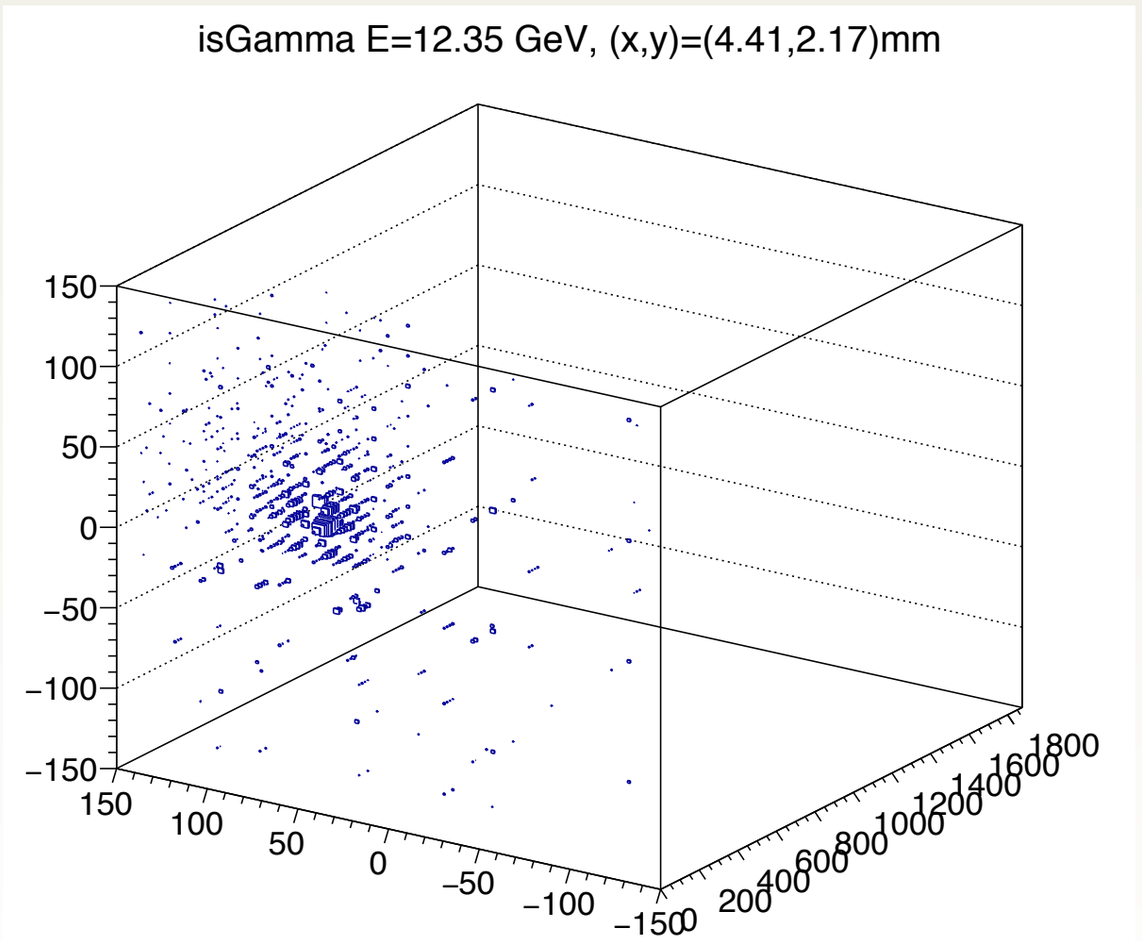
Sample result

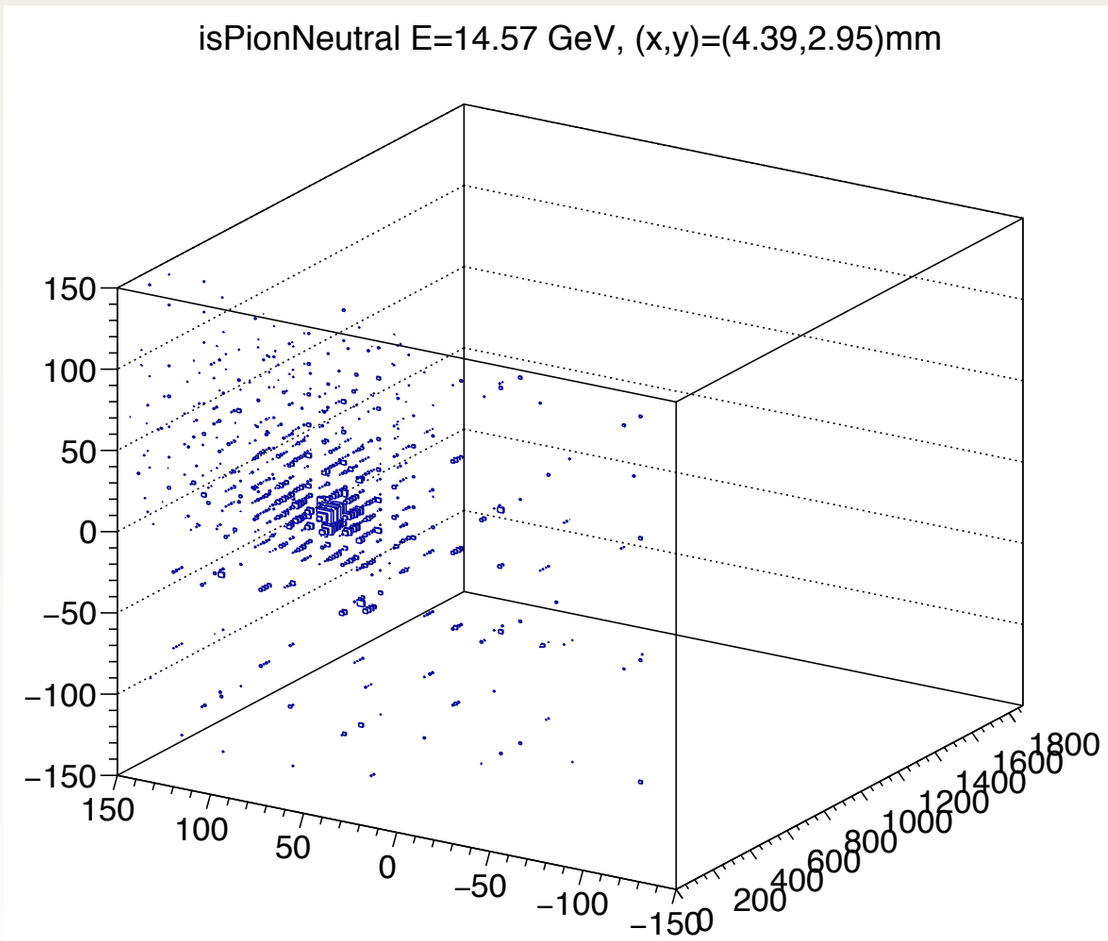


Particle ID

Focus on the most difficult ID problem: γ / π^0

Setup: Single particle, uniform energy distribution 1-100 GeV, uniform position distribution [-5, 5] cm × [-5, 5] cm





Low-energy events in x>0, y>0 quadrature

Starting point - binning method

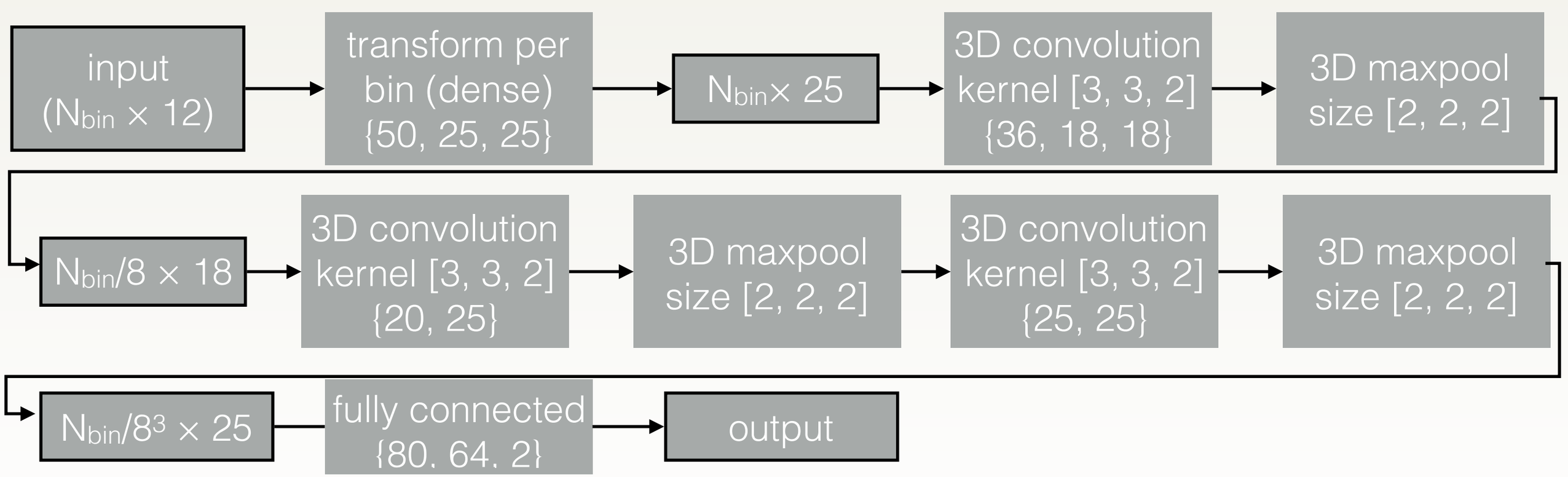
Bin the input space into a grid of 16×16×25

- Bin size 18.75mm in x and y, by layer in z

Each bin contains up to 4 rechits

Bin features: [energy, dx, dy] × 4
dx, dy: relative x and y positions of the hits from the bin center

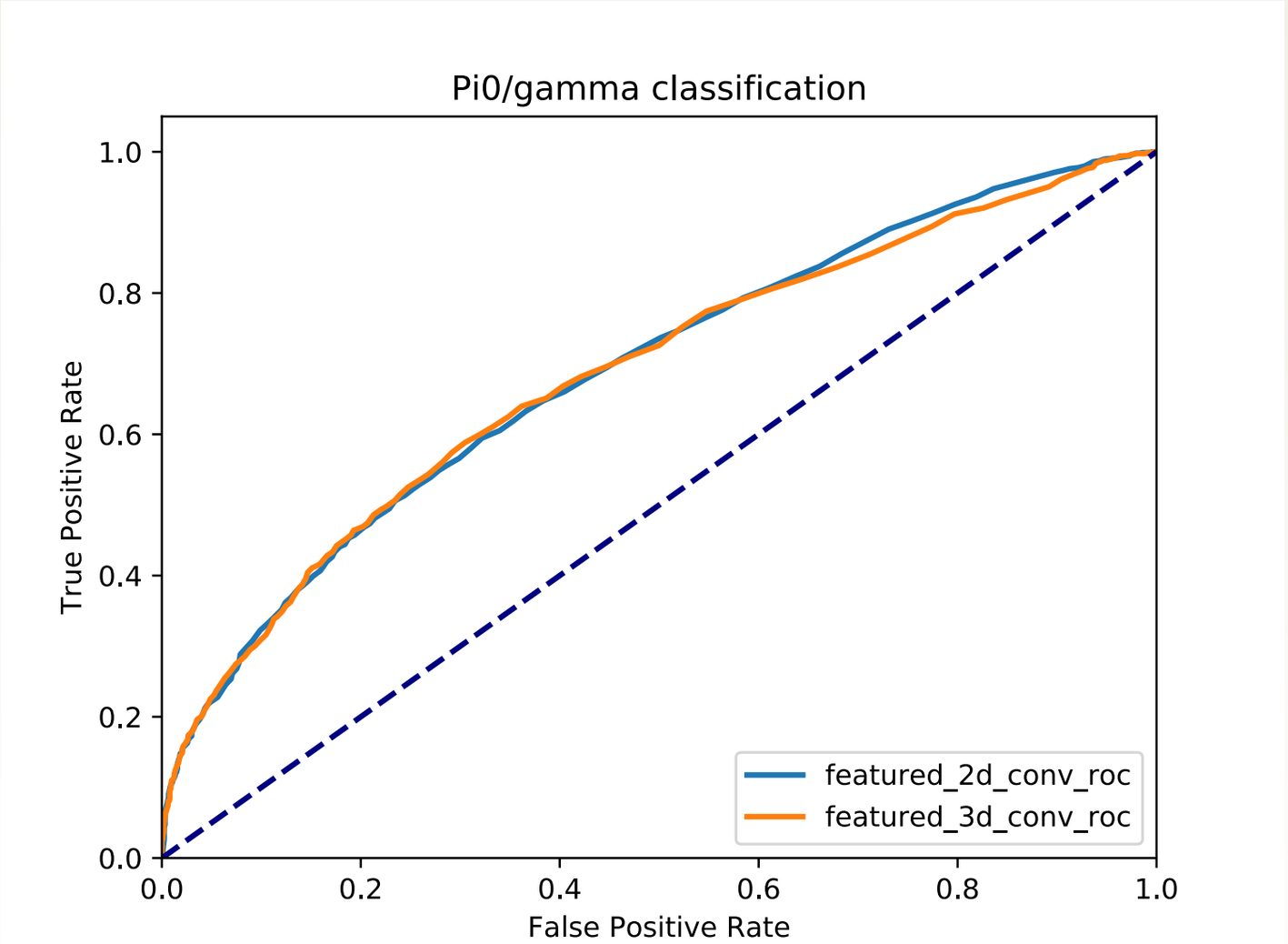
Architecture:



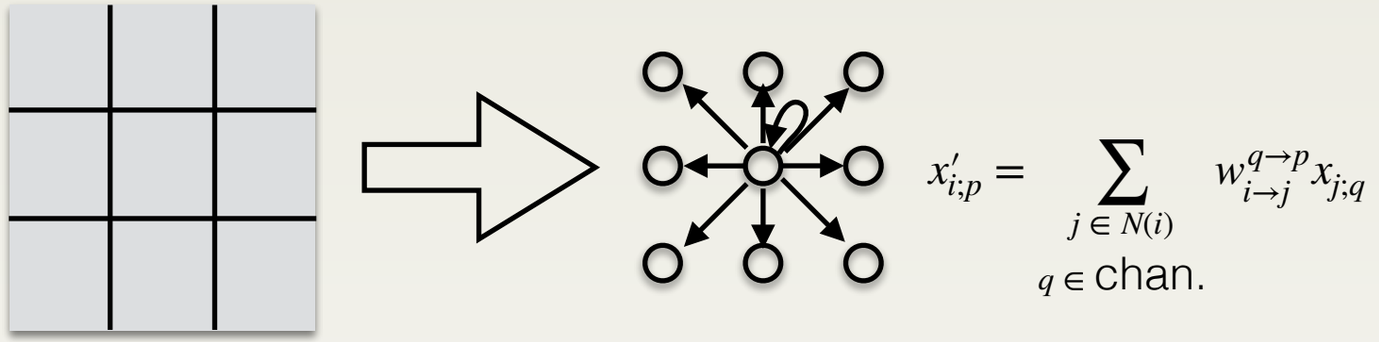
Binning method performance

ROC area-under-curve 0.68

~Identical performance with an alternative architecture based on 2D convolution in xy × dense layer in z

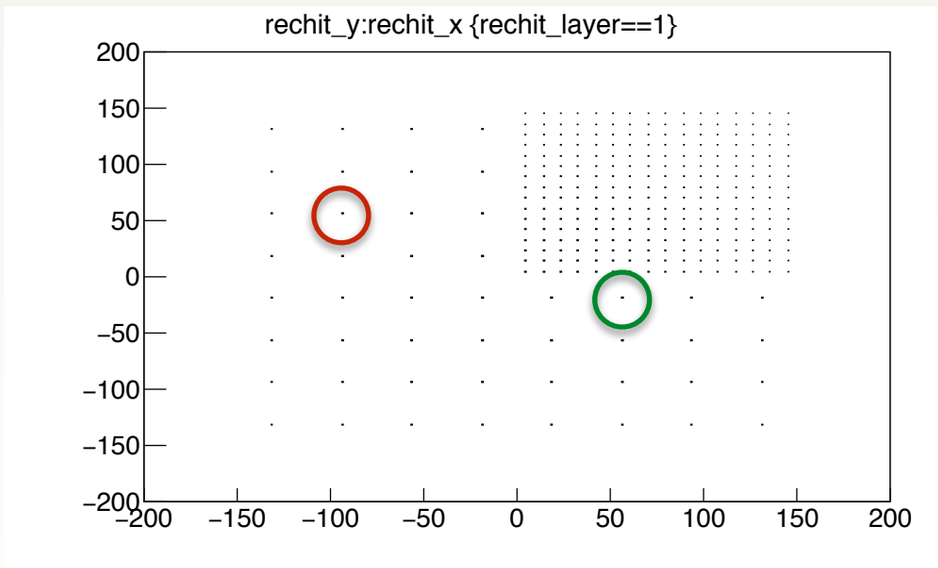


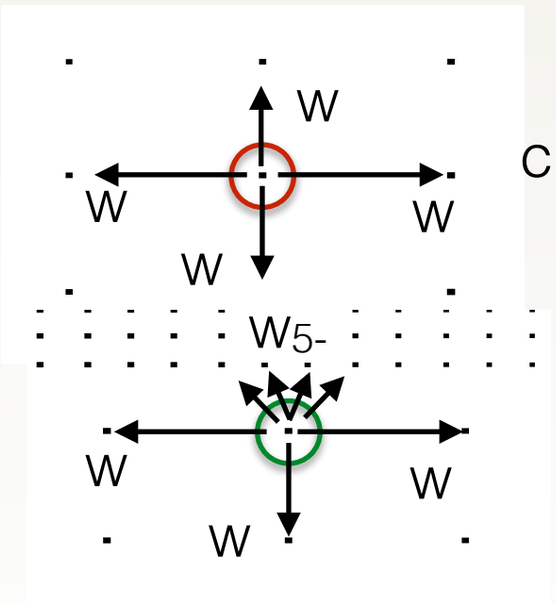
Convolution is a weighted sum over edges of directed graphs



$$x'_{i;p} = \sum_{\substack{j \in N(i) \\ q \in \text{chan.}}} w_{i \to j}^{q \to p} x_{j;q}$$

Generalize: multiple classes of directed graphs from the knowledge of the geometry (weights common within class)



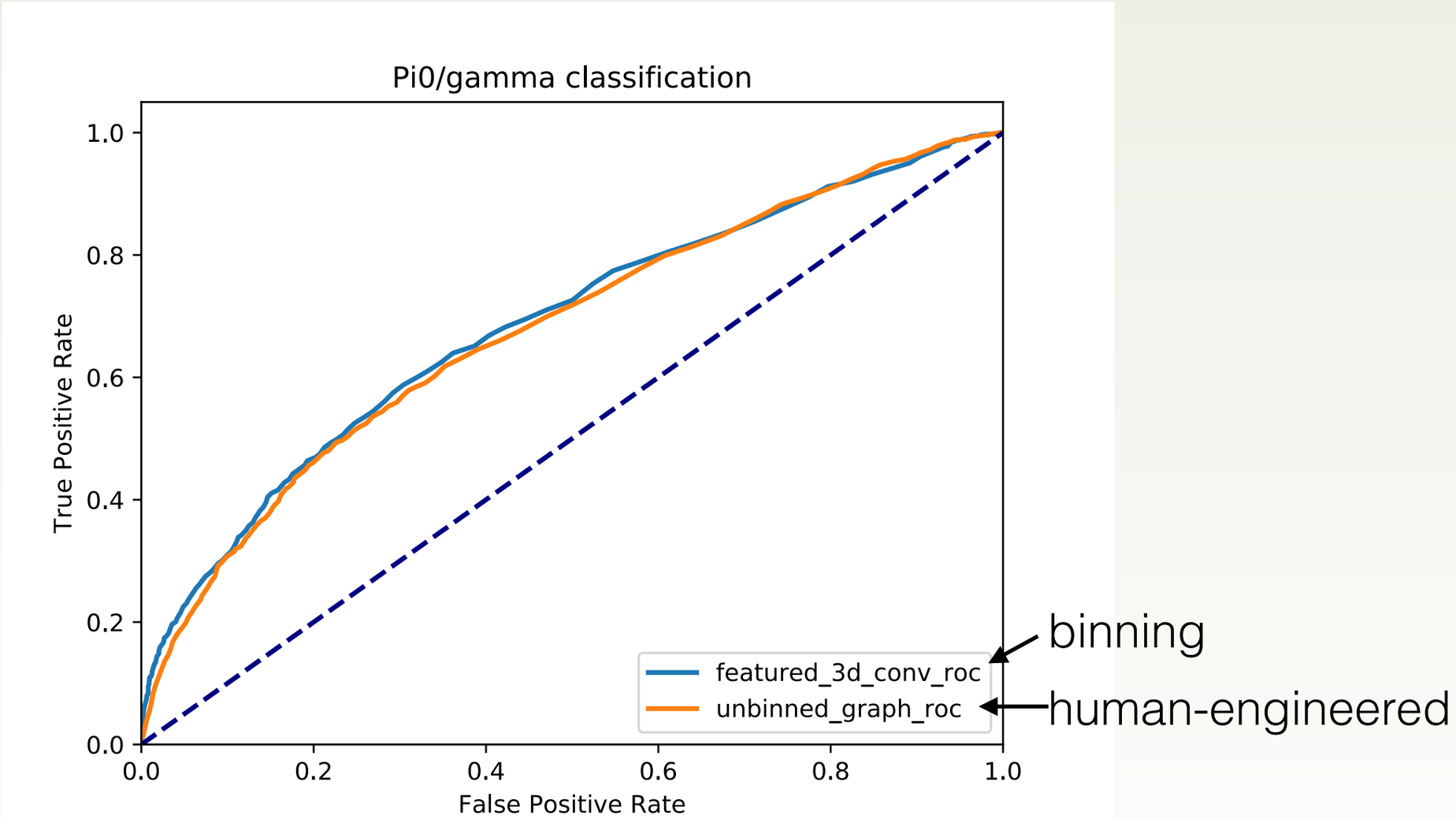


class 1

class 2

Human-engineered adjacency performance

Still ~identical performance (ROCAUC 0.67) to binning method



Summary

DGCNN not training (yet)

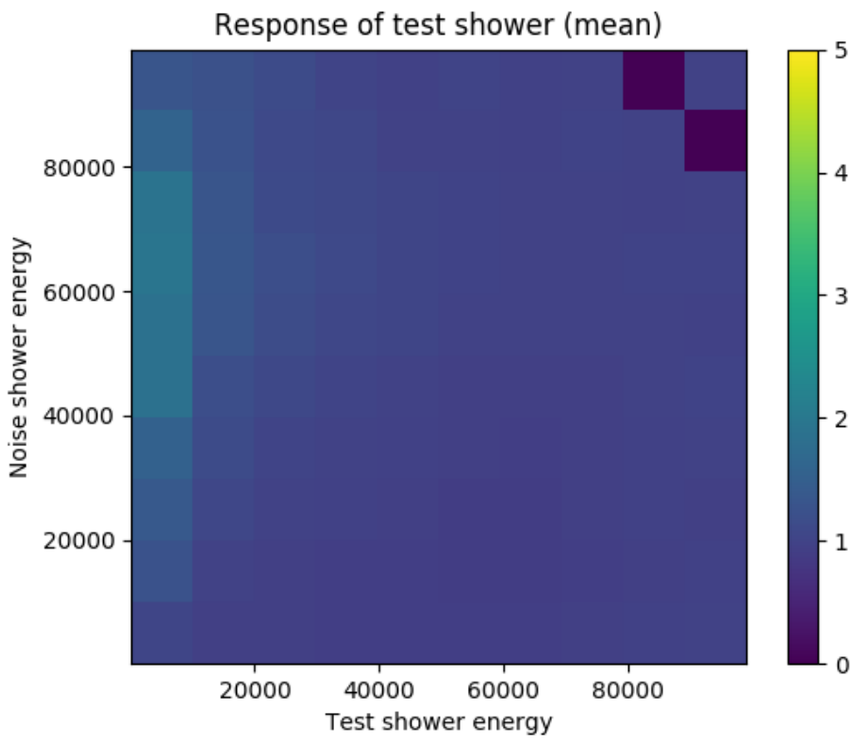
Reason under investigation

Champion: Seeded graph neural network

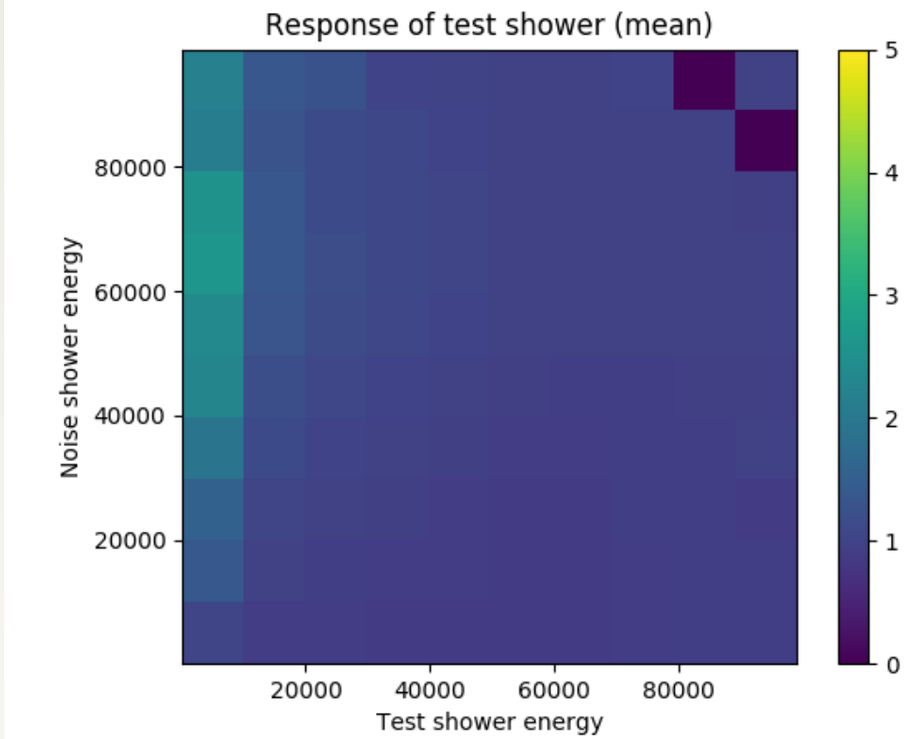
Runner up: Binning based CNN

THE END

Appendex - Comparison with a random seed

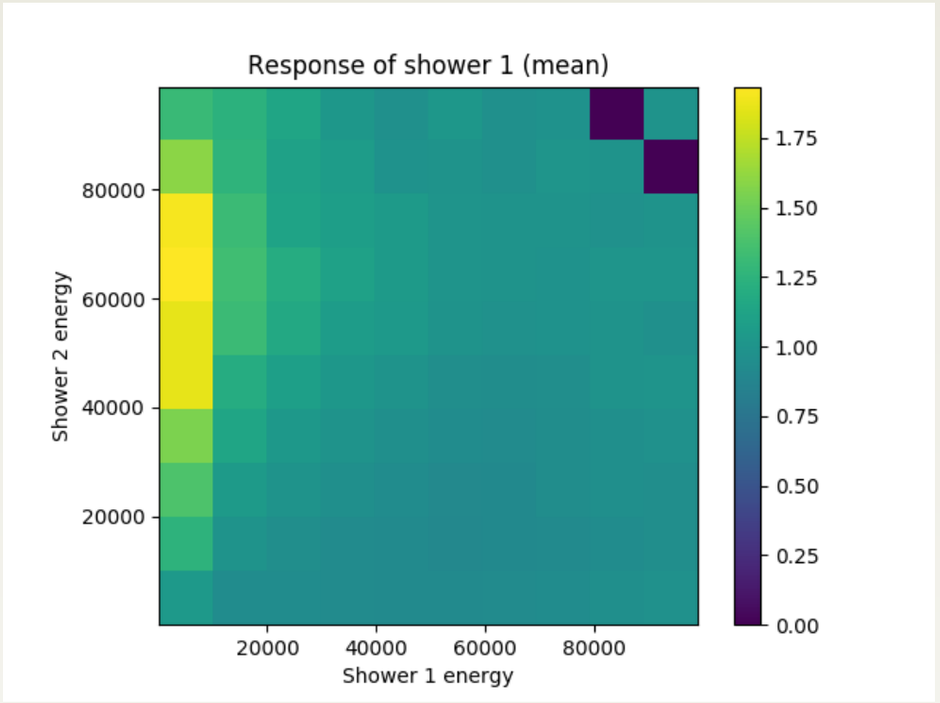


Truth seeds (2 seeds)

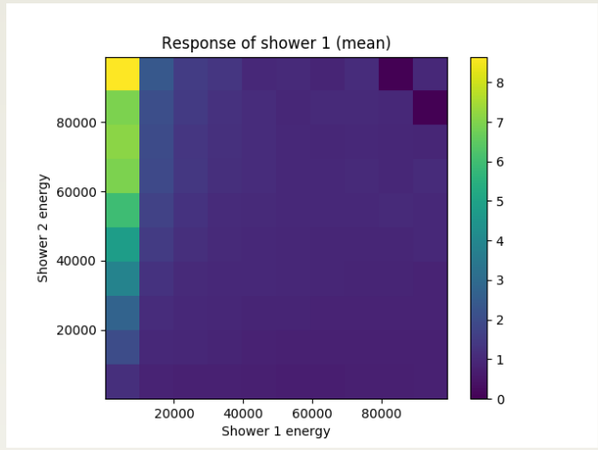


Truth seeds + one random (3 seeds)

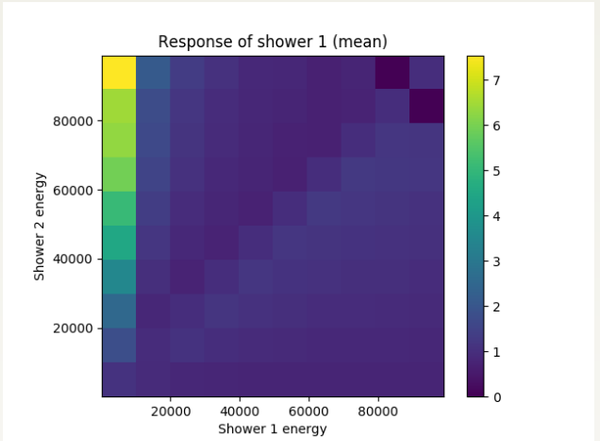
Appendix - Different scales response



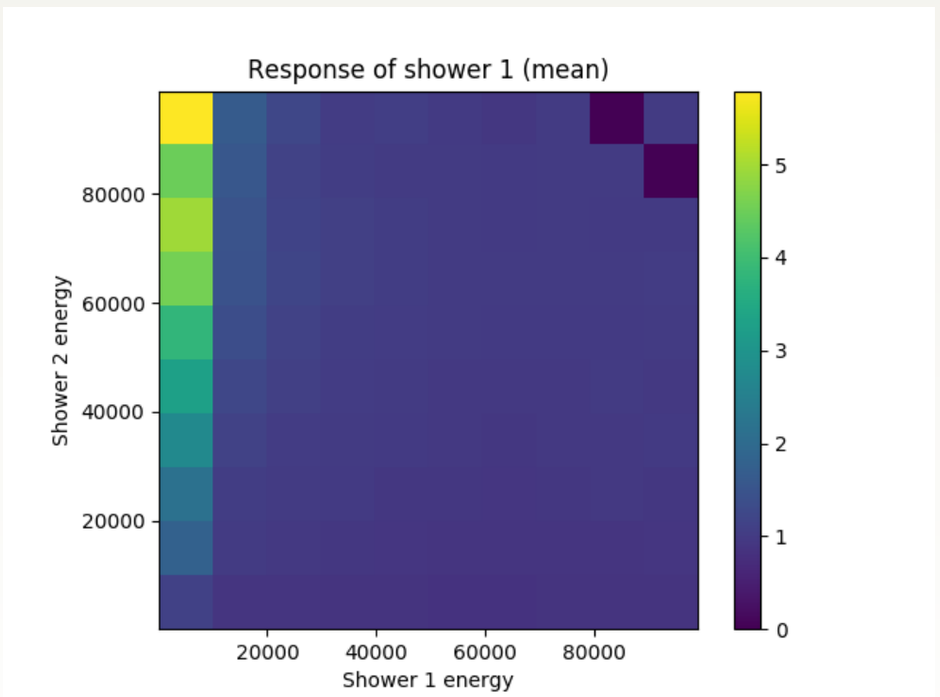
Seeded



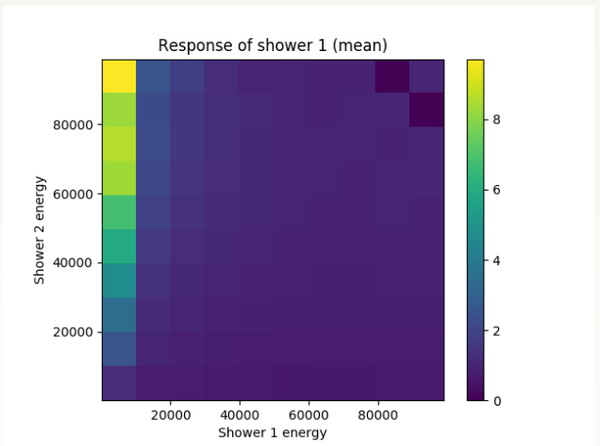
LSTM



GCN



Binning



DGN