

# **Development of the Pytorch Neuro Trigger**

---

Tobias Jülg

07.09.2022

Max Planck Institute for Physics

# Outline

---

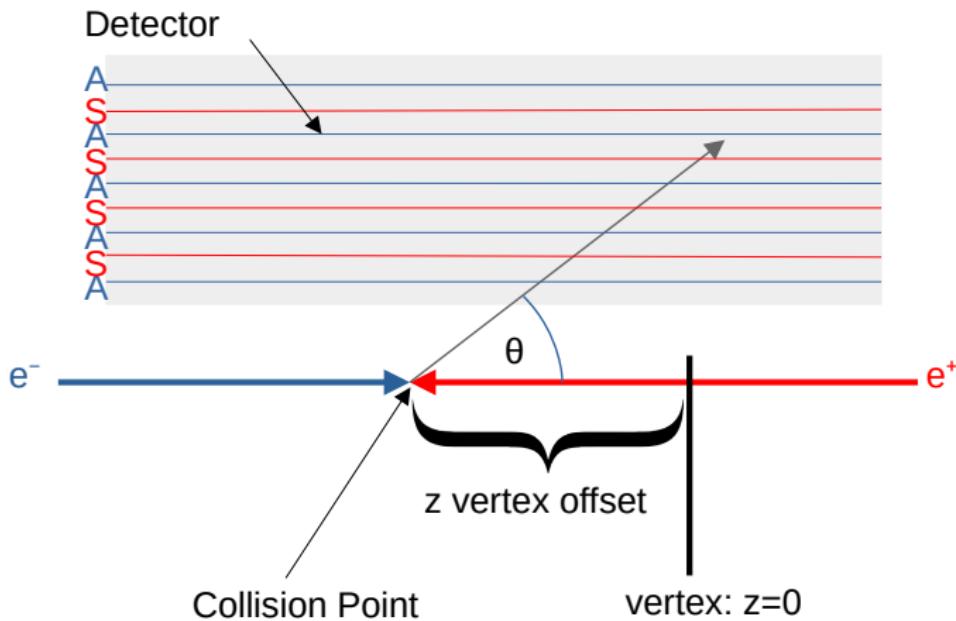
1. Introduction
2. Motivation
3. Configuration and Training
4. Extensibility
5. Feed-down Problem and Reweighting
6. Results

# Introduction

---

# What do we want to predict?

- $z$ -vertex
- $\theta$  angle
- Detector: 5 axial and 4 stereo superlayers

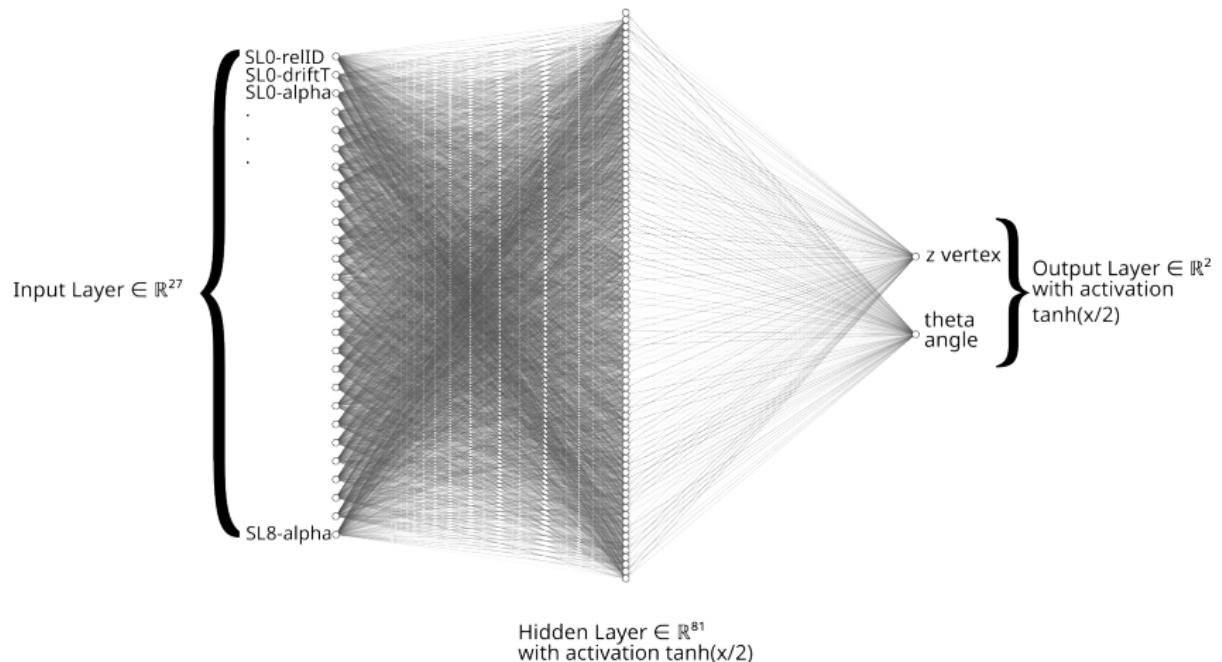


## How to predict $z$ and $\theta$ ?

*Neural Network* for  $z$  and  $\theta$  prediction of the  $e^+e^-$  collision

- Input: 9 layers with
  - SLx-relID: Angle relative to 2D track  $\phi$
  - SLx-driftT: Drift time
  - SLx-alpha: Crossing angle  $\alpha$ $\rightarrow \mathbb{R}^{27}$
- Output:
  - Collision's z-vertex
  - $\theta$  angle of the resulting particle $\rightarrow \mathbb{R}^2$
- One hidden layer with 81 neurons
- $\tanh\left(\frac{x}{2}\right)$  as activation function

# Network Architecture



## Motivation

---

## Motivation

Why was it neccessary to replace the old BASF2 FANN network training?

## Motivation

Why was it necessary to replace the old BASF2 FANN network training?

- FANN uses training and optimization algorithms from the 90's

# Motivation

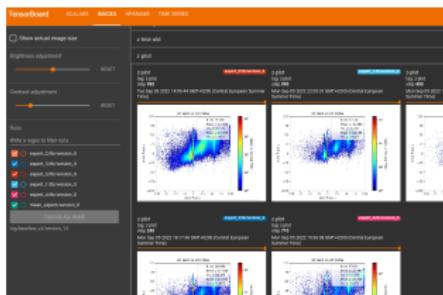
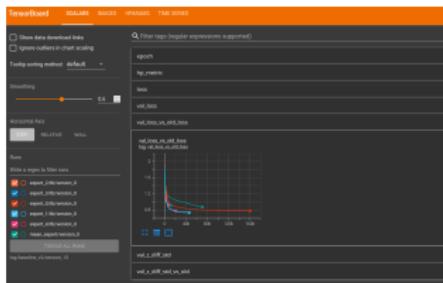
Why was it necessary to replace the old BASF2 FANN network training?

- FANN uses training and optimization algorithms from the 90's
- Improved algorithms in PyTorch
  - Stochastical gradient descent
  - Modern weight optimizer: Adam
  - L2 regularization / weight decay
  - Sophisticated random weight initialization strategies

# Motivation

Why was it necessary to replace the old BASF2 FANN network training?

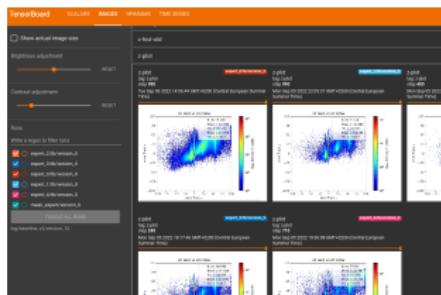
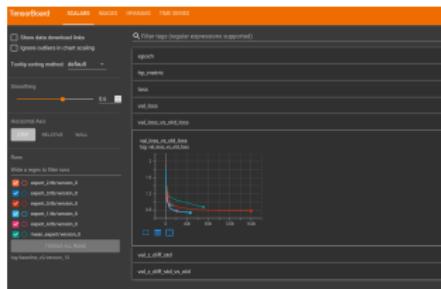
- FANN uses training and optimization algorithms from the 90's
- Improved algorithms in PyTorch
  - Stochastical gradient descent
  - Modern weight optimizer: Adam
  - L2 regularization / weight decay
  - Sophisticated random weight initialization strategies
- Live graphical training supervision through tensorboard



## Motivation

Why was it necessary to replace the old BASF2 FANN network training?

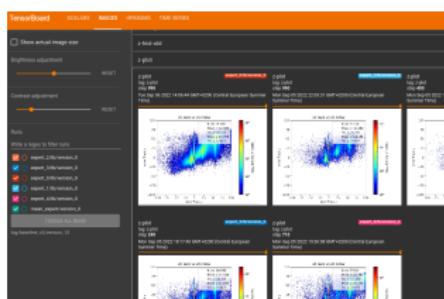
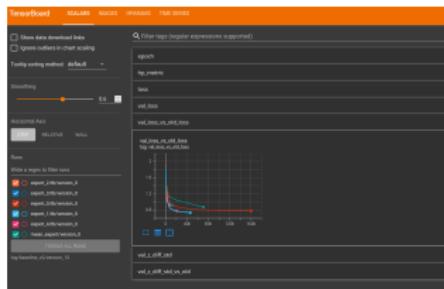
- FANN uses training and optimization algorithms from the 90's
  - Improved algorithms in PyTorch
    - Stochastical gradient descent
    - Modern weight optimizer: Adam
    - L2 regularization / weight decay
    - Sophisticated random weight initialization strategies
  - Live graphical training supervision through tensorboard
  - Modular and decoupled from BASF2



# Motivation

Why was it necessary to replace the old BASF2 FANN network training?

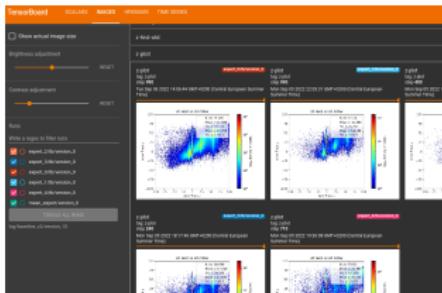
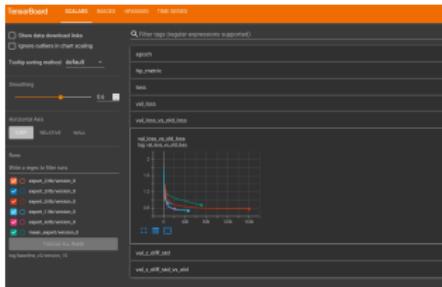
- FANN uses training and optimization algorithms from the 90's
- Improved algorithms in PyTorch
  - Stochastical gradient descent
  - Modern weight optimizer: Adam
  - L2 regularization / weight decay
  - Sophisticated random weight initialization strategies
- Live graphical training supervision through tensorboard
- Modular and decoupled from BASF2
- Flexible configuration which does not require code changes to test different hyperparameter settings



# Motivation

Why was it necessary to replace the old BASF2 FANN network training?

- FANN uses training and optimization algorithms from the 90's
- Improved algorithms in PyTorch
  - Stochastical gradient descent
  - Modern weight optimizer: Adam
  - L2 regularization / weight decay
  - Sophisticated random weight initialization strategies
- Live graphical training supervision through tensorboard
- Modular and decoupled from BASF2
- Flexible configuration which does not require code changes to test different hyperparameter settings
- Reproducability build-in through extensive logging



## **Configuration and Training**

---

# Folder Structure

nnt-pytorch

- changelog.md
- docs
  - class.diagram.dia
  - class.diagram.png
  - class.diagram.svg
  - norm\_inf\_bounds.png
  - norm\_non\_inf\_bounds.png
  - uniform.png
  - zhist.png
- README.md
- requirements.txt
- neuro\_trigger
  - configs.py
  - \_\_init\_\_.py

neuro\_trigger

- lightning
  - \_\_init\_\_.py
  - mean\_tb\_logger.py
  - pl\_module.py
- main.py
- pytorch
  - \_\_init\_\_.py
  - dataset\_filters.py
  - dataset.py
  - model.py
- tests
  - \_\_init\_\_.py
  - test\_data.csv
  - test\_data\_filter.csv
  - test.py
- utils.py
- visualize.py

## Configure a Training

Trainings are configured in a python dictionary in  
neuro\_trigger/config.py

- All training hyperparameter can be configured like learning rate, batch size, optimizer, network model, ... <sup>1</sup>
- Supports configurations inheritance
- Global hyperparameters vs per-expert hyperparameters
- Hierarchical: Flexible and extensible scheme

---

<sup>1</sup>Extensive list can be found in the README.md documentation

# Configure a Training: Example

Base config to set default parameters:

```
"base": {  
    "version": 1.0,  
    "description": "Some desc.",  
    "learning_rate": 1e-3,  
    "batch_size": 2048,  
    "weight_decay": 1e-6,  
    "in_size": 27,  
    "out_size": 2,  
    "workers": 5,  
    "epochs": 10,  
    "model": "BaselineModel",  
    "loss": "MSELoss",  
    "optim": "Adam",  
    "act": "tanh",  
    "experts": [0, 1, 2, 3, 4],  
    "compare_to": None,  
    "load_pre_trained_weights":  
        None,  
}
```

# Configure a Training: Example

Base config to set default parameters:

```
"base": {  
    "version": 1.0,  
    "description": "Some desc.",  
    "learning_rate": 1e-3,  
    "batch_size": 2048,  
    "weight_decay": 1e-6,  
    "in_size": 27,  
    "out_size": 2,  
    "workers": 5,  
    "epochs": 10,  
    "model": "BaselineModel",  
    "loss": "MSELoss",  
    "optim": "Adam",  
    "act": "tanh",  
    "experts": [0, 1, 2, 3, 4],  
    "compare_to": None,  
    "load_pre_trained_weights":  
        None,  
}
```

Advanced config which inherits from base:

```
"my_base_extension": {  
    "extends": "base",  
    "description": "My ext.",  
    "act": "tanh/2",  
    "epochs": 1000,  
    "expert_3": {  
        "batch_size": 128,  
        "epochs": 2000,  
    },  
    "expert_4": {  
        "batch_size": 16,  
        "epochs": 4000,  
    },  
    "compare_to":  
        "base/version_4",  
}
```

# Training CLI

To start a training the neuro\_trigger/main.py CLI has to be used:

```
usage: main.py [-h] [-p] [-s] mode
```

Tool to start the neuro trigger training.

positional arguments:

mode	Config mode to use, must be defined in config.py
------	---

optional arguments:

-h, --help	show this help message and exit
-p, --production	If the flag is not given code will run in debug mode otherwise production mode
-s, --solo_expert	Whether one or several experts are used for training

## Start Training and Tensorboard

- Start a production training

```
source venv/bin/activate
export PYTHONPATH="$PYTHONPATH:."
python neuro_trigger/main.py my_base_extension -p
```

## Start Training and Tensorboard

- Start a production training

```
source venv/bin/activate
export PYTHONPATH="$PYTHONPATH:."
python neuro_trigger/main.py my_base_extension -p
```

- View the log path

```
cat log/log.txt
```

# Start Training and Tensorboard

- Start a production training

```
source venv/bin/activate
export PYTHONPATH="$PYTHONPATH:."
python neuro_trigger/main.py my_base_extension -p
```

- View the log path

```
cat log/log.txt
```

- Start Tensorboard

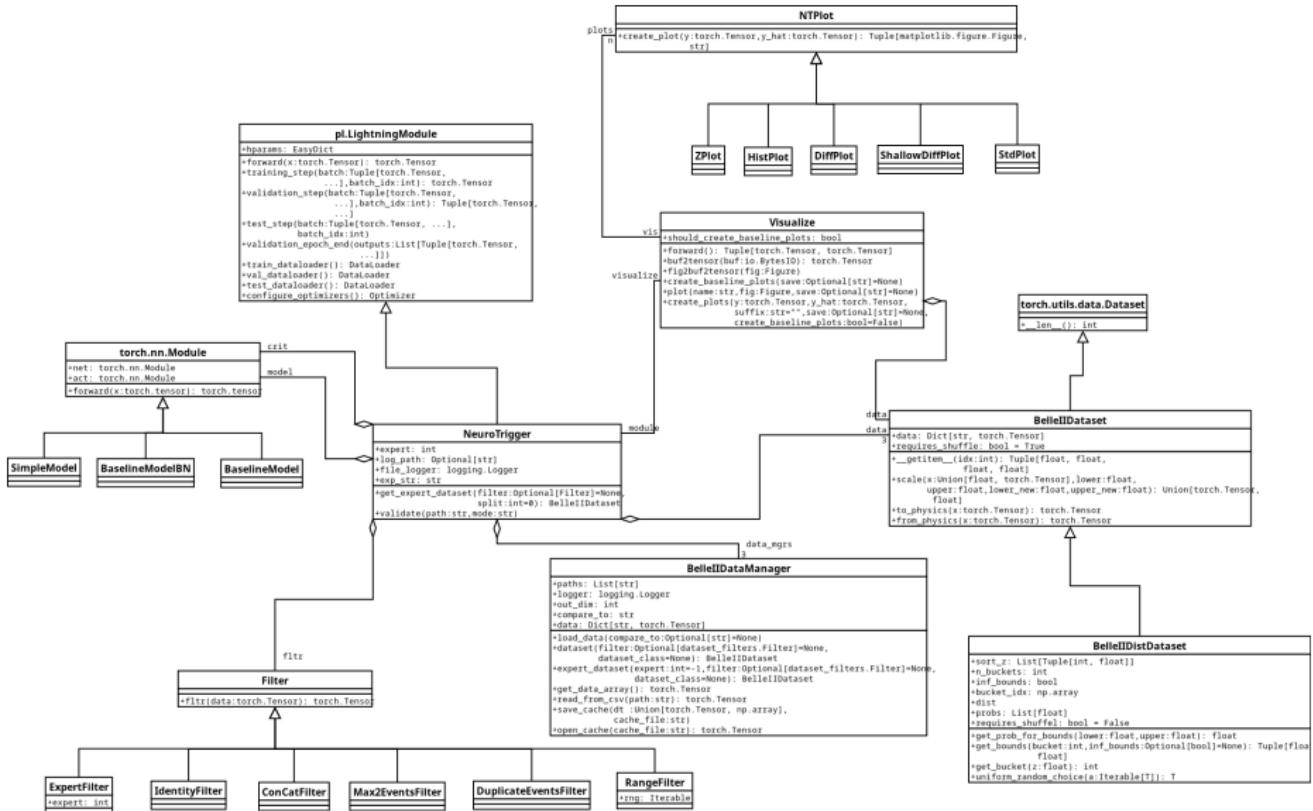
```
tensorboard --logdir=log/my_base_extension/
version_0
```

# Live Demo!

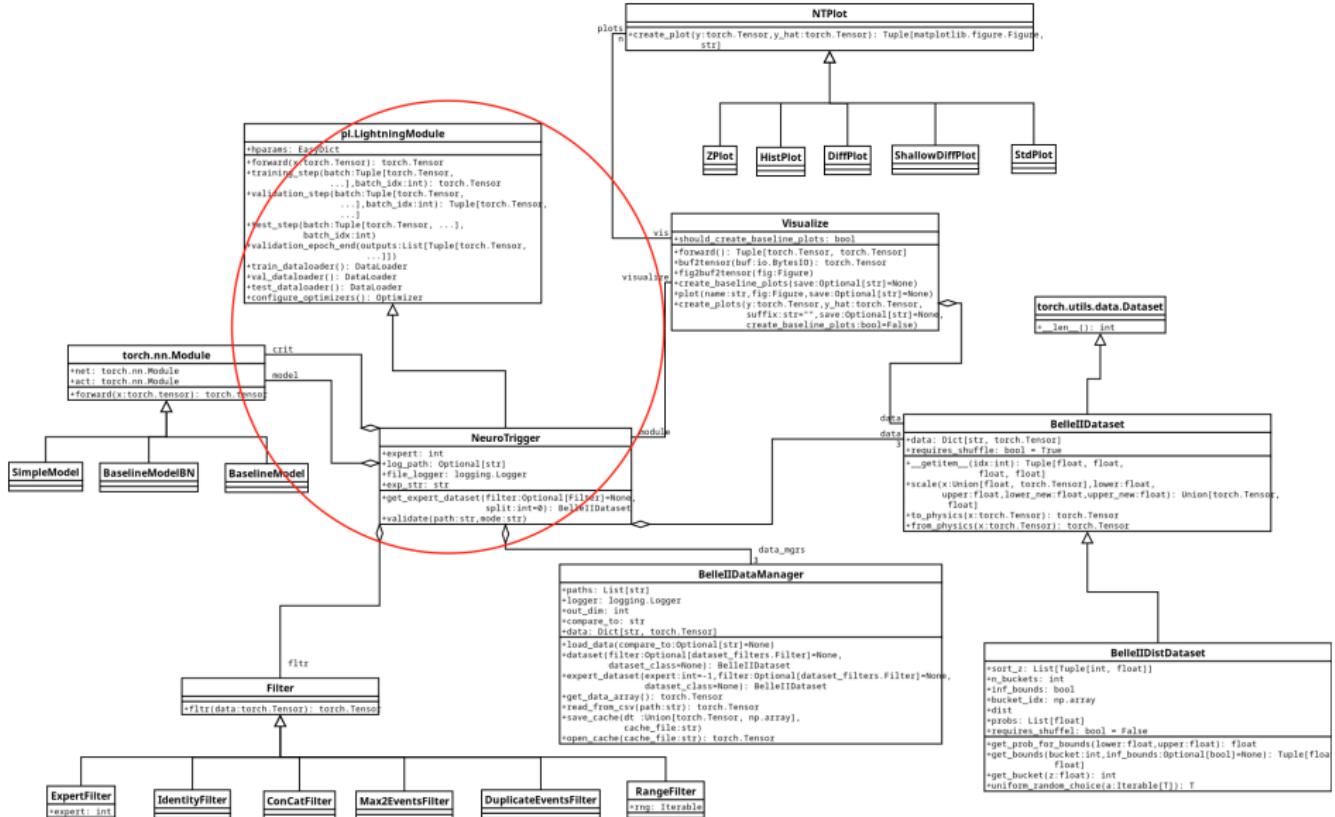
## Extensibility

---

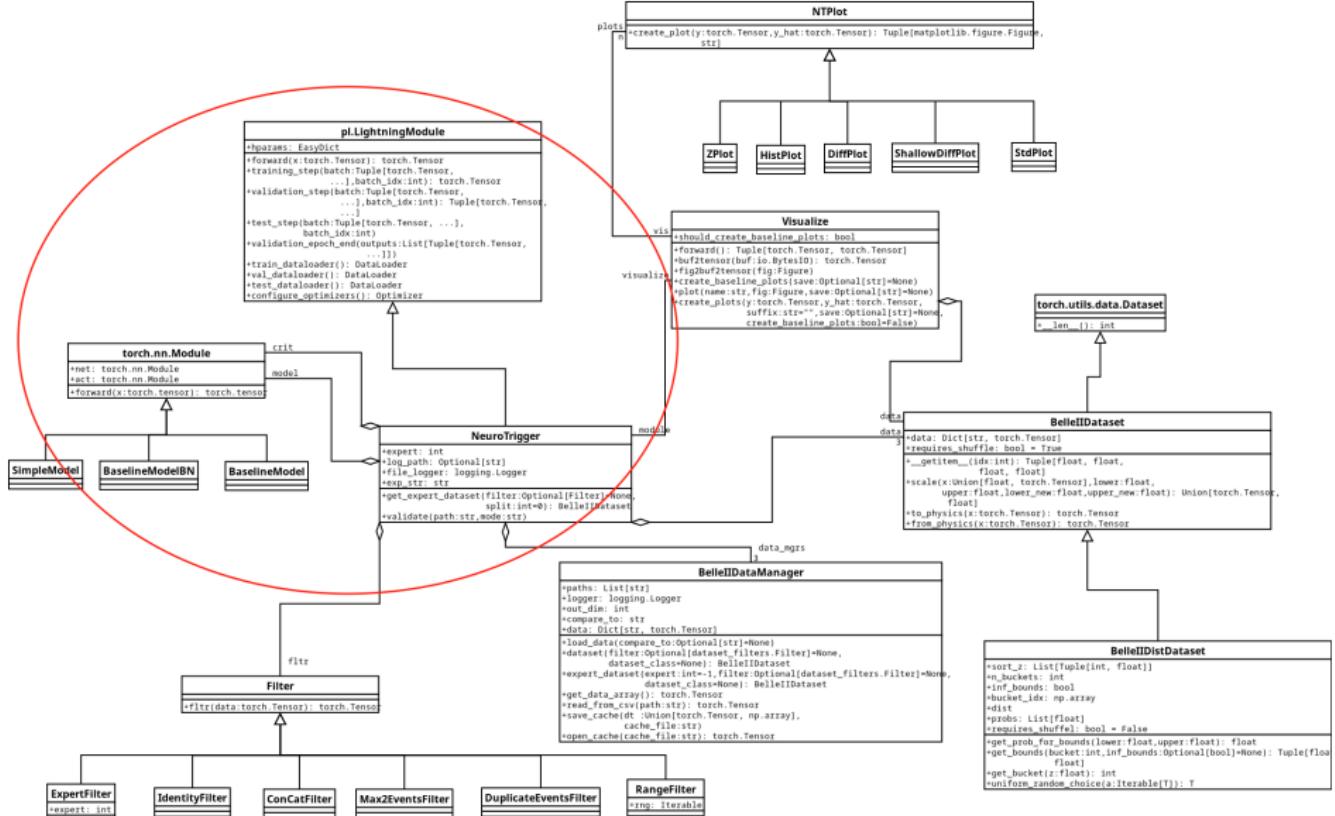
# Software Architecture



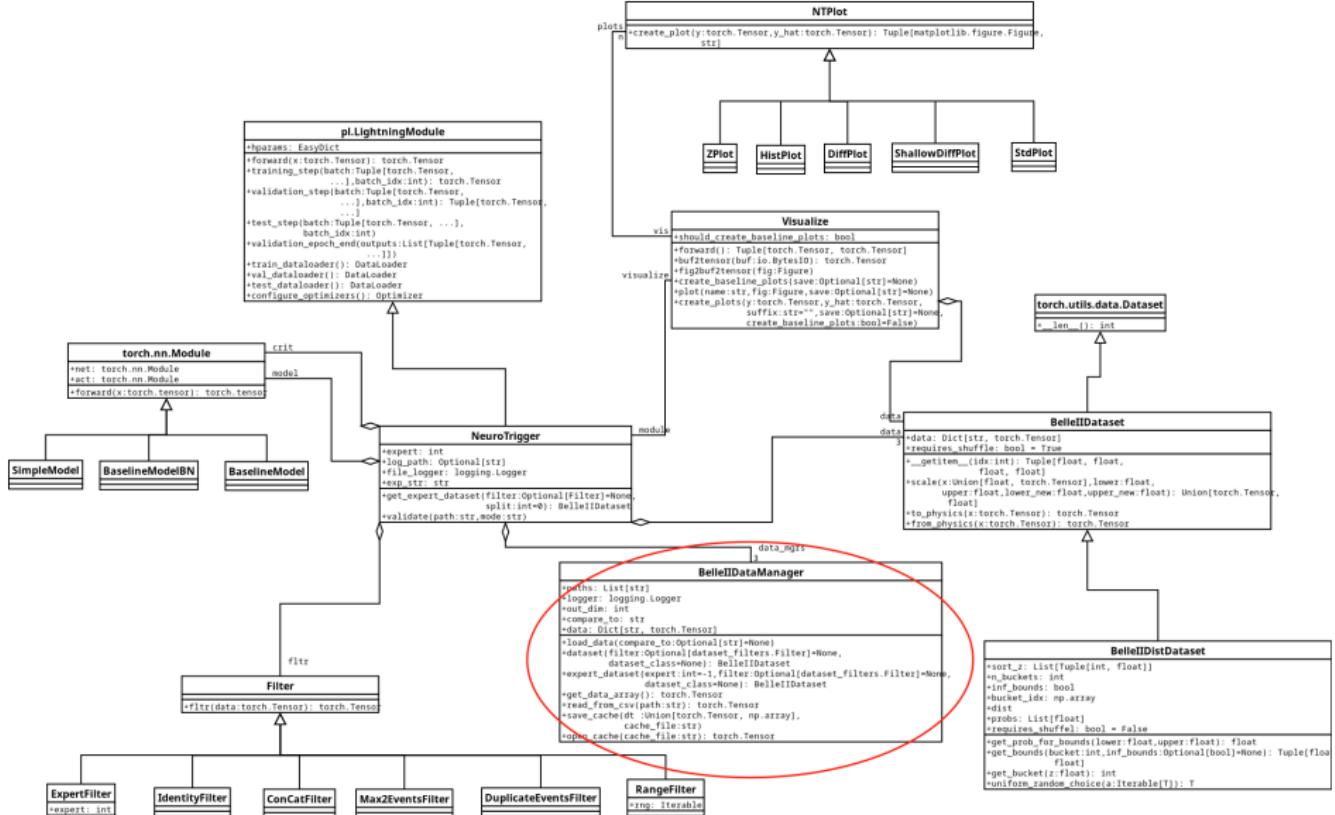
# Software Architecture



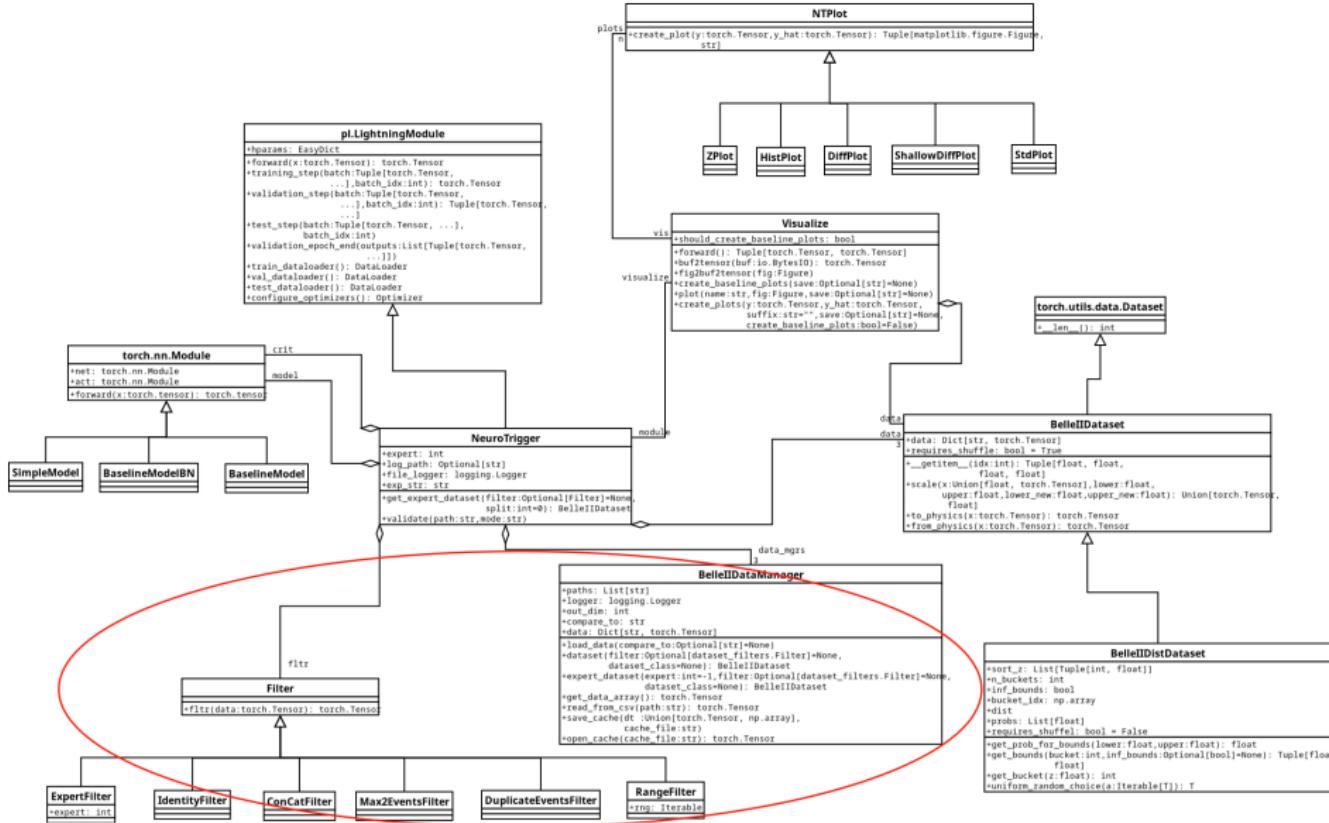
# Software Architecture



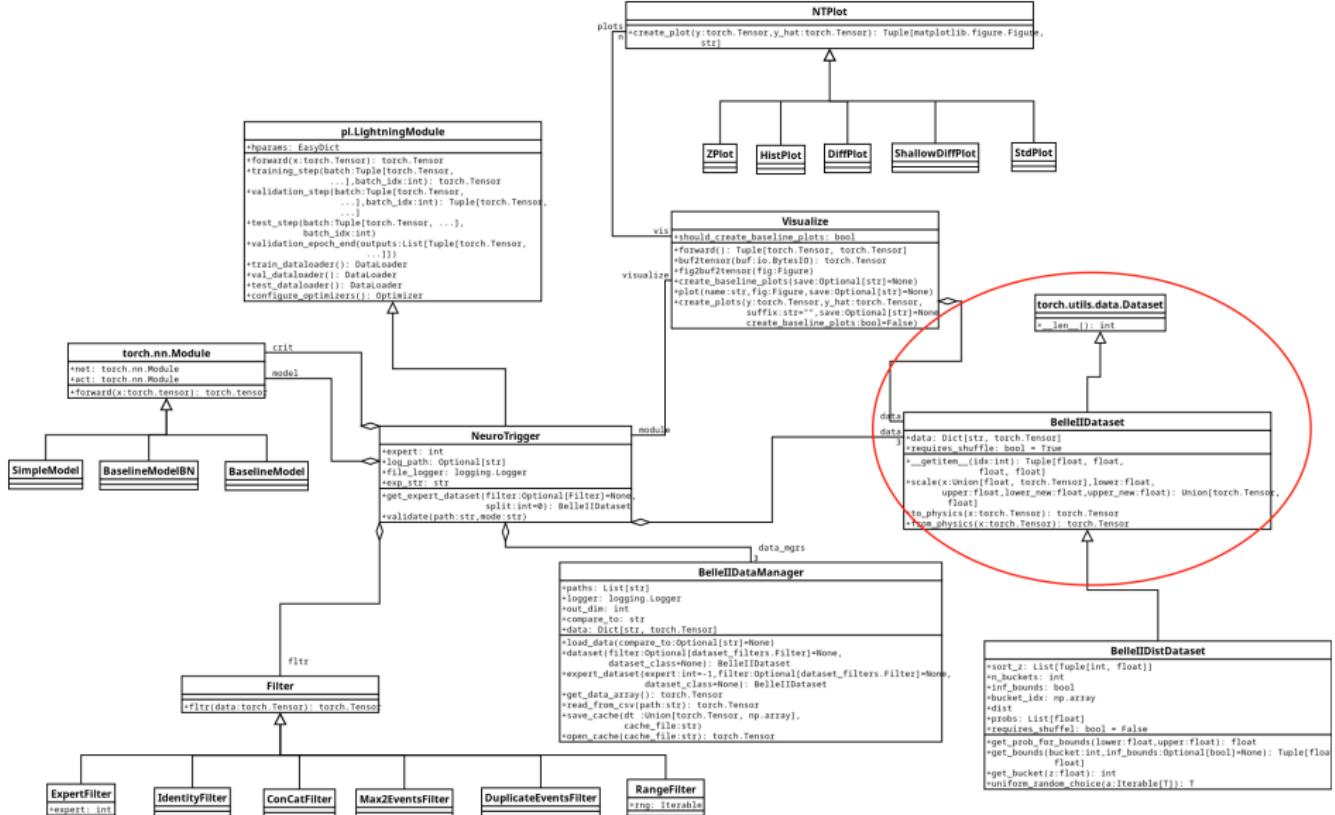
# Software Architecture



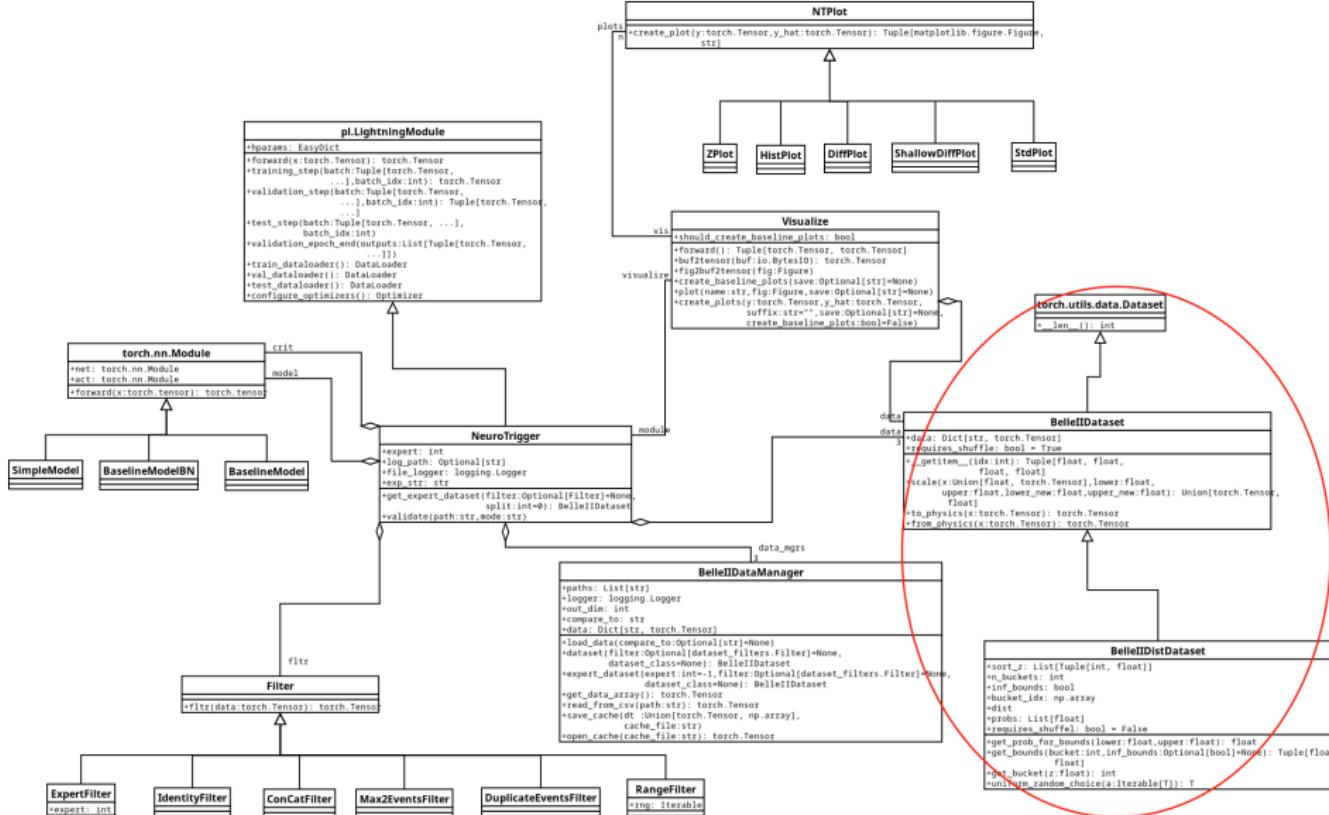
# Software Architecture



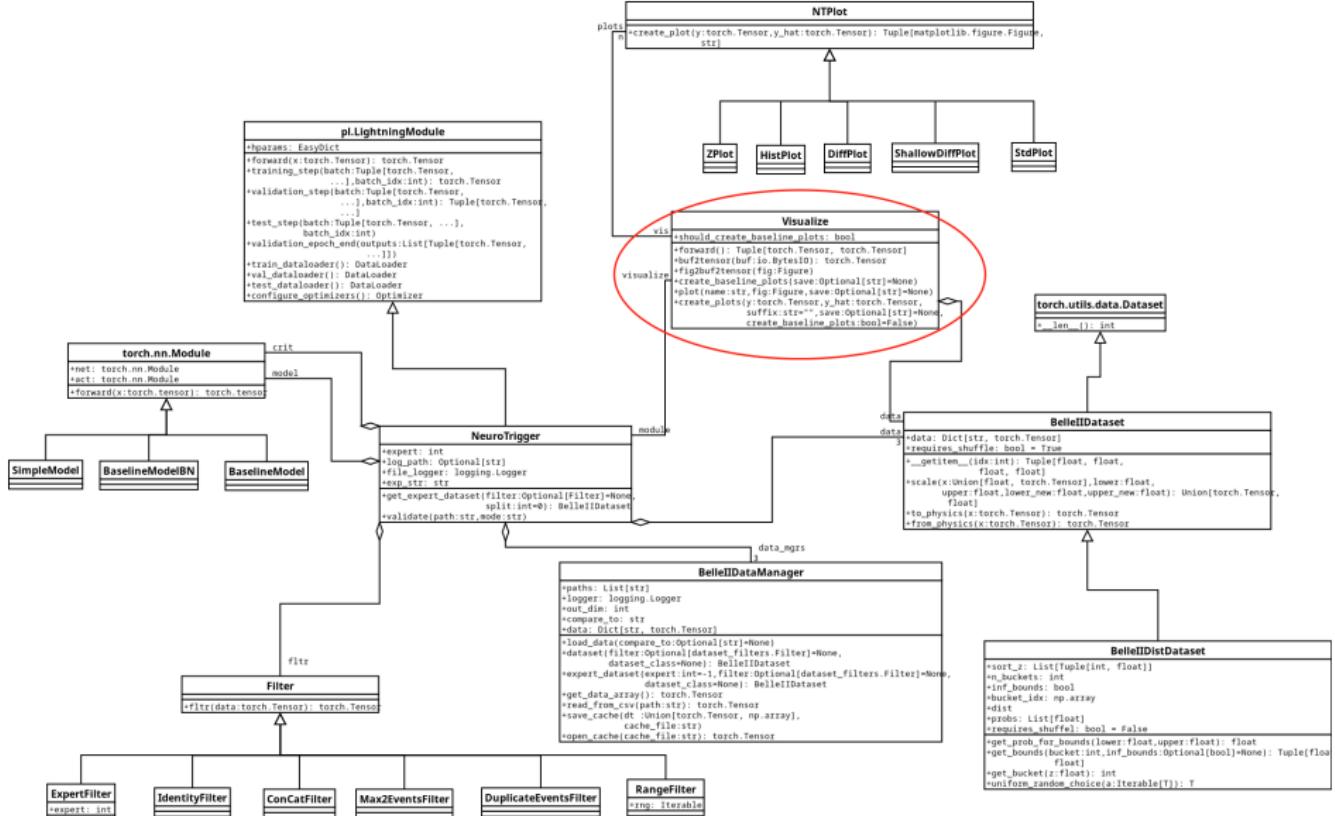
# Software Architecture



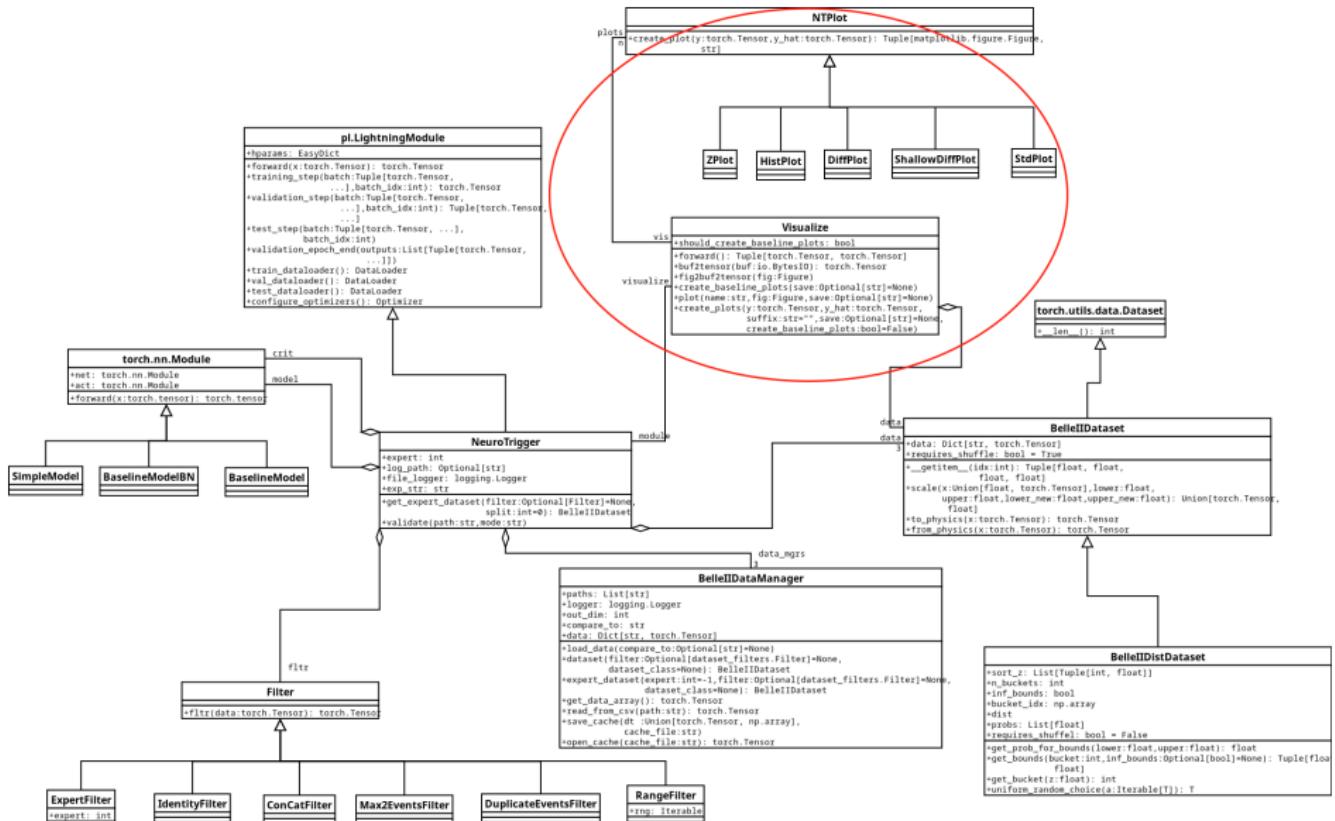
# Software Architecture



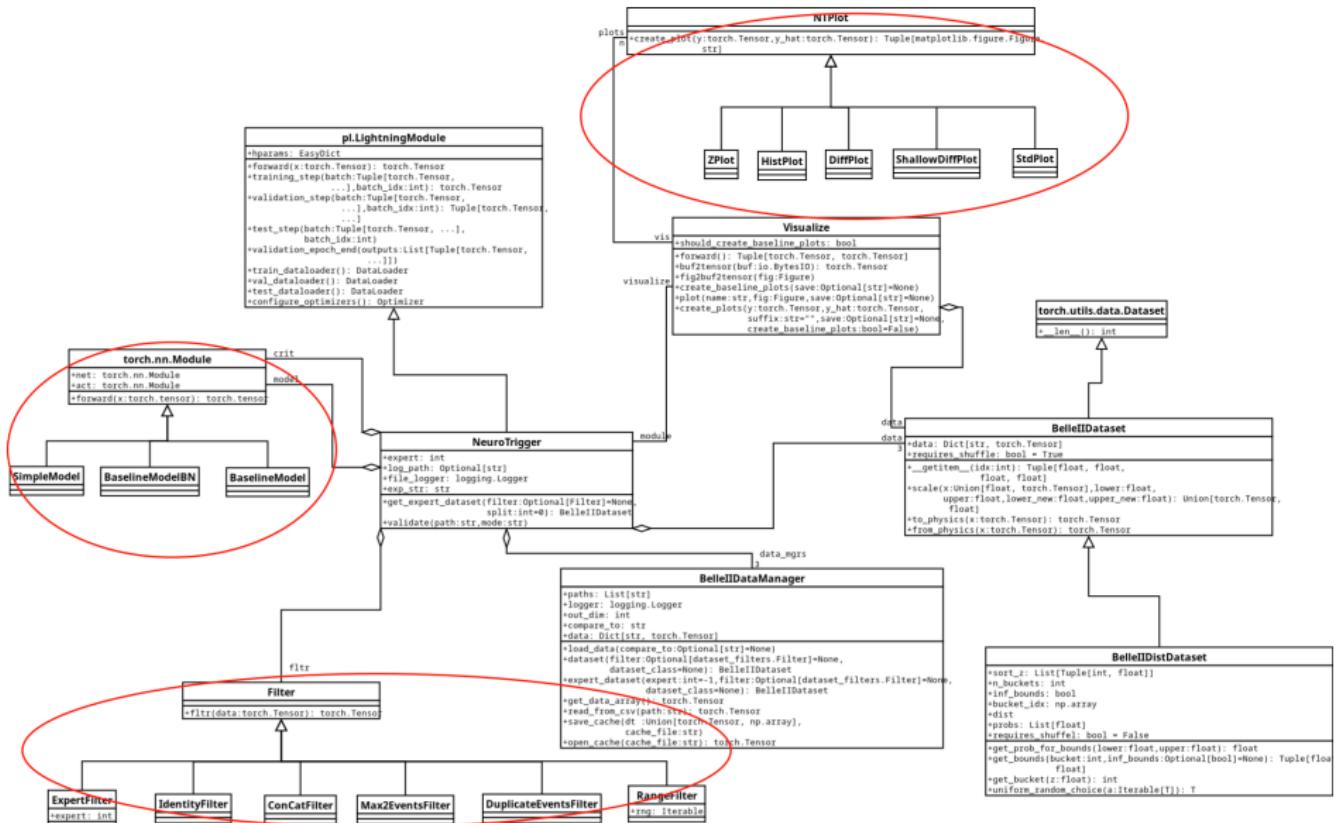
# Software Architecture



# Software Architecture

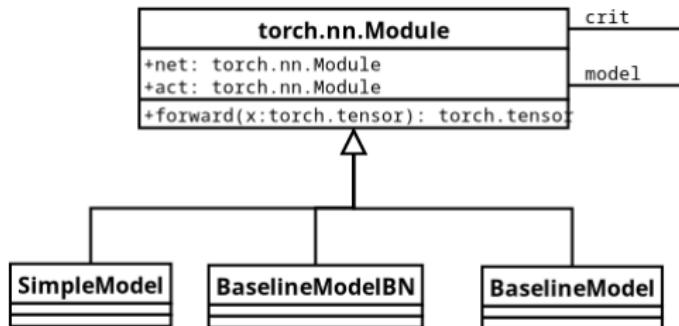


# Software Architecture



# New Network Models

- Network models are defined using PyTorch Modules
- Expected constructor arguments:
  - inp: input vector size, usually 27
  - out: output vector size, 2 for  $z$  and  $\theta$ , 1 for only  $z$
  - act: Activation function (PyTorch Module)
- PyTorch Module needs to implement the forward function



# New Network Models II

Example: Current two layer FC network

```
class BaselineModel(nn.Module):
```

# New Network Models II

Example: Current two layer FC network

```
class BaselineModel(nn.Module):
    def __init__(self,
                 inp: int = 27,
                 out: int = 2,
                 act: Optional[nn.Module]=None):
```

# New Network Models II

Example: Current two layer FC network

```
class BaselineModel(nn.Module):
    def __init__(self,
                 inp: int = 27,
                 out: int = 2,
                 act: Optional[nn.Module]=None):
        super().__init__()
        act = act or nn.Tanh()
        self.net = nn.Sequential(
            nn.Linear(inp, 81),
            act,
            nn.Linear(81, out),
            act,
        )
```

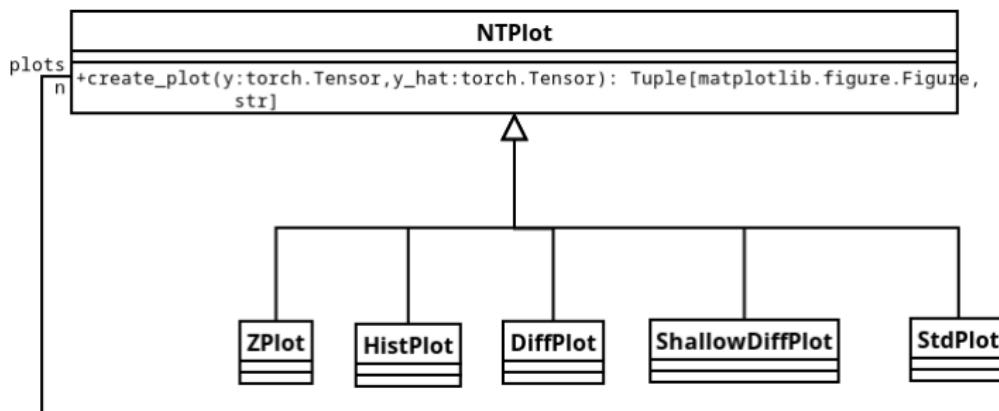
# New Network Models II

Example: Current two layer FC network

```
class BaselineModel(nn.Module):
    def __init__(self,
                 inp: int = 27,
                 out: int = 2,
                 act: Optional[nn.Module]=None):
        super().__init__()
        act = act or nn.Tanh()
        self.net = nn.Sequential(
            nn.Linear(inp, 81),
            act,
            nn.Linear(81, out),
            act,
        )
    def forward(self, x: torch.Tensor) -> torch.Tensor:
        return self.net(x)
```

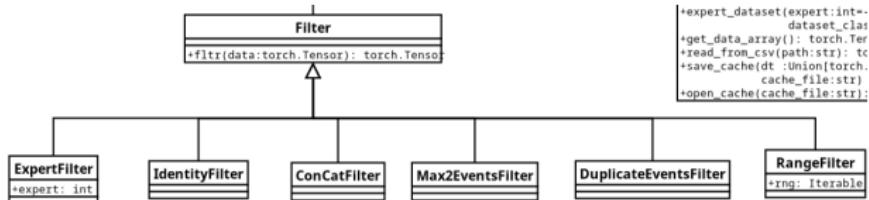
# New Plots and Graphs

- Subclass from `visualize.NTPlot`
- Override the `create_plot` method
  - Gets prediction and ground truth (neuro and reco z)
  - Must return a matplotlib figure and a figure name



# New Dataset filters

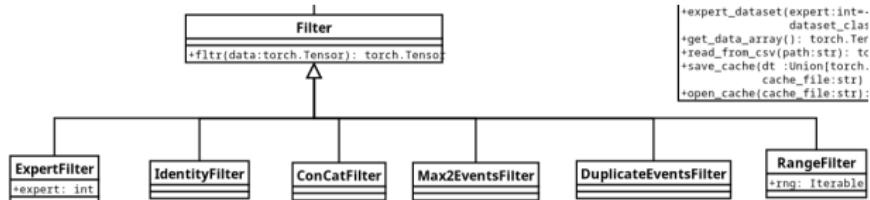
- Subclass from `dataset_filters.Filter`
- Override the `fltr` method
  - Gets data dictionary<sup>2</sup>
  - Must return boolean array with entries set to one that should be kept



<sup>2</sup> Keys and dimensions:  $x \in \mathbb{R}^{N \times 27}$ ,  $y \in \mathbb{R}^{N \times 2}$ ,  $\text{expert} \in \mathbb{R}^N$ ,  $\text{y\_hat\_old} \in \mathbb{R}^N$ , ...

# New Dataset filters

- Subclass from `dataset_filters.Filter`
- Override the `fltr` method
  - Gets data dictionary<sup>2</sup>
  - Must return boolean array with entries set to one that should be kept

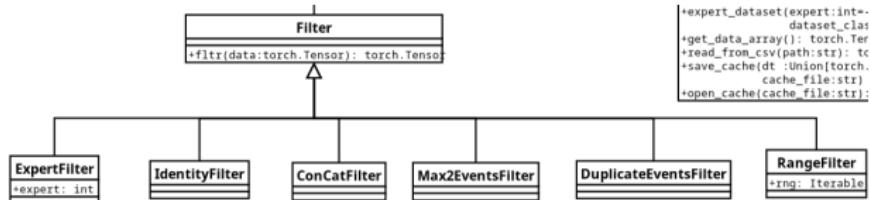


Example: Keep only positive z values

<sup>2</sup> Keys and dimensions:  $x \in \mathbb{R}^{N \times 27}$ ,  $y \in \mathbb{R}^{N \times 2}$ ,  $\text{expert} \in \mathbb{R}^N$ ,  $\text{y_hat.old} \in \mathbb{R}^N$ , ...

# New Dataset filters

- Subclass from `dataset_filters.Filter`
- Override the `fltr` method
  - Gets data dictionary<sup>2</sup>
  - Must return boolean array with entries set to one that should be kept



Example: Keep only positive z values

```
class PositiveZFilter(Filter):
    def fltr(self, data: Dict[str, torch.Tensor]) -> torch.Tensor:
        z_data = data['y'][:,0]
        return z_data > 0
```

<sup>2</sup> Keys and dimensions:  $x \in \mathbb{R}^{N \times 27}$ ,  $y \in \mathbb{R}^{N \times 2}$ ,  $\text{expert} \in \mathbb{R}^N$ ,  $\text{y\_hat\_old} \in \mathbb{R}^N$ , ...

## Dataset filters in Configuration

Use the new filter in your config (filter needs to be defined in `dataset_filters.py`):

```
"some_config": {  
    # ...  
    "filter": "dataset_filters.PositiveZFilter()",  
}
```

# Dataset filters in Configuration

Use the new filter in your config (filter needs to be defined in `dataset_filters.py`):

```
"some_config": {  
    # ...  
    "filter": "dataset_filters.PositiveZFilter()",  
}
```

Combine several filters with the `ConCatFilter`:

```
"some_config": {  
    # ...  
    "filter": "dataset_filters.ConCatFilter([  
        dataset_filters.PositiveZFilter(),  
        dataset_filters.RangeFilter(range(100))  
    ])",  
}
```

## Dataset filters in Configuration

Use the new filter in your config (filter needs to be defined in `dataset_filters.py`):

```
"some_config": {  
    # ...  
    "filter": "dataset_filters.PositiveZFilter()",  
}
```

Combine several filters with the `ConCatFilter`:

```
"some_config": {  
    # ...  
    "filter": "dataset_filters.ConCatFilter([  
        dataset_filters.PositiveZFilter(),  
        dataset_filters.RangeFilter(range(100))  
    ])",  
}
```

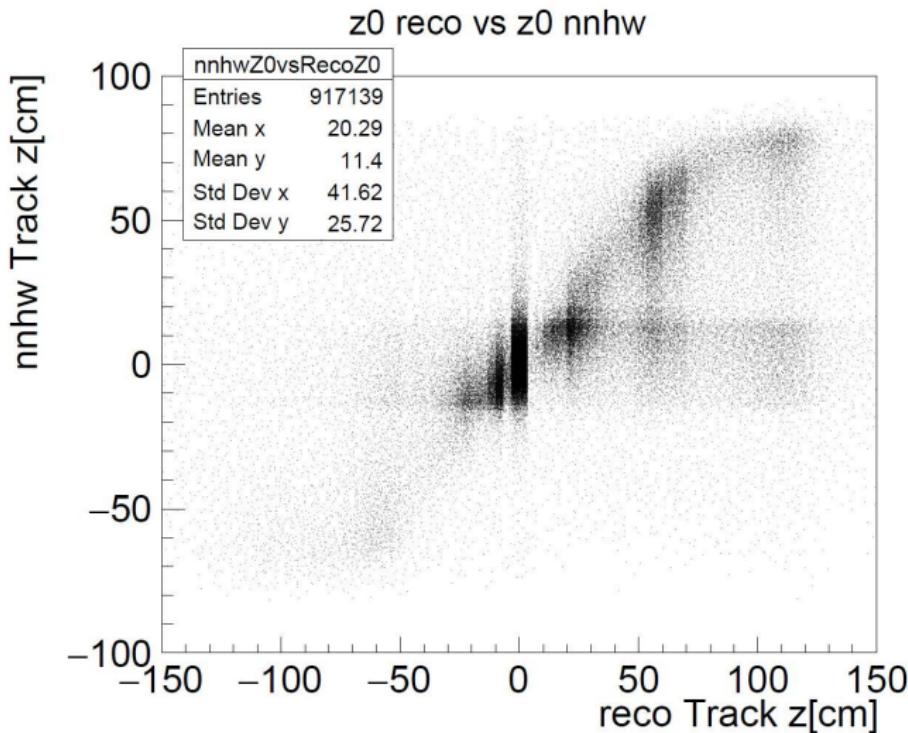
→ Only positive z values **and** only the first one hundred samples

## **Feed-down Problem and Reweighting**

---

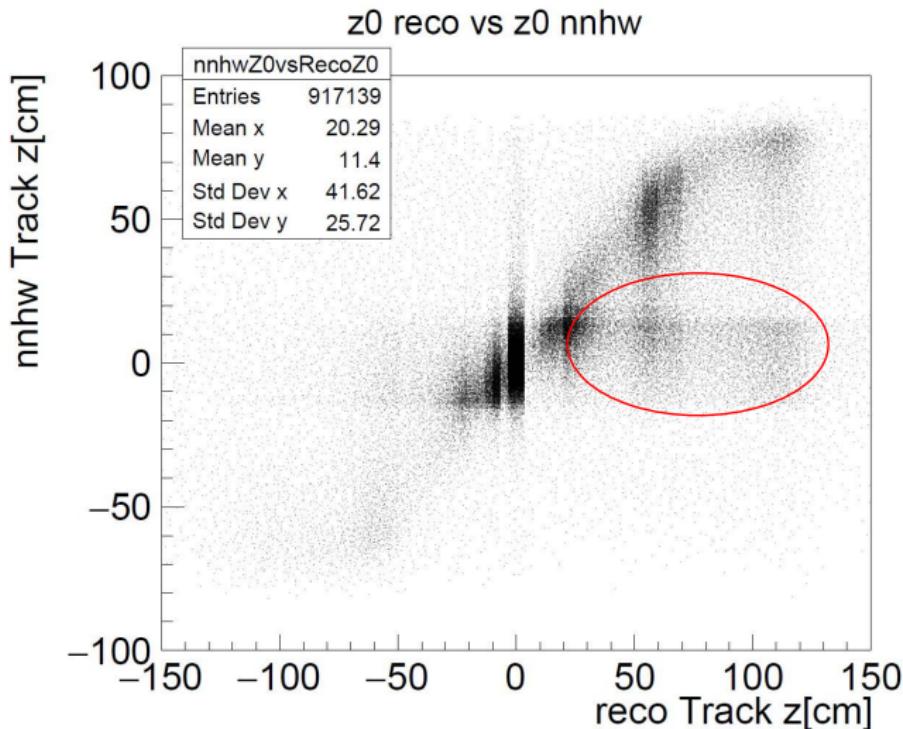
# The Feed-Down Problem

Feed-Down in the pre-PyTorch training:



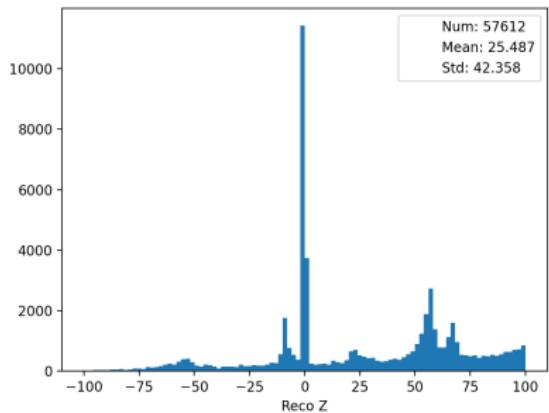
# The Feed-Down Problem

Feed-Down in the pre-PyTorch training:



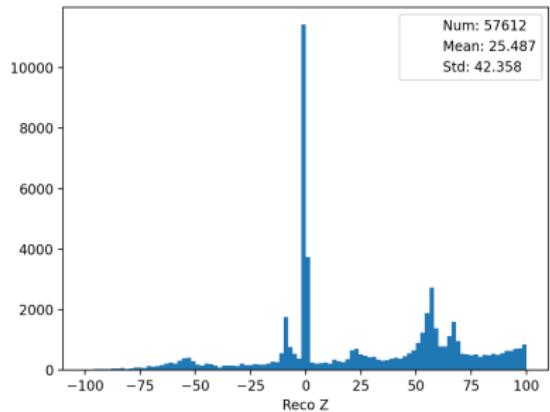
# Reweighting: Root Problem & Idea

- A lot of data at  $\hat{z} = 0$



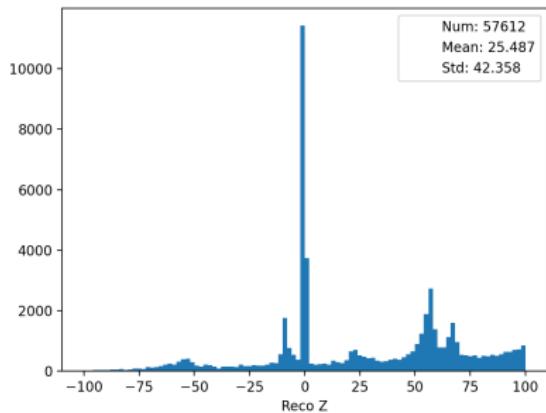
# Reweighting: Root Problem & Idea

- A lot of data at  $\hat{z} = 0$
- Bias towards predicting  $z = 0$



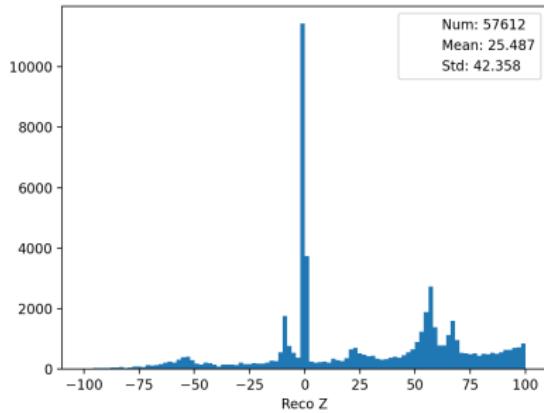
# Reweighting: Root Problem & Idea

- A lot of data at  $\hat{z} = 0$
  - Bias towards predicting  $z = 0$
  - Idea: Present the network with more data of the edge regions by duplicating them
- Upsampling



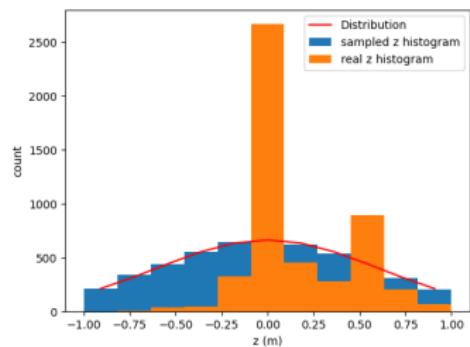
# Reweighting: Root Problem & Idea

- A lot of data at  $\hat{z} = 0$
- Bias towards predicting  $z = 0$
- Idea: Present the network with more data of the edge regions by duplicating them
  - Upsampling
- Try to keep a similar distribution and avoid uniform distribution
  - Area with more data is also more important



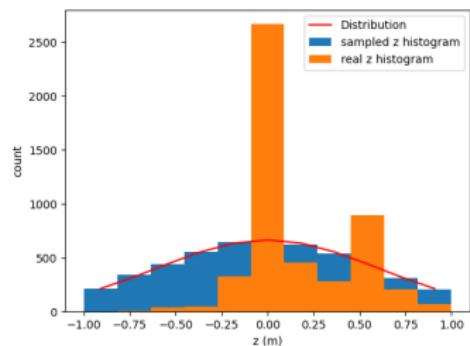
# Reweighting: Algorithm

- Choose a continuous probability density function  $f(x)$  over  $z$   
e.g. a normal distribution with certain mean and variance



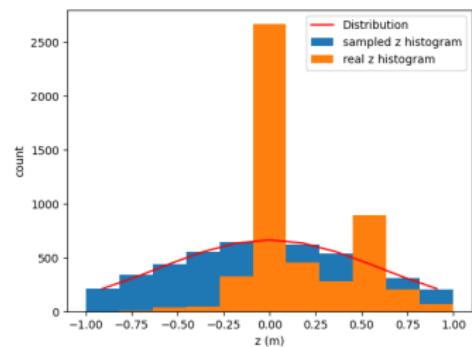
# Reweighting: Algorithm

- Choose a continuous probability density function  $f(x)$  over  $z$   
e.g. a normal distribution with certain mean and variance
- Divide the  $z$  range into  $n$  equally size buckets  $b_i = [b_{i_l}, b_{i_u}] \forall i \in [n]$



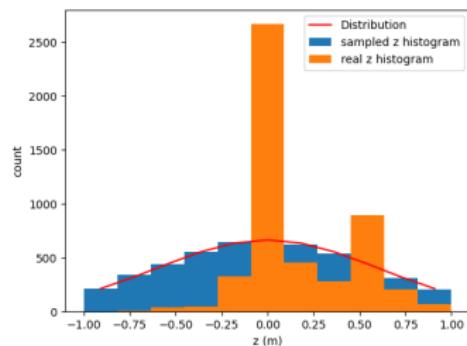
# Reweighting: Algorithm

- Choose a continuous probability density function  $f(x)$  over  $z$   
e.g. a normal distribution with certain mean and variance
- Divide the  $z$  range into  $n$  equally size buckets  $b_i = [b_{i_l}, b_{i_u}] \forall i \in [n]$
- Bucket probability given by CDF:  
$$p_i = \int_{b_{i_l}}^{b_{i_u}} f(x) dx$$



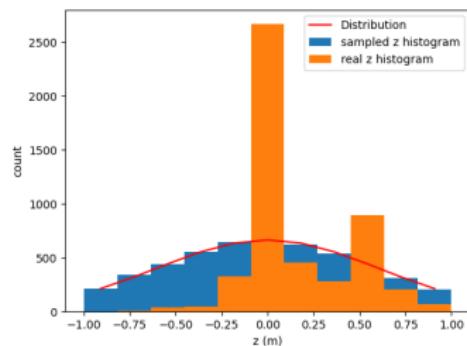
# Reweighting: Algorithm

- Choose a continuous probability density function  $f(x)$  over  $z$   
e.g. a normal distribution with certain mean and variance
- Divide the  $z$  range into  $n$  equally size buckets  $b_i = [b_{i_l}, b_{i_u}] \forall i \in [n]$
- Bucket probability given by CDF:  
 $p_i = \int_{b_{i_l}}^{b_{i_u}} f(x) dx$
- To sample with an item:



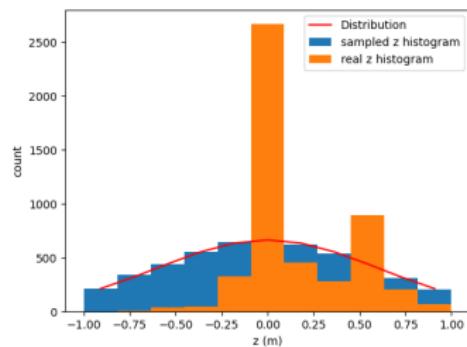
# Reweighting: Algorithm

- Choose a continuous probability density function  $f(x)$  over  $z$   
e.g. a normal distribution with certain mean and variance
- Divide the  $z$  range into  $n$  equally size buckets  $b_i = [b_{i_l}, b_{i_u}] \forall i \in [n]$
- Bucket probability given by CDF:  
 $p_i = \int_{b_{i_l}}^{b_{i_u}} f(x) dx$
- To sample with an item:
  - Pick  $a$  according the probabilities  $p_i$



# Reweighting: Algorithm

- Choose a continuous probability density function  $f(x)$  over  $z$   
e.g. a normal distribution with certain mean and variance
- Divide the  $z$  range into  $n$  equally size buckets  $b_i = [b_{i_l}, b_{i_u}] \forall i \in [n]$
- Bucket probability given by CDF:  
 $p_i = \int_{b_{i_l}}^{b_{i_u}} f(x) dx$
- To sample with an item:
  - Pick a according the probabilities  $p_i$
  - Within the bucket, sample uniform randomly



## Reweighting: Configuration

- Reweightings are configured with a hierarchical syntax
- Example:
  - $n = 11$  buckets
  - Normal distribution with  $\mu = 0$  and  $\sigma = 0.4$

## Reweighting: Configuration

- Reweightings are configured with a hierarchical syntax
- Example:
  - $n = 11$  buckets
  - Normal distribution with  $\mu = 0$  and  $\sigma = 0.4$

```
"some_config": {  
    # ...  
}
```

## Reweighting: Configuration

- Reweightings are configured with a hierarchical syntax
- Example:
  - $n = 11$  buckets
  - Normal distribution with  $\mu = 0$  and  $\sigma = 0.4$

```
"some_config": {  
    # ...  
    "dist": {  
        },  
    }  
}
```

## Reweighting: Configuration

- Reweightings are configured with a hierarchical syntax
- Example:
  - $n = 11$  buckets
  - Normal distribution with  $\mu = 0$  and  $\sigma = 0.4$

```
"some_config": {  
    # ...  
    "dist": {  
        "n_buckets": 11,  
  
    },  
}
```

# Reweighting: Configuration

- Reweightings are configured with a hierarchical syntax
- Example:
  - $n = 11$  buckets
  - Normal distribution with  $\mu = 0$  and  $\sigma = 0.4$

```
"some_config": {  
    # ...  
    "dist": {  
        "n_buckets": 11,  
        "norm": {  
            "mean": 0,  
            "std": 0.4,  
        },  
    },  
}
```

# Reweighting: Configuration

- Reweightings are configured with a hierarchical syntax
- Example:
  - $n = 11$  buckets
  - Normal distribution with  $\mu = 0$  and  $\sigma = 0.4$

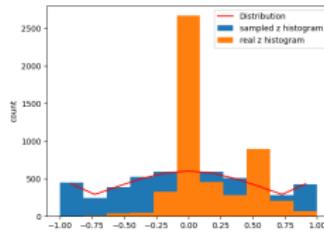
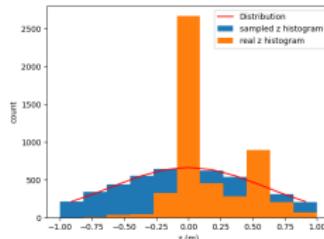
```
"some_config": {  
    # ...  
    "dist": {  
        "n_buckets": 11,  
        "norm": {  
            "mean": 0,  
            "std": 0.4,  
        },  
        "inf_bounds": False,  
    },  
}
```

# Reweighting: Configuration

- Reweightings are configured with a hierarchical syntax
- Example:
  - $n = 11$  buckets
  - Normal distribution with  $\mu = 0$  and  $\sigma = 0.4$

Infinite bounds vs non finite bounds:

```
"some_config": {  
    # ...  
    "dist": {  
        "n_buckets": 11,  
        "norm": {  
            "mean": 0,  
            "std": 0.4,  
        },  
        "inf_bounds": False,  
    },  
}
```



## Results

---

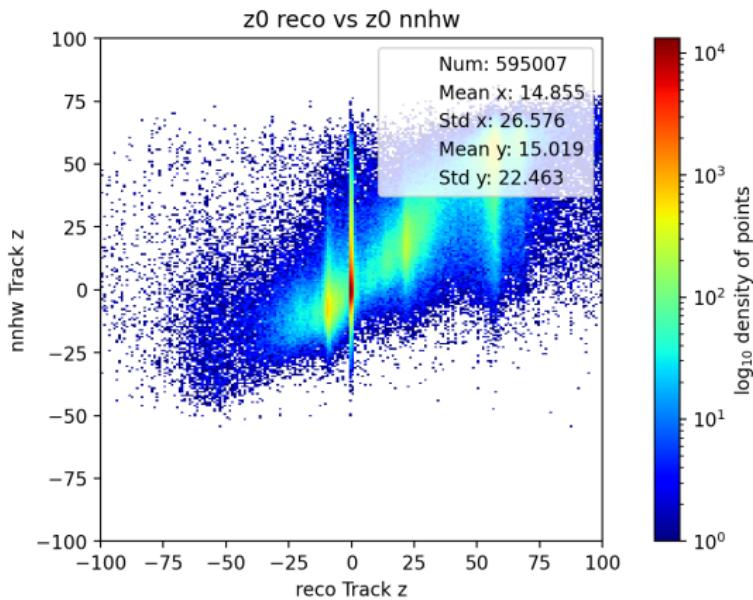
# Numeric Results

**Table 1:** Validation loss vs Old loss

	Baseline	Tanh	Tanh BN	Softsign	Reweight	Events Filter
Expert 0	0.766	0.742	0.709	0.737	1.159	1.016
Expert 1	0.736	0.703	0.696	0.710	1.074	1.047
Expert 2	0.928	0.851	0.830	0.831	1.475	1.406
Expert 3	0.908	0.780	0.760	0.770	1.559	1.067
Expert 4	0.779	0.784	0.683	0.692	1.256	1.259
Mean	0.823	0.772	0.735	0.748	1.305	1.159

# Z Plot

Neuro  $z$  vs reco  $z$  for expert 0 of the current Trigger:



# Conclusion

- Interestingly, the first PyTorch training gave the highest gain, further optimization with regards to the feed-down problem even worsened outcome

# Conclusion

- Interestingly, the first PyTorch training gave the highest gain, further optimization with regards to the feed-down problem even worsened outcome
- Most gain through modern training techniques

# Conclusion

- Interestingly, the first PyTorch training gave the highest gain, further optimization with regards to the feed-down problem even worsened outcome
  - Most gain through modern training techniques
- Further Improvements
  - Open for potential for different network architectures
  - Large hyperparameter optimization should be done
  - Use more and more diverse data to train!
  - Overall plots: Cumbersome to look at all experts

**Questions?**