Physics Data Analysis with Neural Networks

Daniel Lersch

July 6, 2021

Overview

- This presentation and jupyter notebooks are available at:

  http://hadron.physics.fsu.edu/~dlersch/GlueXPID_with_Networks/

- Content:

1.) Introduction to neural networks

2.) Implementation in physics data analysis:
   - Scikit
   - Tensorflow / Keras

3.) Performance evaluation

4.) Hyper parameter optimization (optional)

Search for $\eta \to e^+e^-\gamma$ in GlueX

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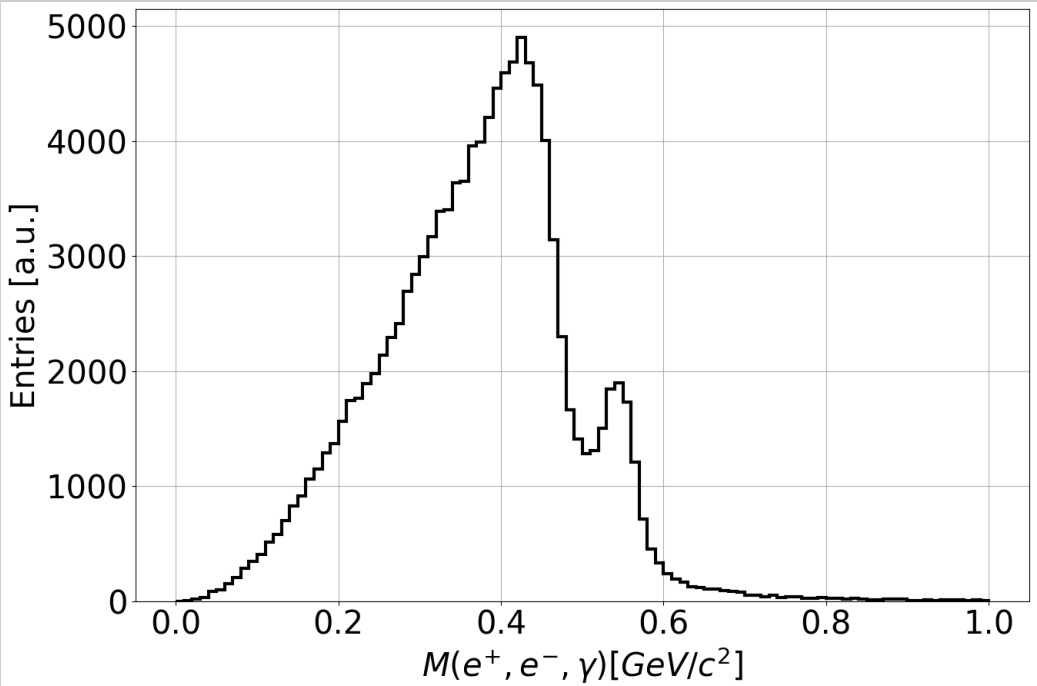

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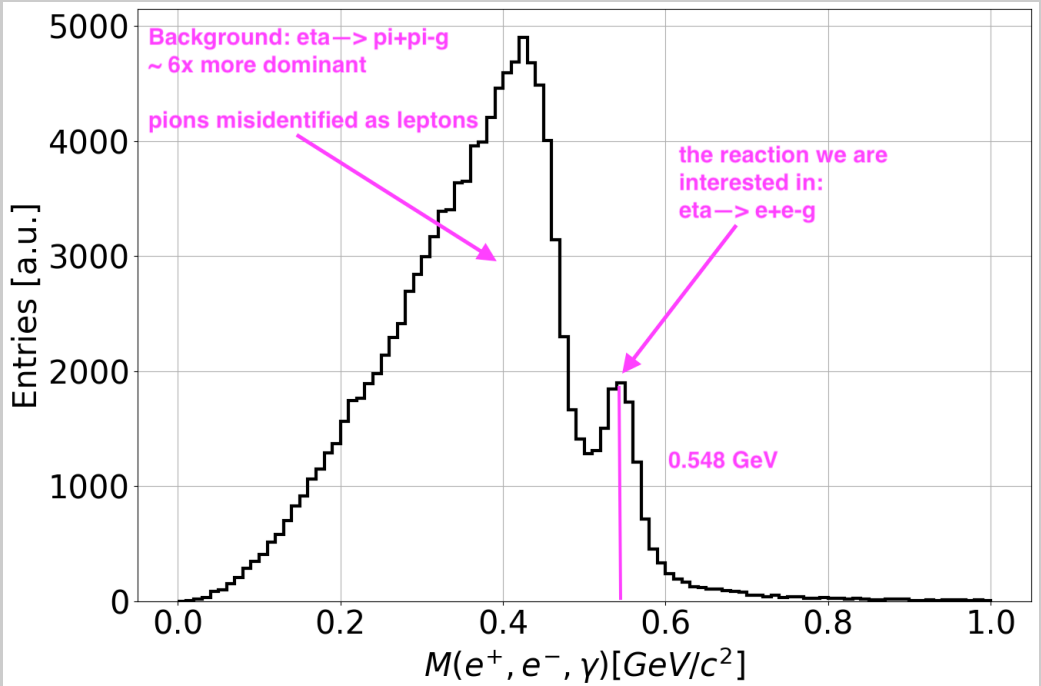
  i.e. $M(e^+, e^-, \gamma) = m_\eta = 0.548\,\mathrm{GeV/c^2}$



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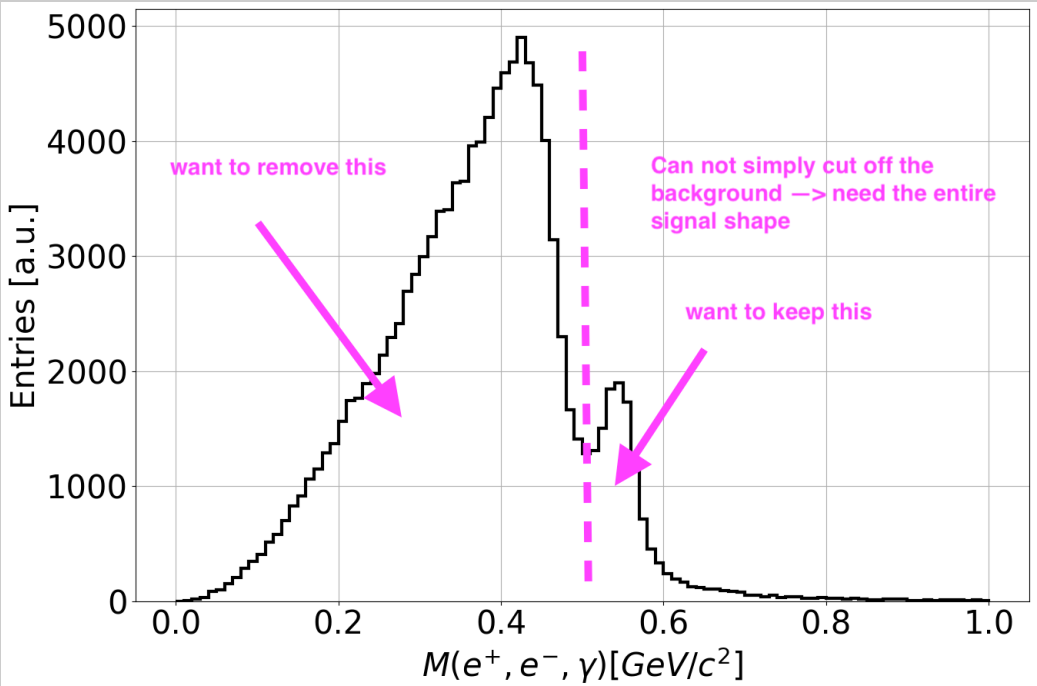

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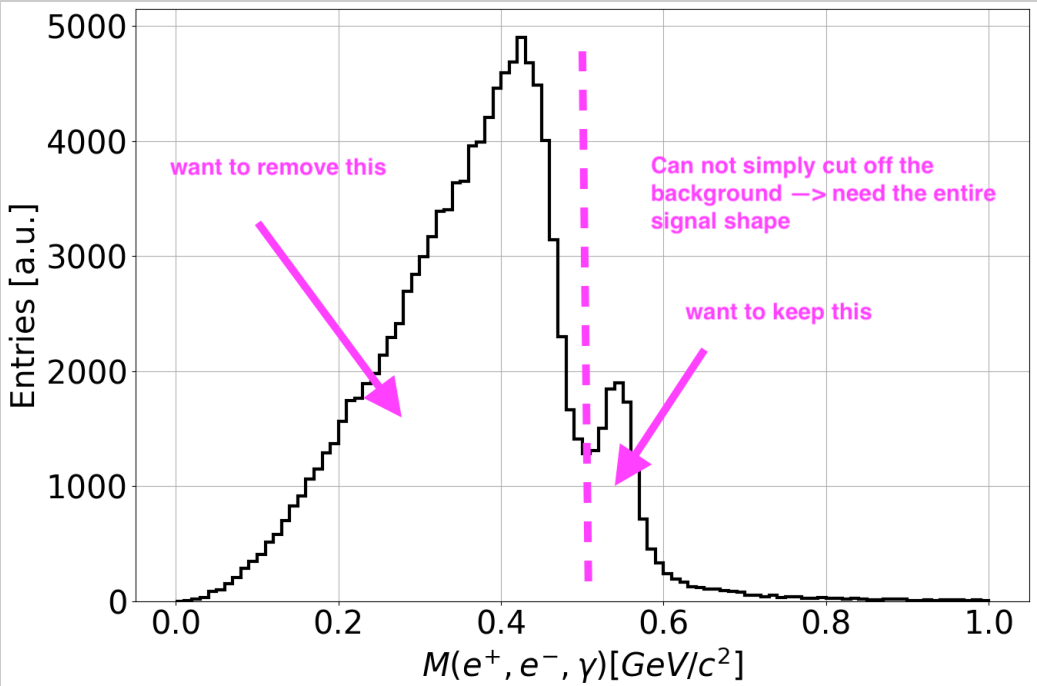

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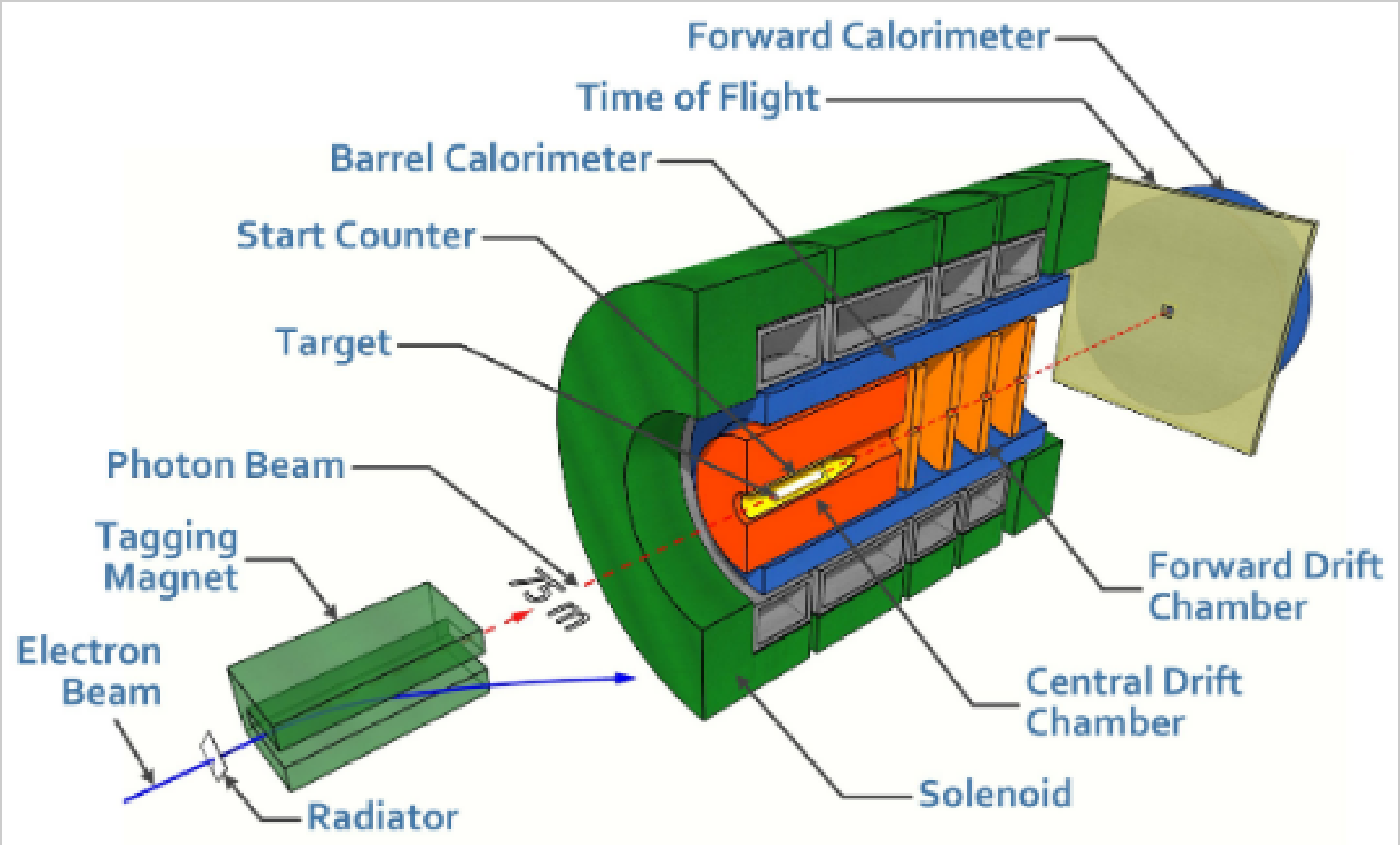
- **Approach:** Use neural networks to suppress $\eta \to \pi^+\pi^-\gamma$ background

The Gluonic Excitation Experiment (GlueX)



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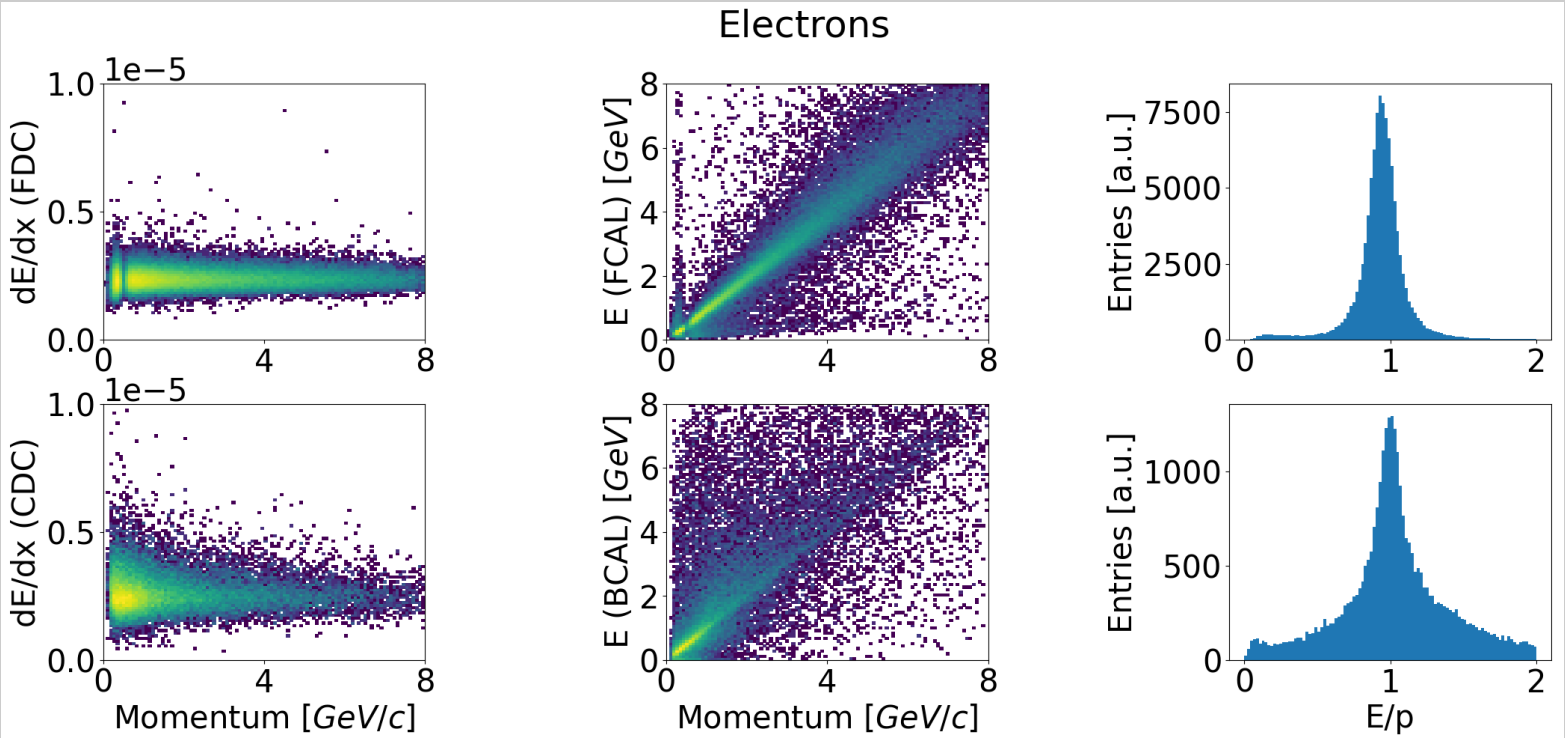
- Look at simulations



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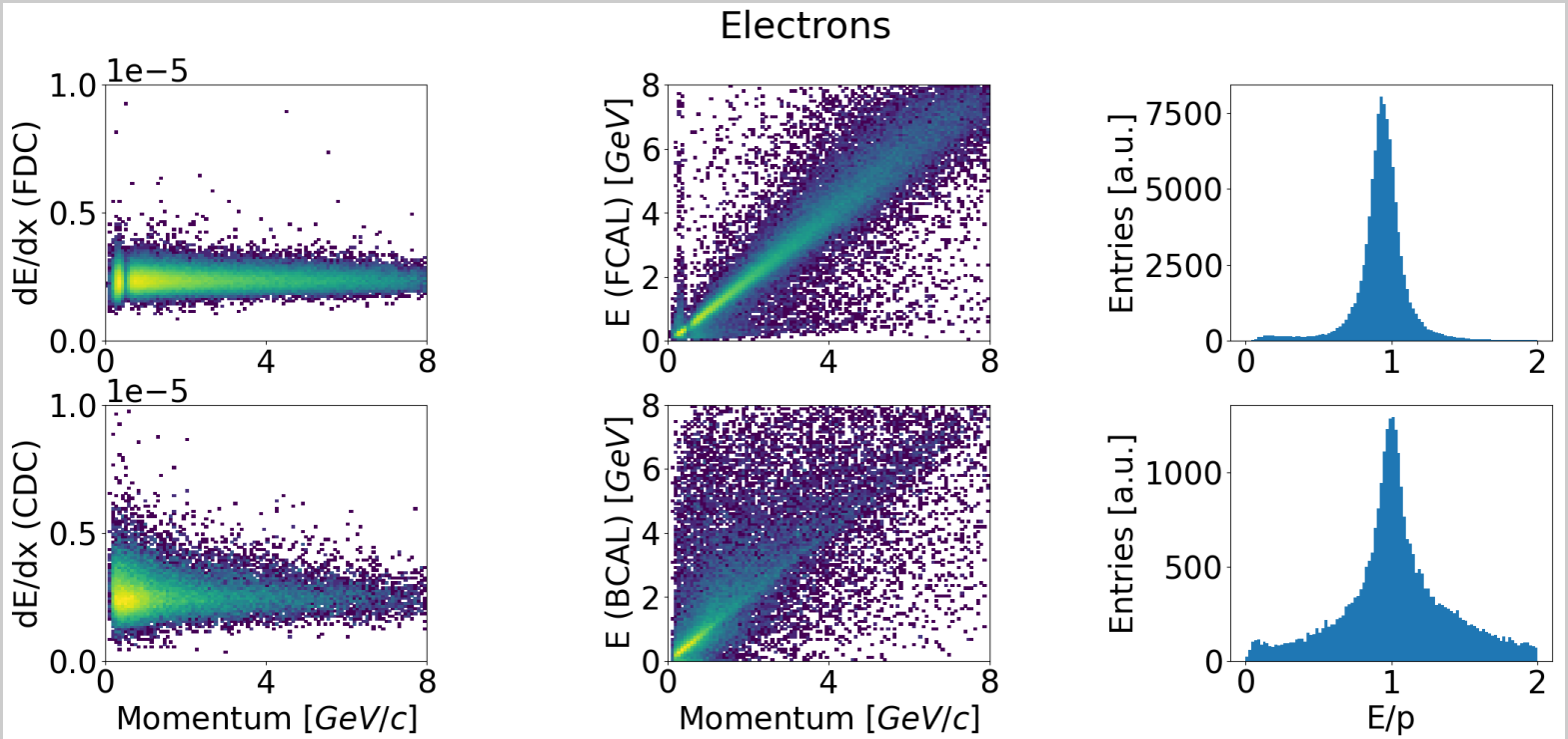

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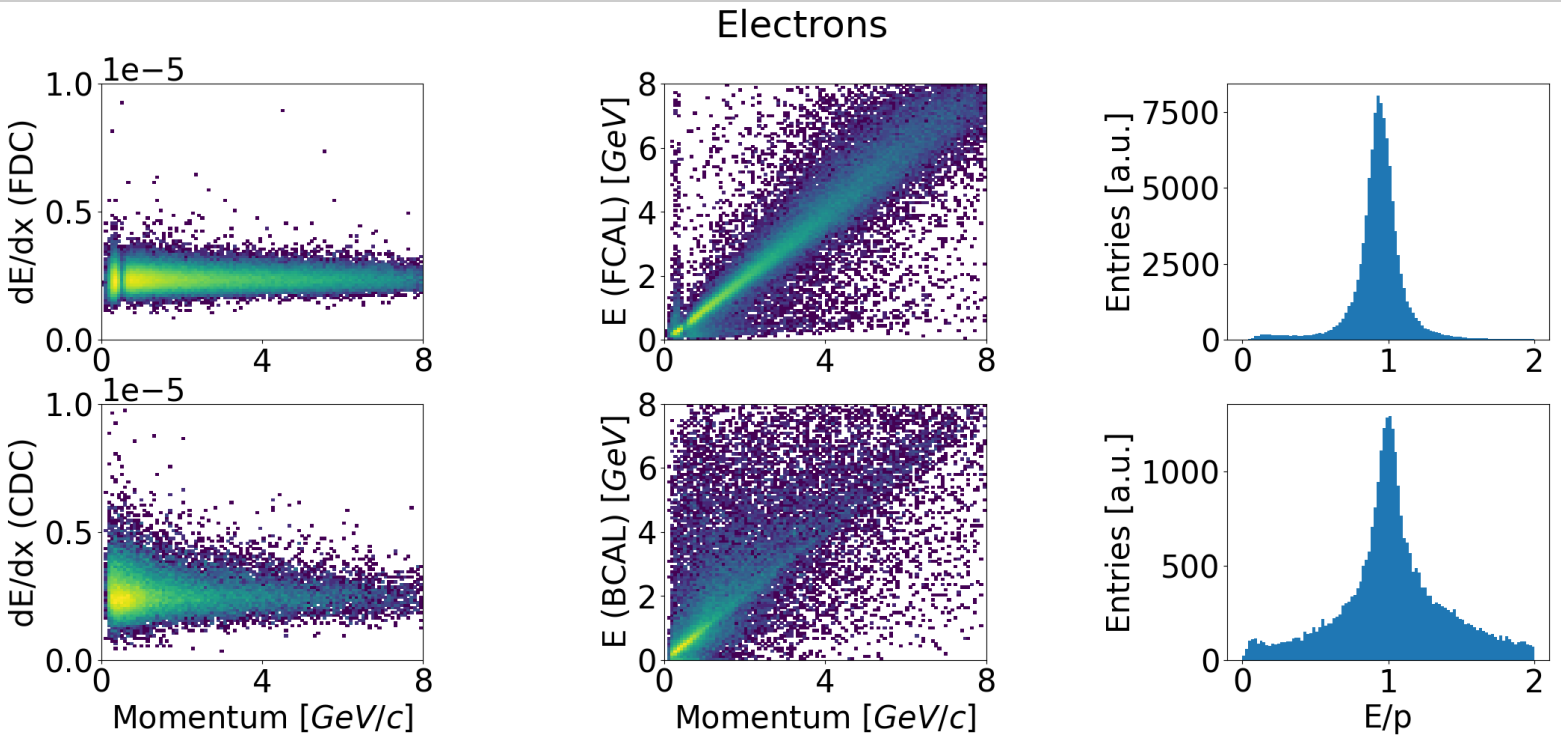

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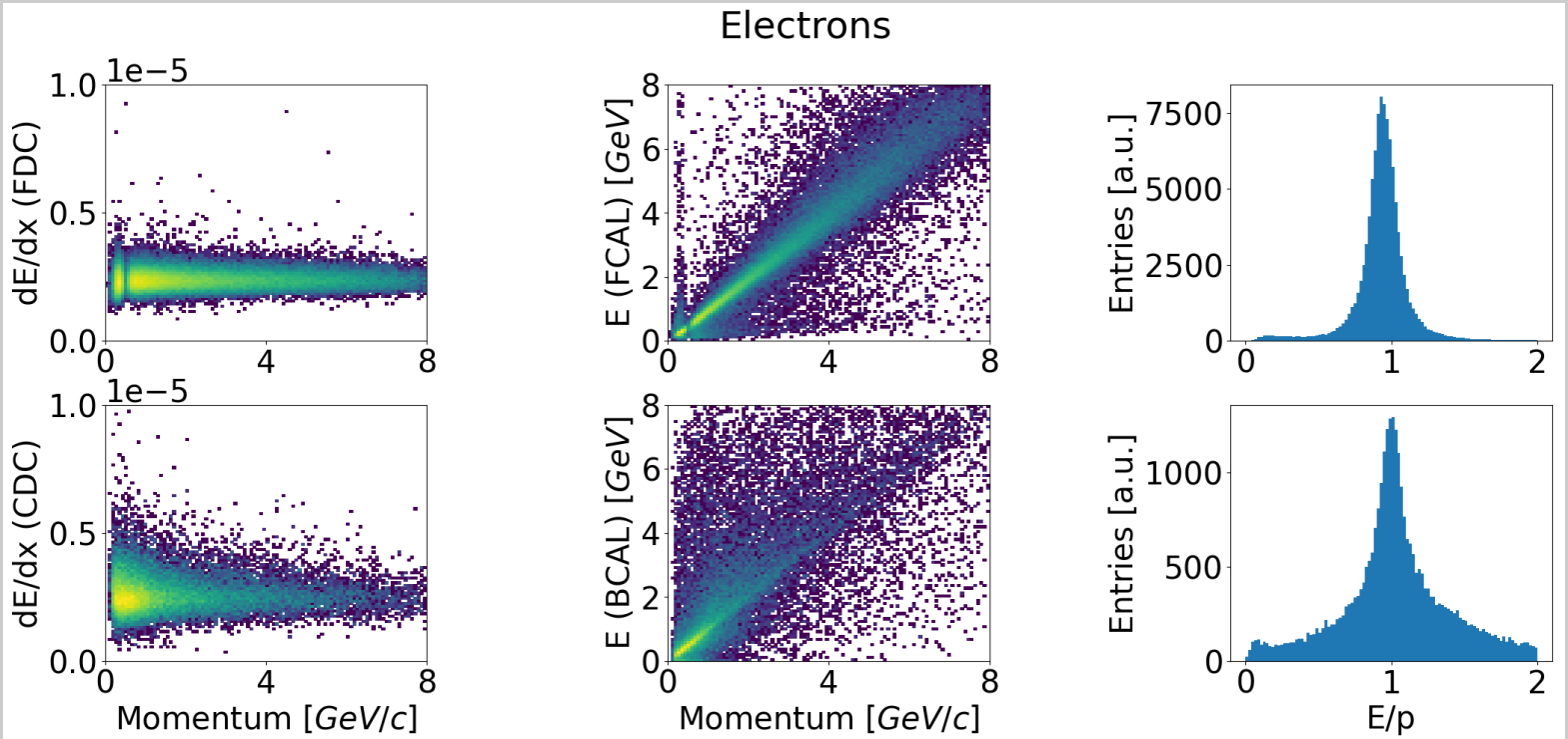

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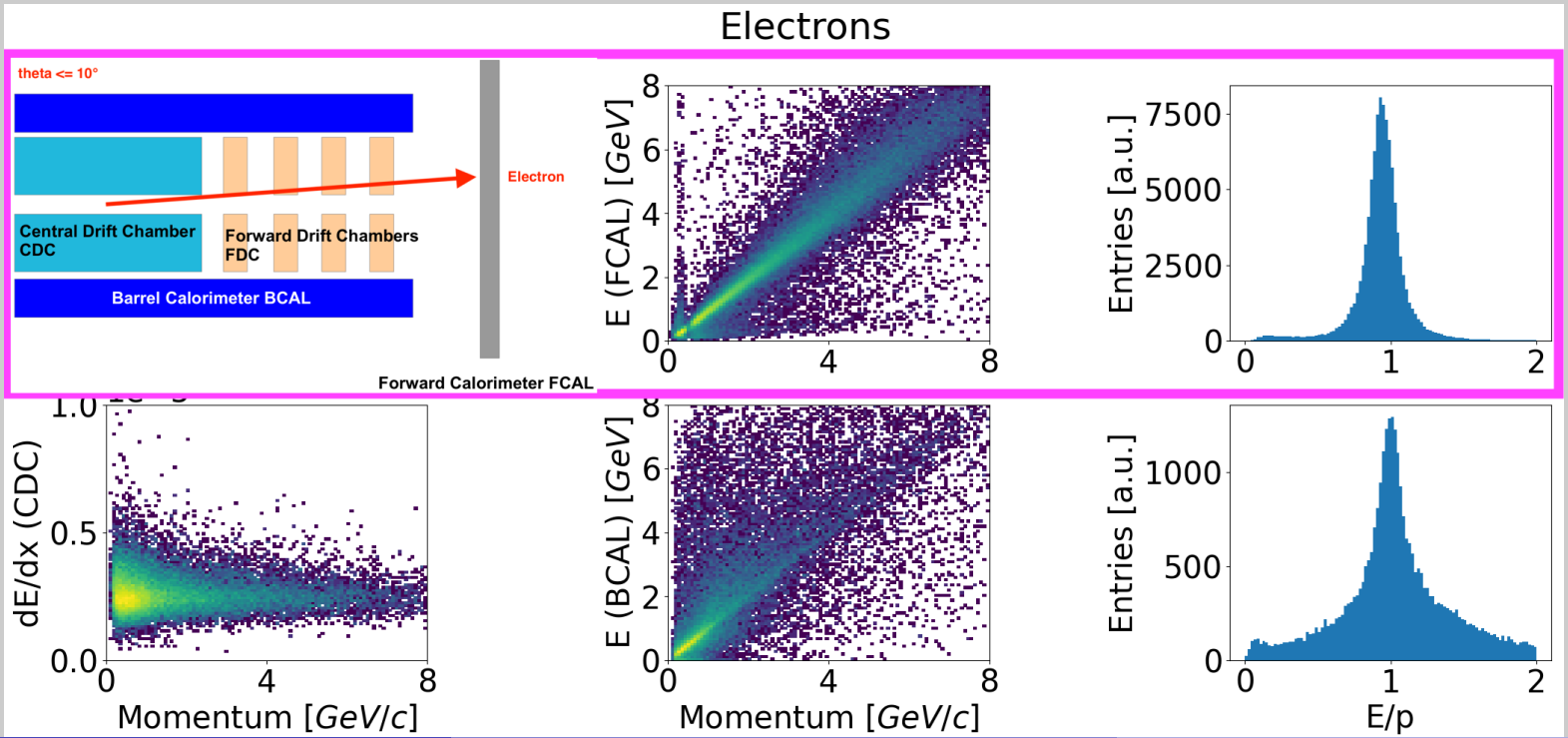

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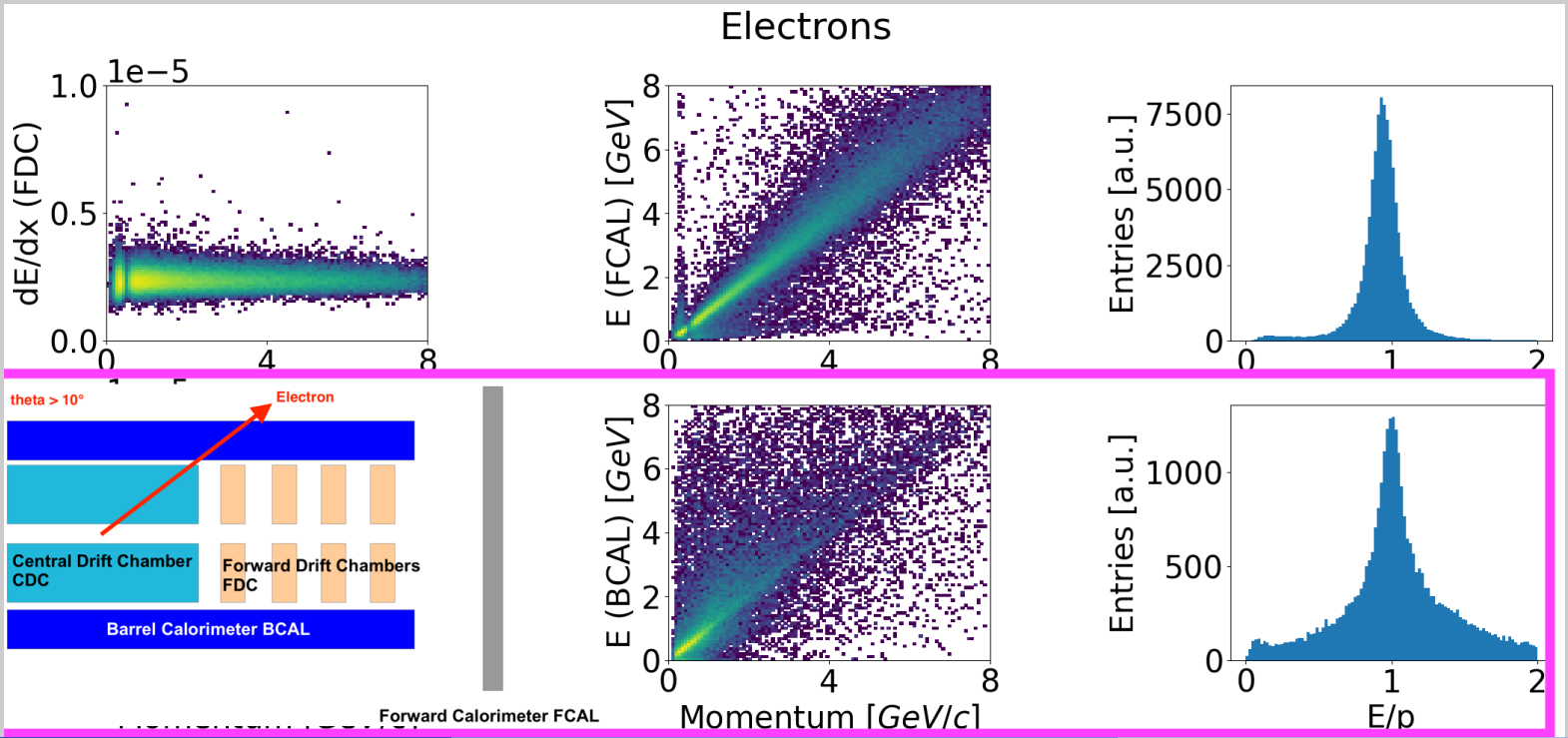

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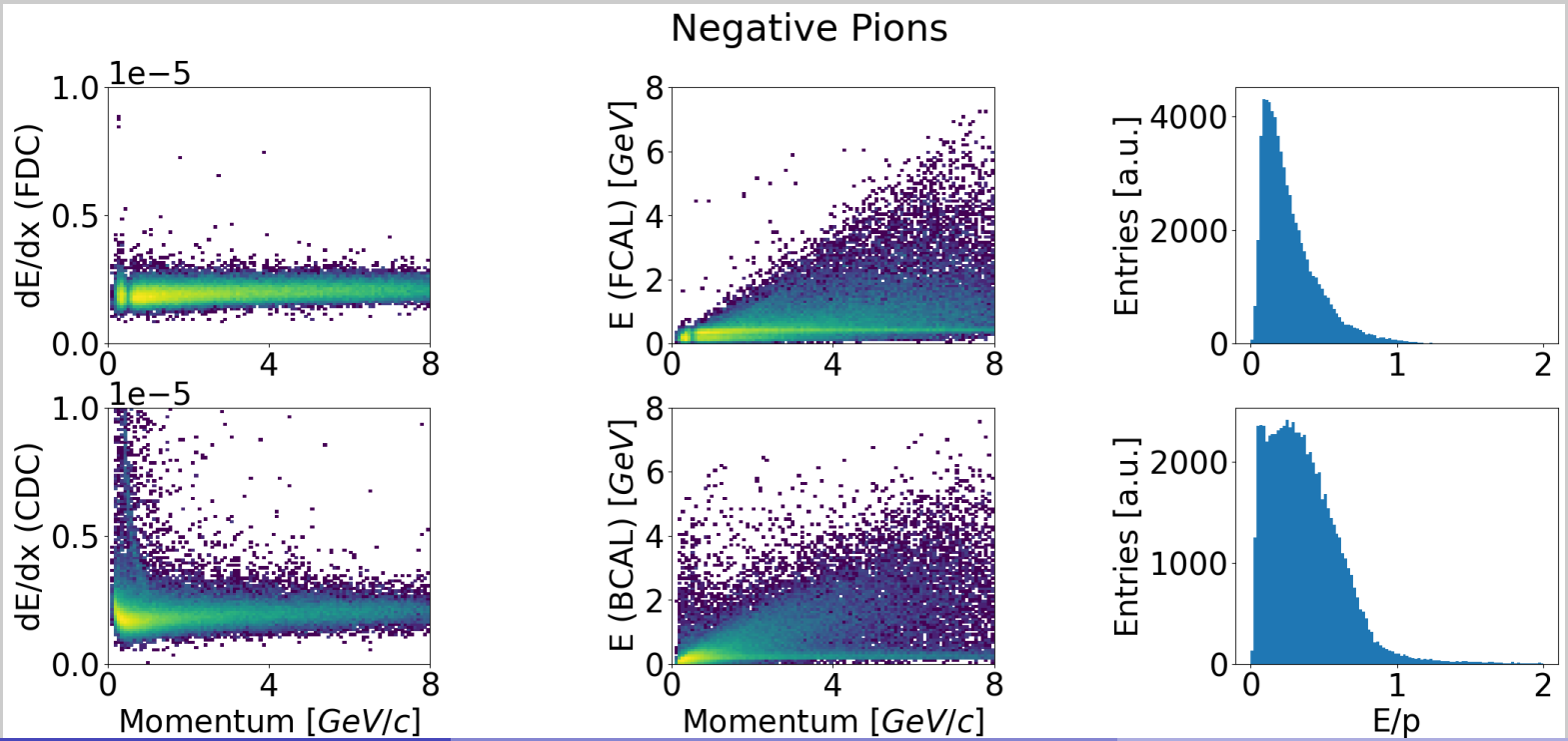

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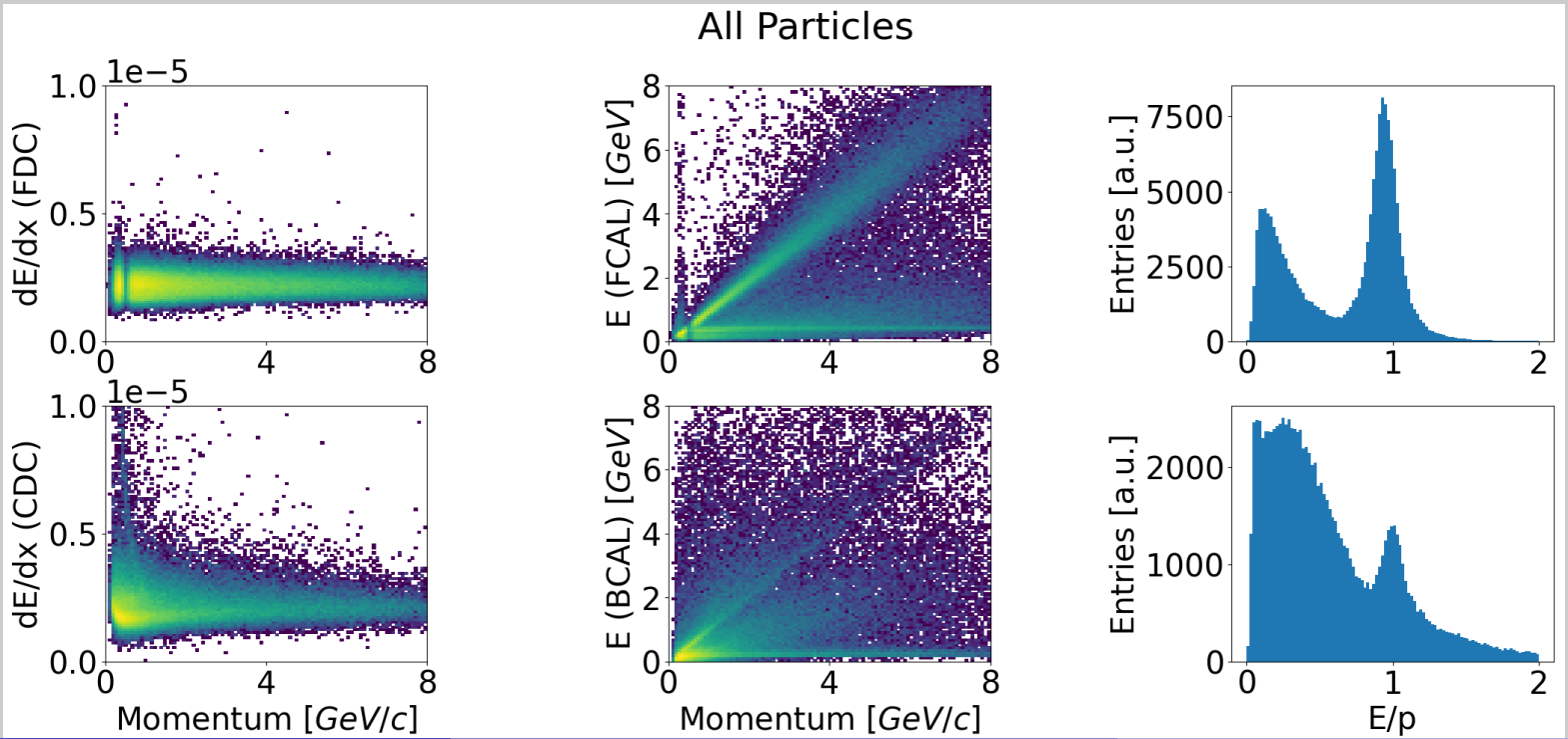

Reference Analysis

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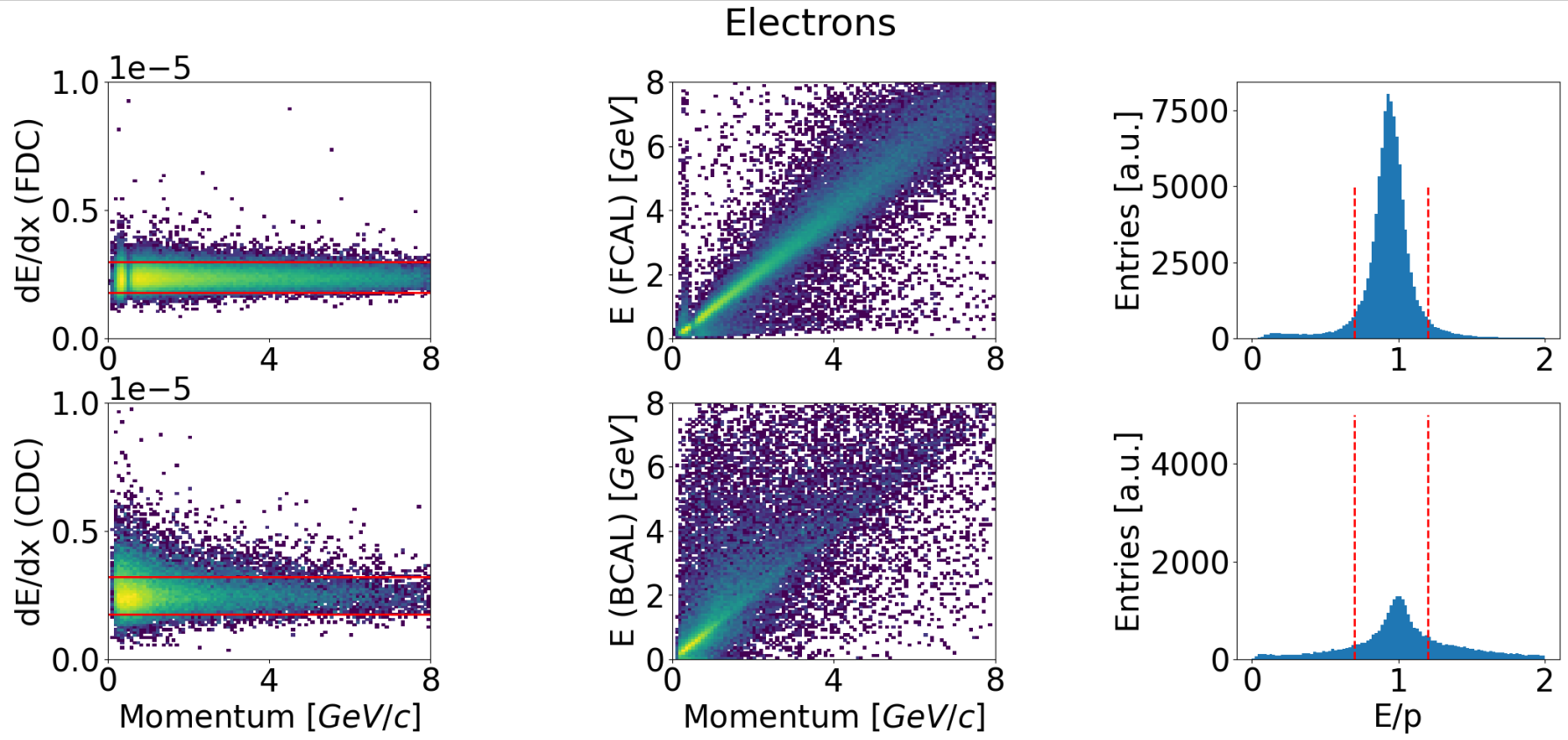

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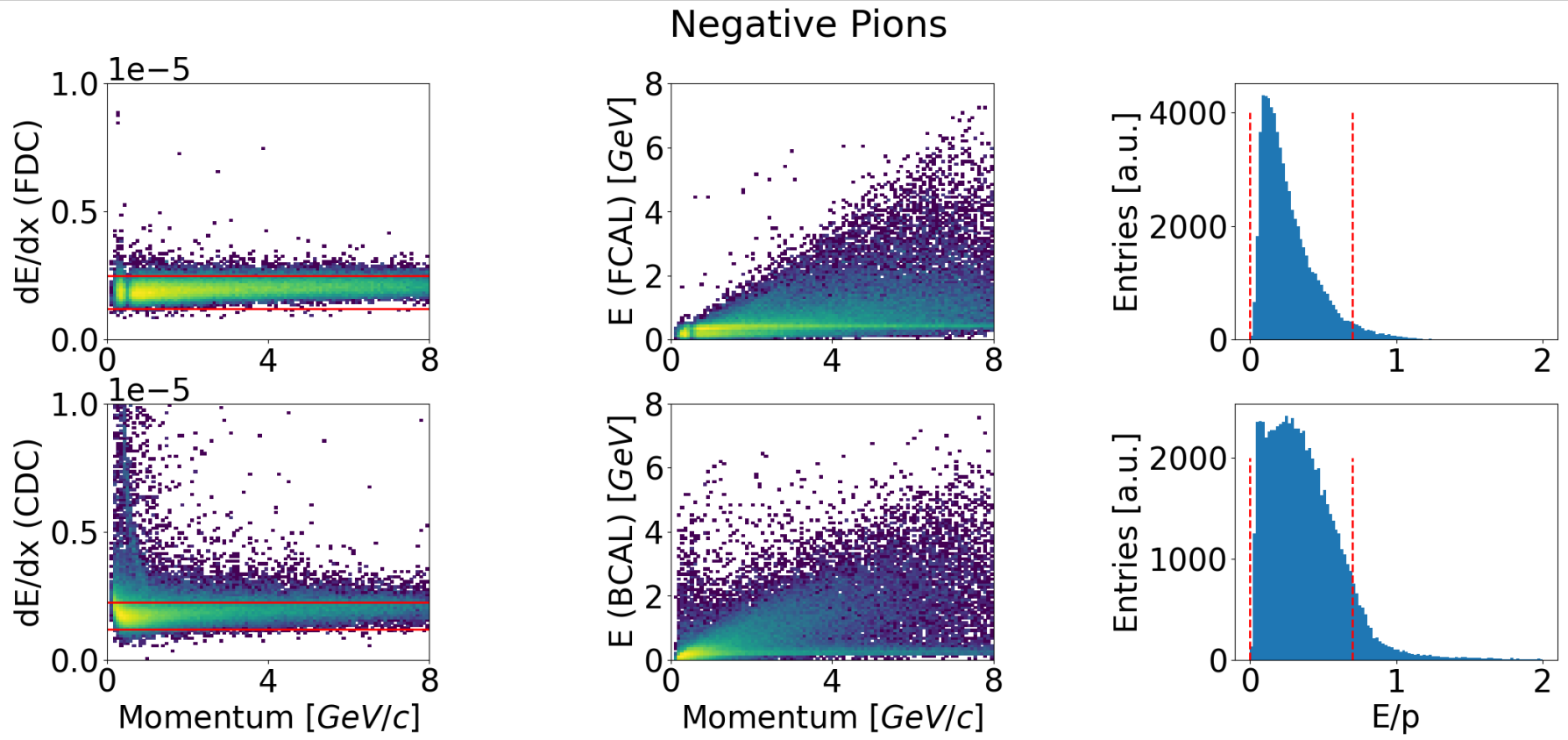

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- These are the building blocks for nearly all classification performance metrics

Identification Rates

Particle	True Positive Rate (TPR)	False Positive Rate (FPR)
Electrons	0.85	0.11
Negative Pions	0.89	0.15

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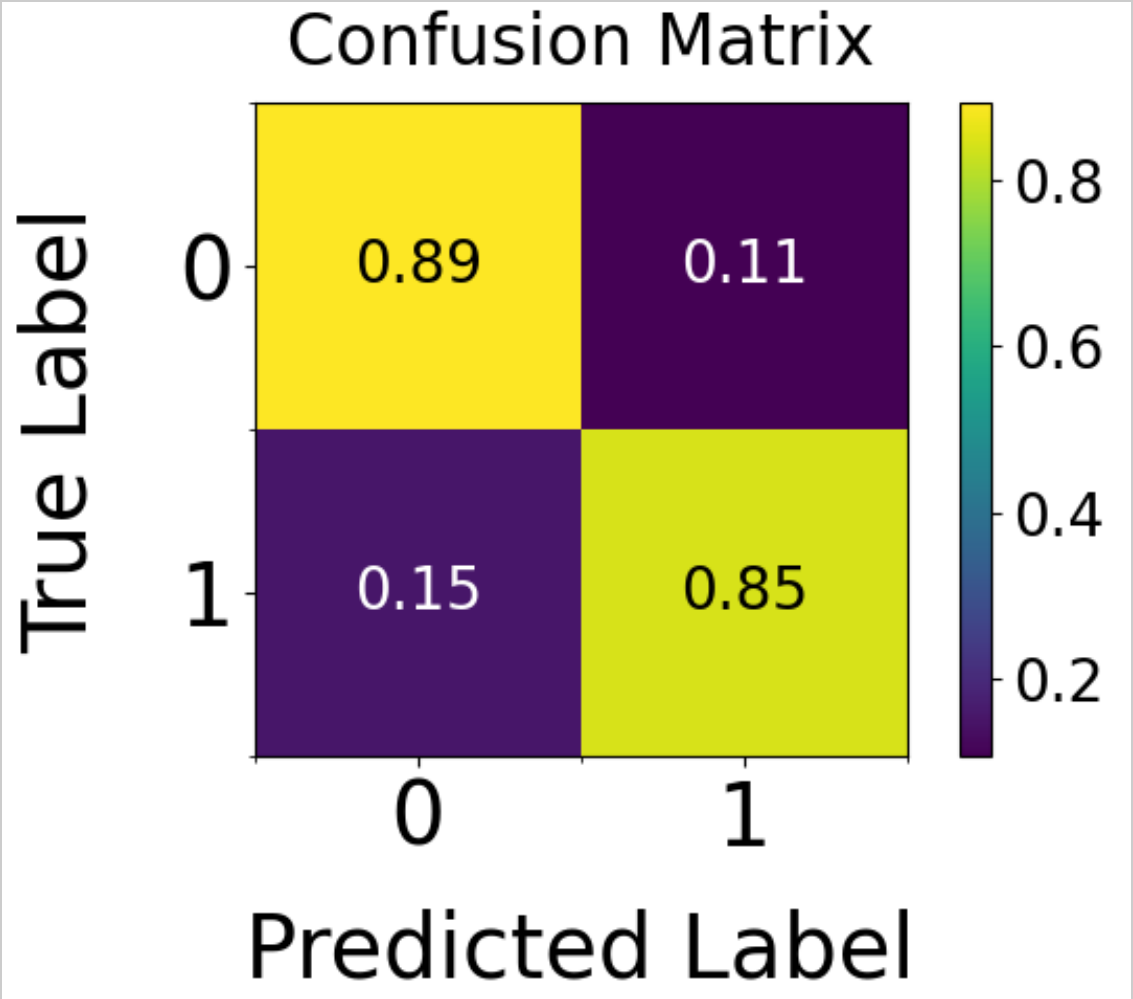
The Confusion Matrix



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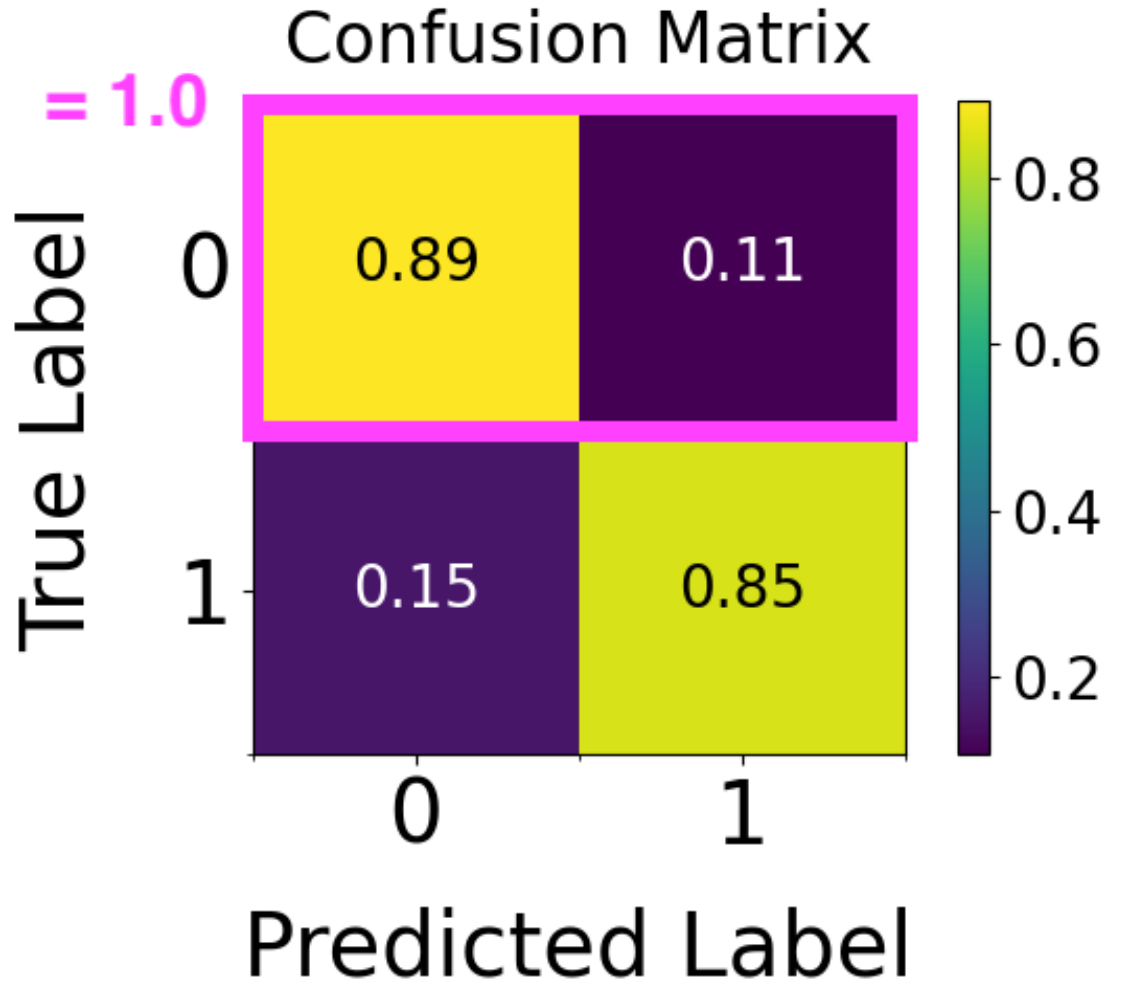

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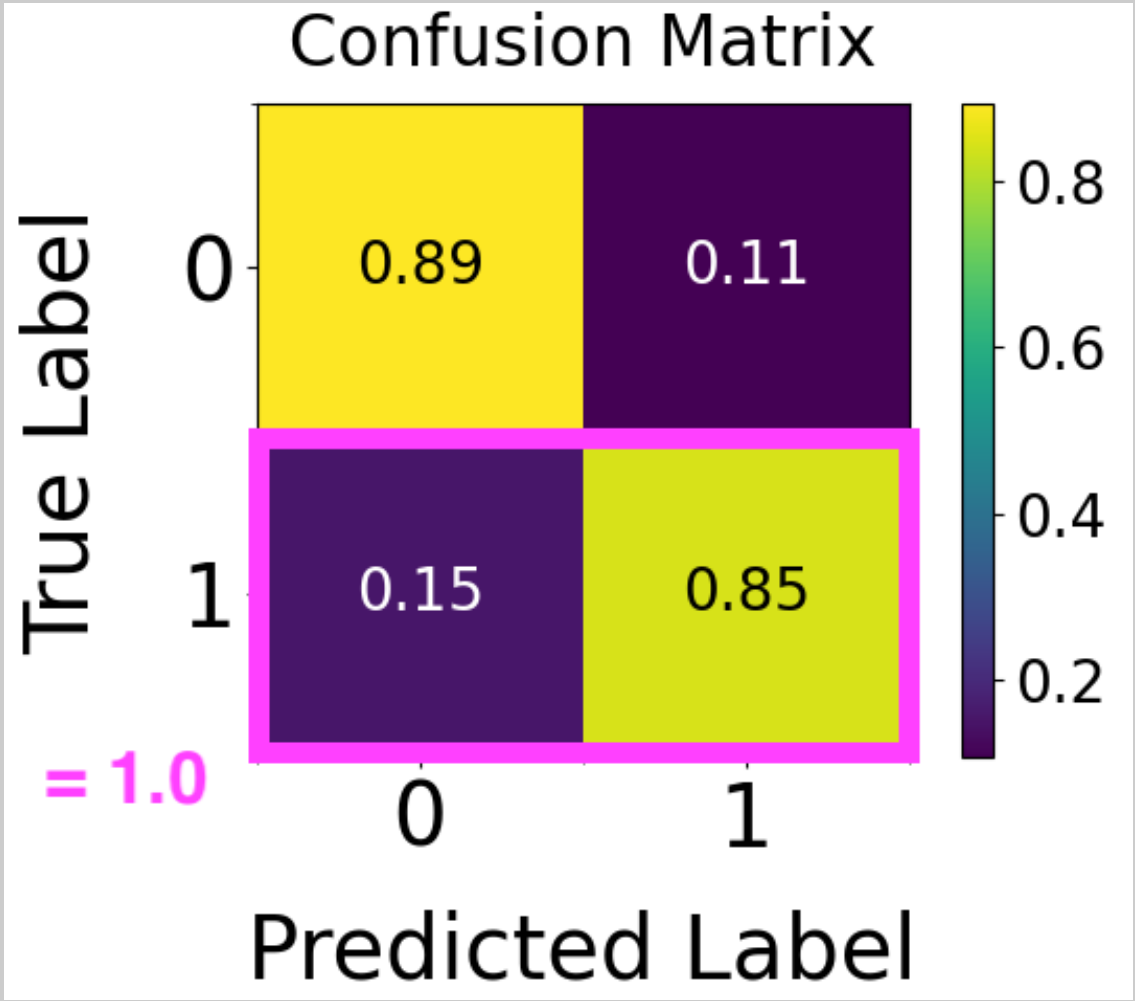

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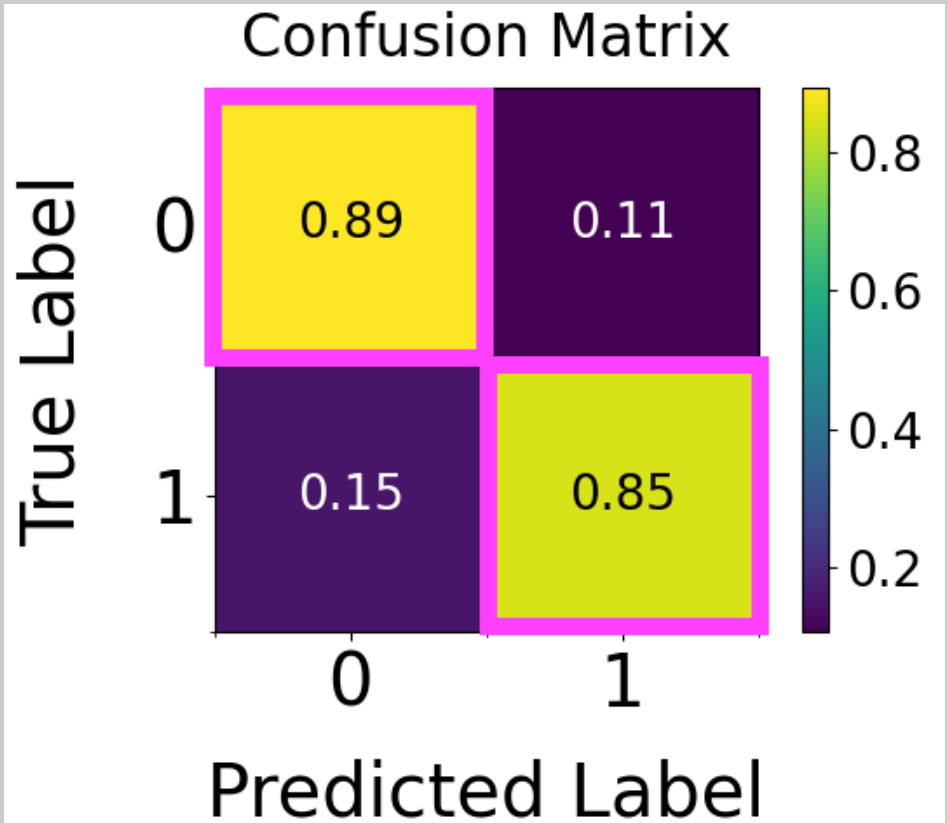
The Accuracy

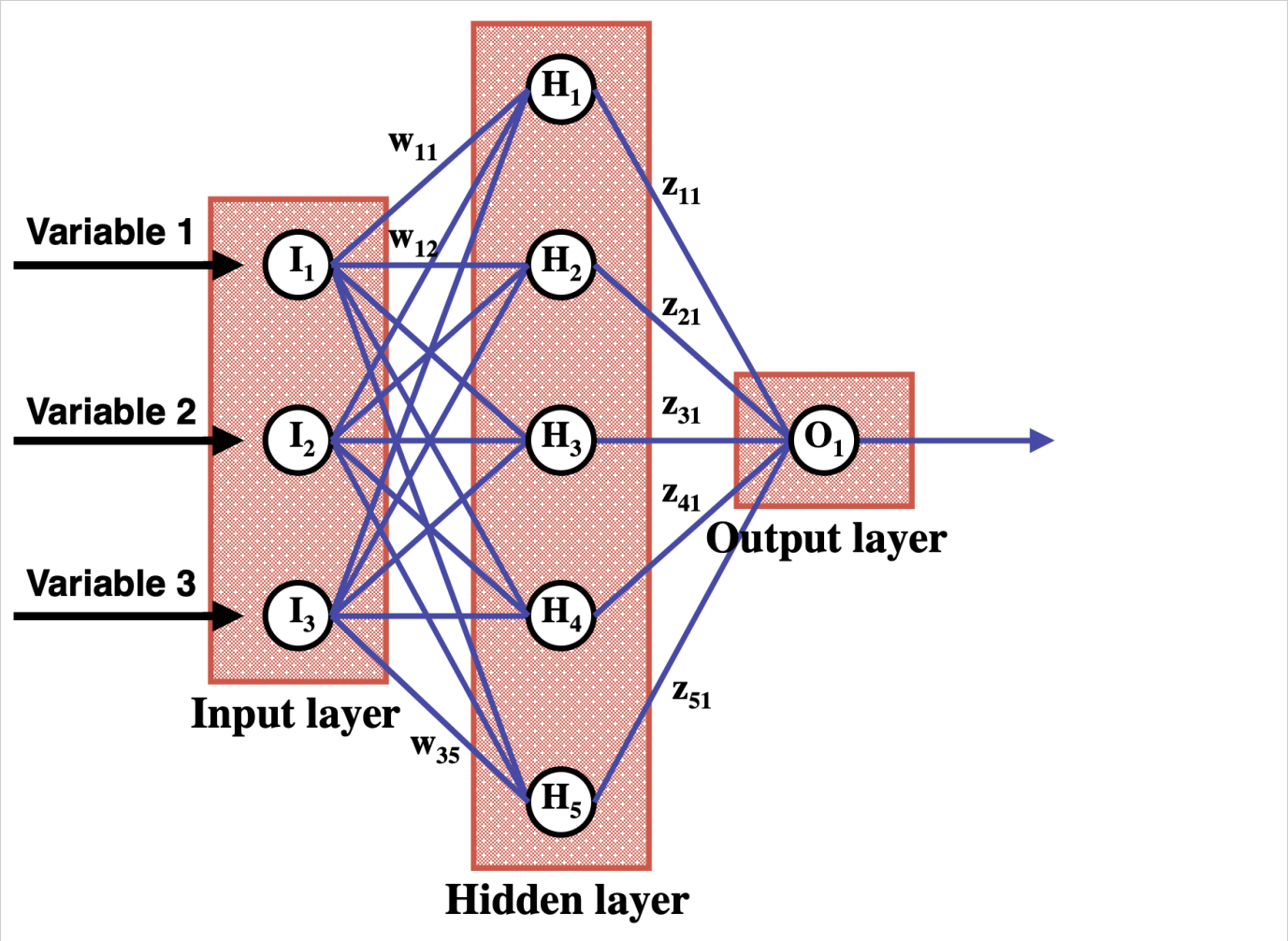
- Many performance metrics can be (directly) derived from the confusion matrix
- **Example: Accuracy** $= \vec{diag} \cdot \vec{R} = \sum_{i}^{\#species} TPR(i) \cdot R(i)$
- R(i) denotes abundance of each particle species in the data
- Balanced data (each species equally represented): R(i) = 1 / number species
- **Here: R(i) = 0.5 and Accuracy** $= 0.89 \cdot 0.5 + 0.85 \cdot 0.5 = 0.87$



Can we do better?

- Would like to optimize PID $\Rightarrow$ TPR = 1 / FPR = 0
- Could tune E/p by hand $\rightarrow$ Tedious and does not use all information
- Input features:
  1.) Is particle detected in forward / central part of GlueX $\equiv \theta$
  2.) Particle Momentum
  3.) Information from forward drift chamber (FDC)
  4.) Information from forward calorimeter (FCAL)
  5.) Information from central drift chamber (CDC)
  6.) Information from central calorimeter (BCAL)
- **Stone-Weierstrass-Theorem**(1990): "[...] there are no nemesis functions that cannot be modeled by neural networks"

The Multilayer Perceptron



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- **Architecture:** Hidden layers with a set of neurons

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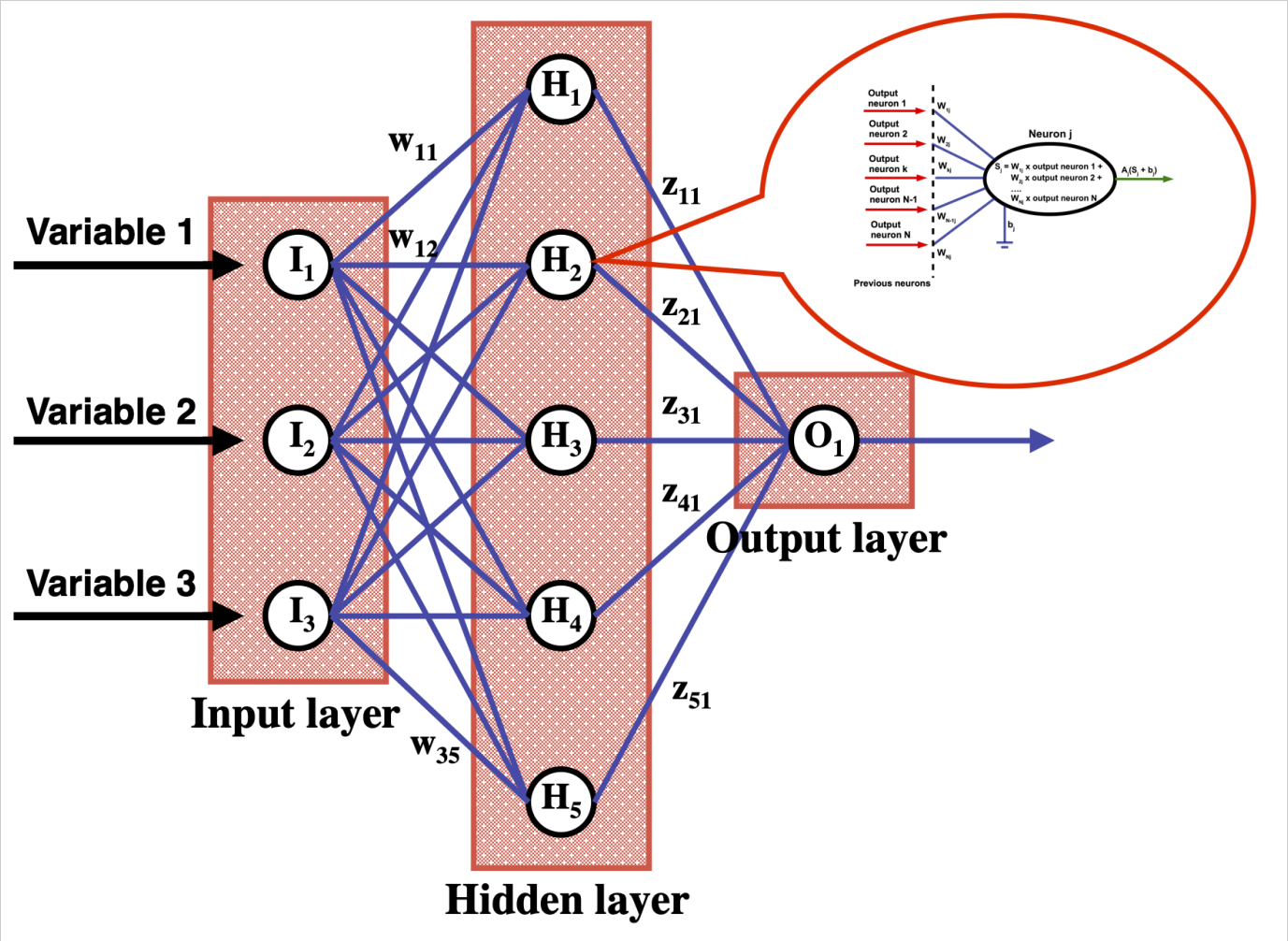

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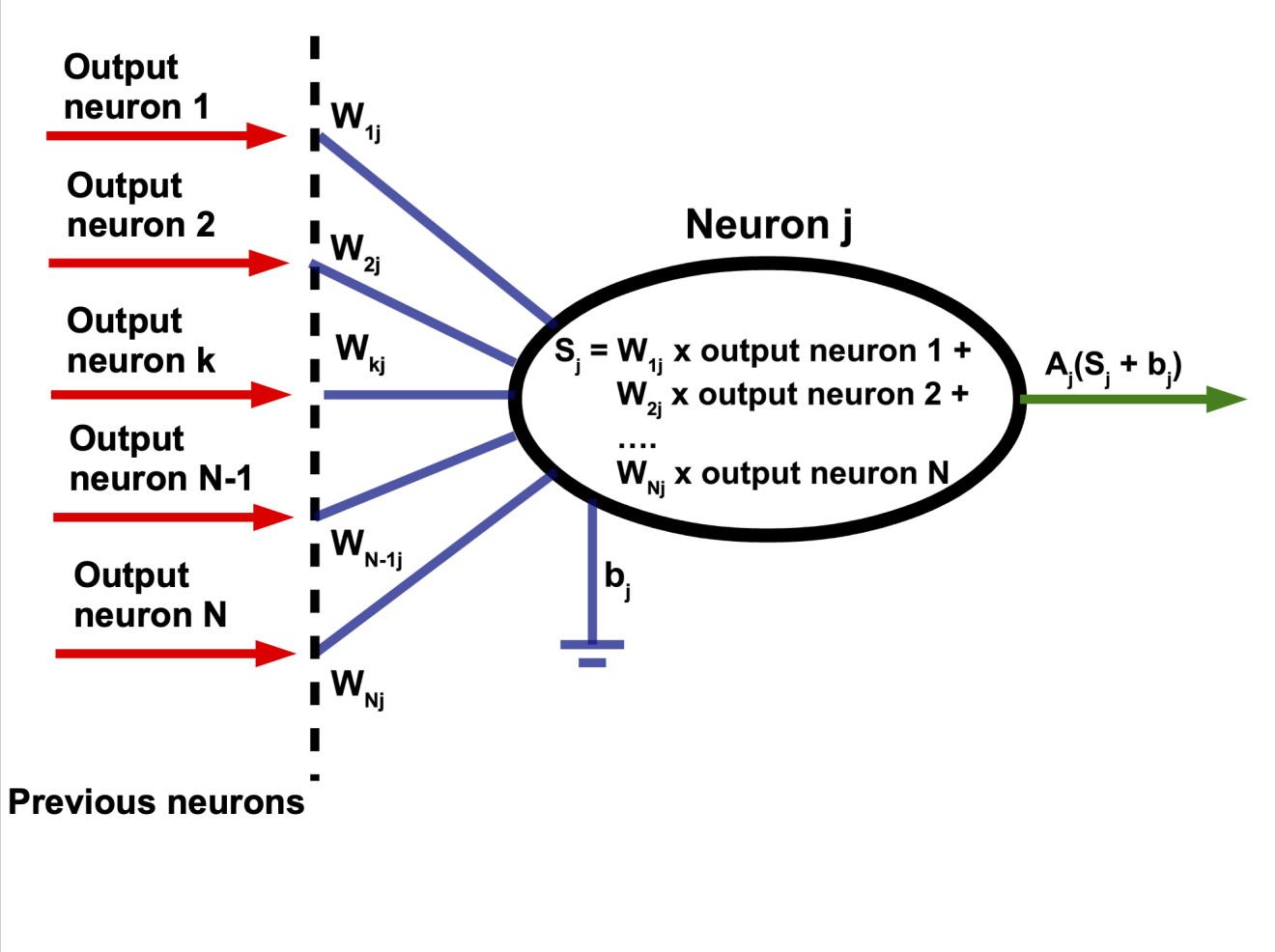
A single Neuron



Basic ingredients:

- Information from previous neurons
- Weights and bias
- Activation function

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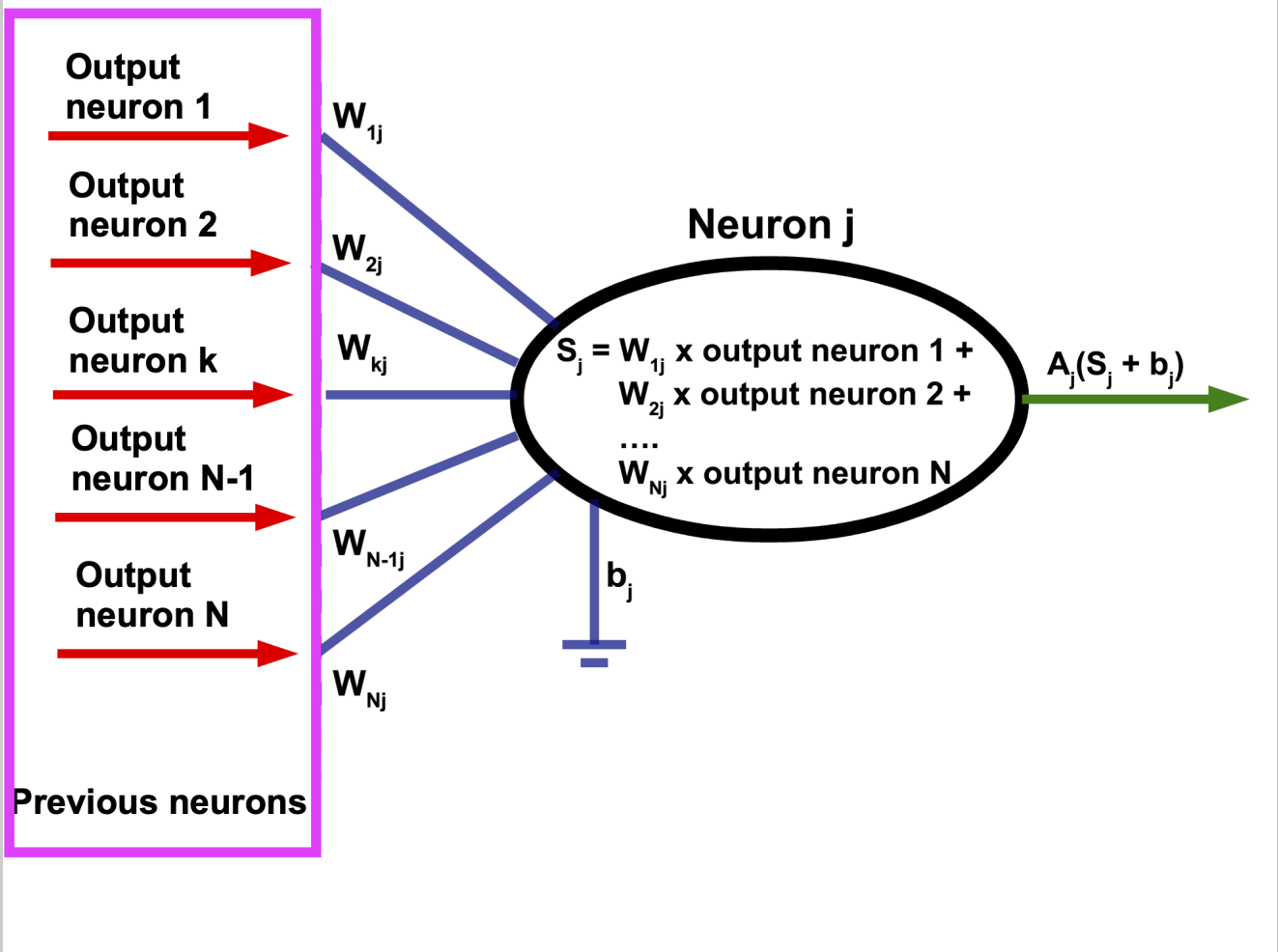

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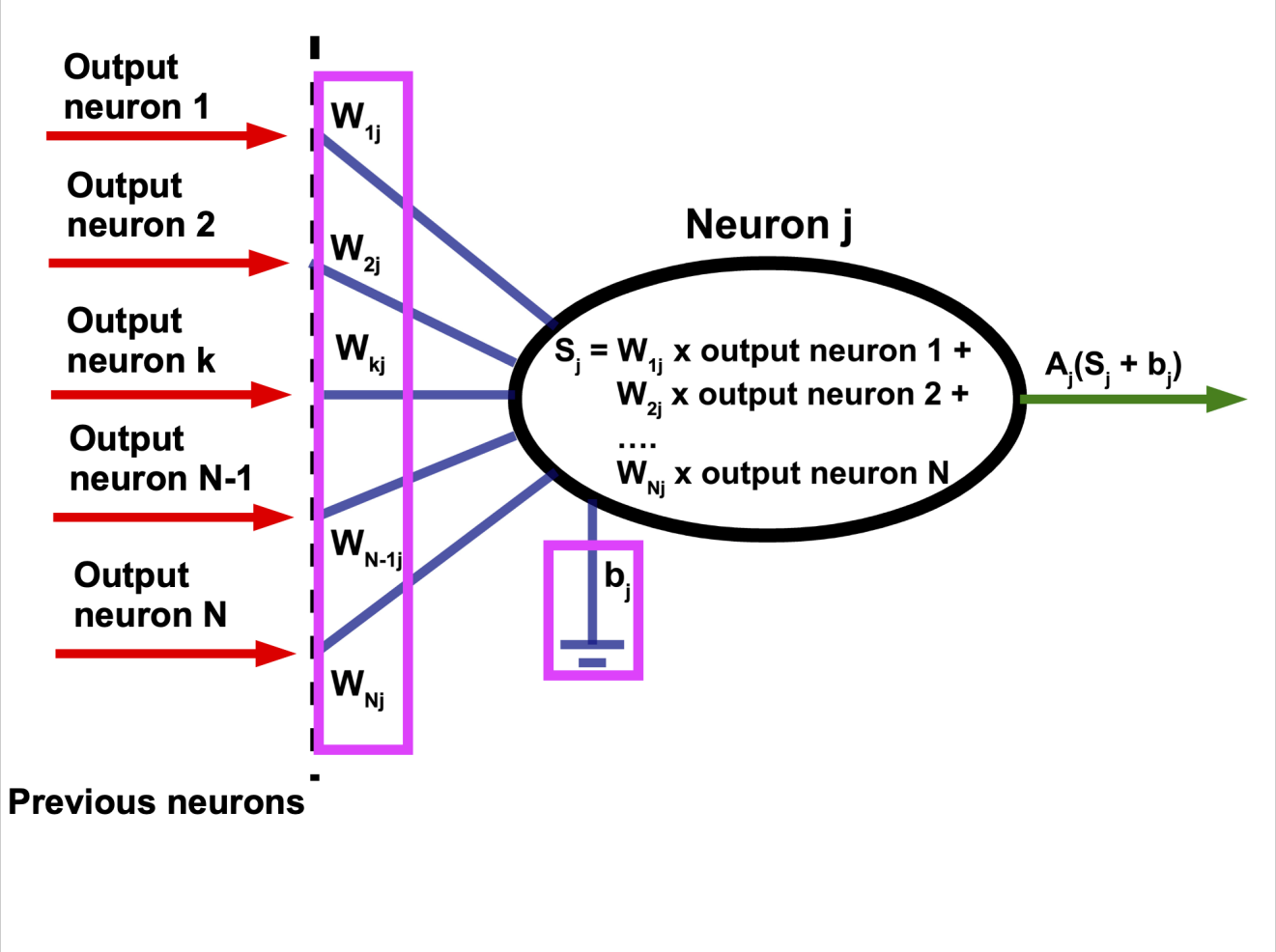

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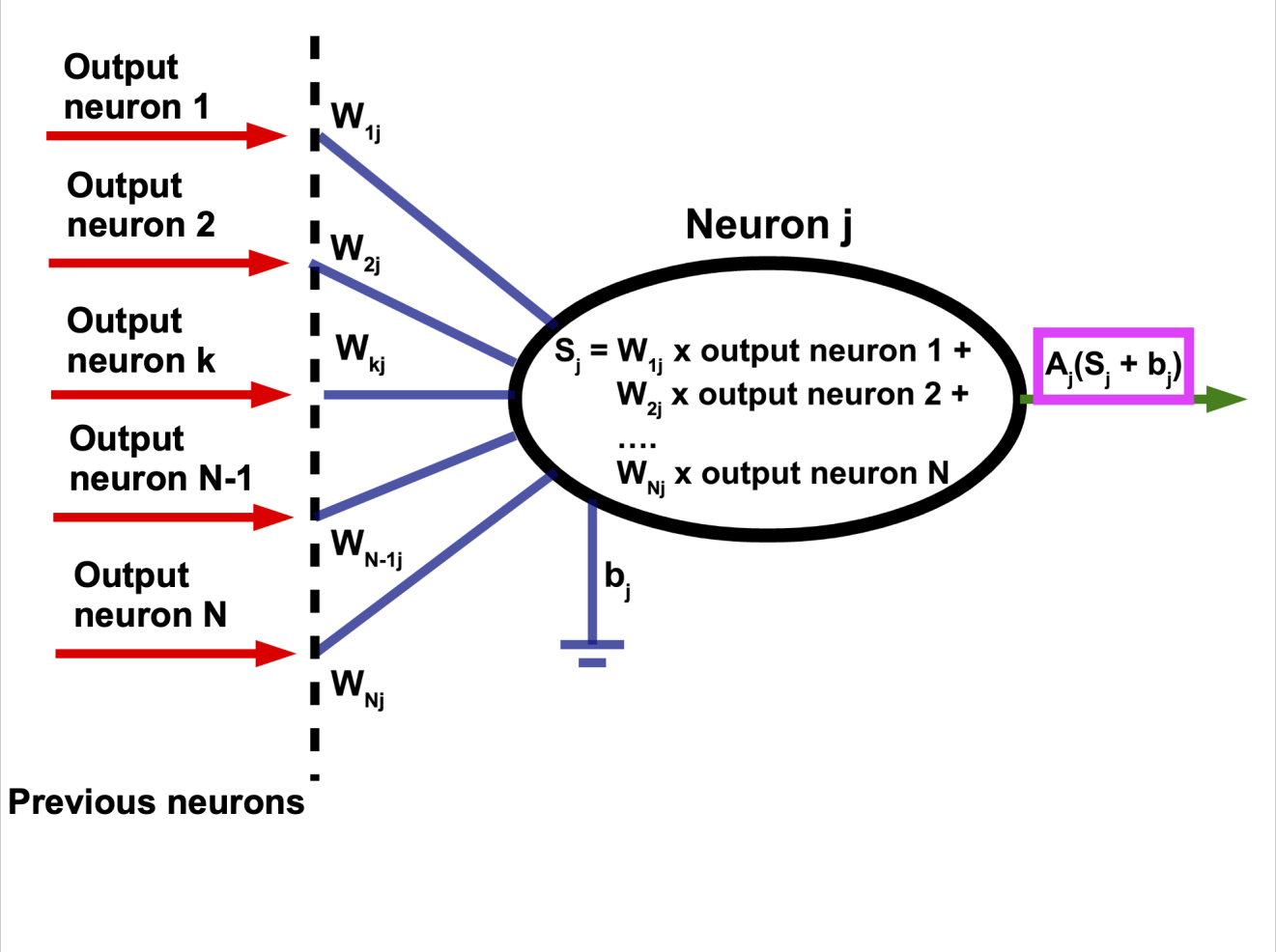

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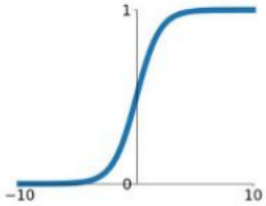
Activation Functions

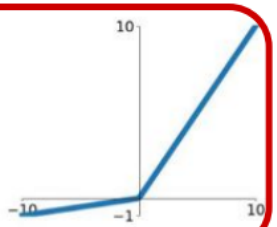
Sigmoid

$$\sigma(x) = \frac{1}{1+e^{-x}}$$



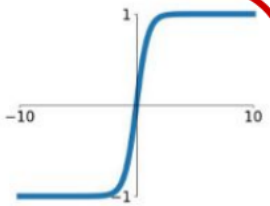
Leaky ReLU

$$\max(0.1x, x)$$



tanh

$$\tanh(x)$$

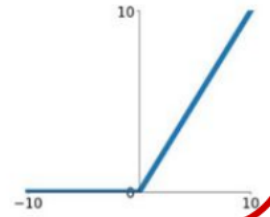


Maxout

$$\max(w_1^T x + b_1, w_2^T x + b_2)$$

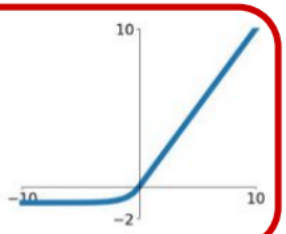
ReLU

$$\max(0, x)$$



ELU

$$\begin{cases} x & x \geq 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$$



Most commonly used in modern networks as hidden layer activations

Activation function plots taken from Mustafa Mustafas lecture at the: deep learning for science school 2019

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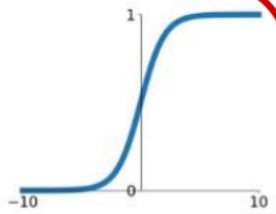

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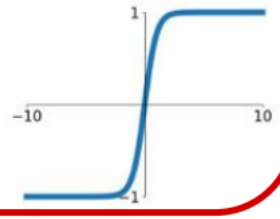

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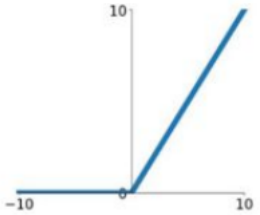

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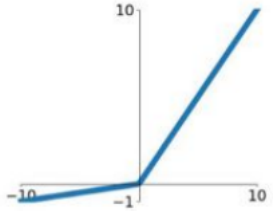

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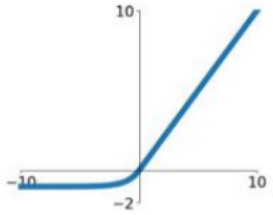
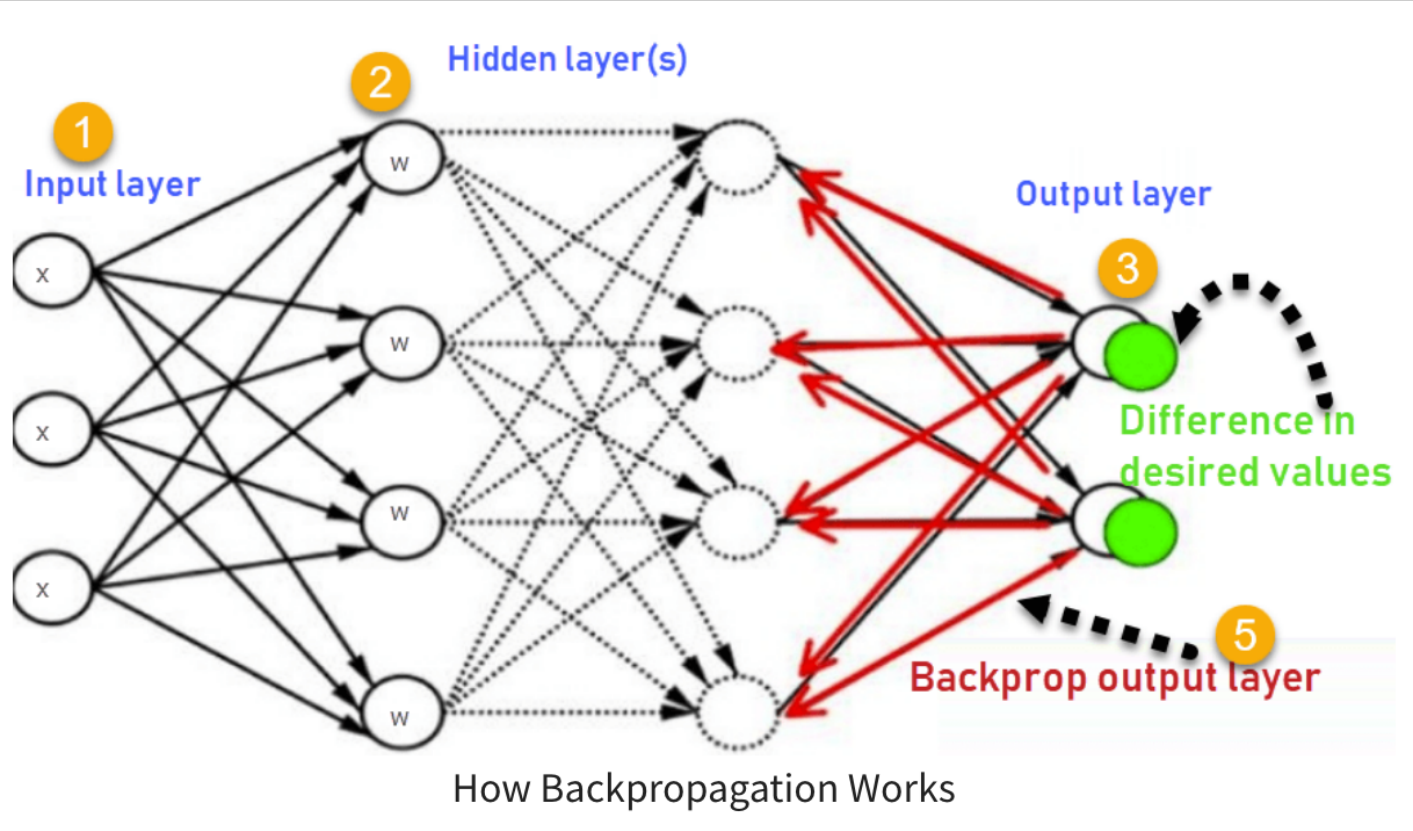


Often used for output layers

Activation function plots taken from Mustafa Mustafas lecture at the: deep learning for science school 2019

Training a Neural Network: Backpropagation

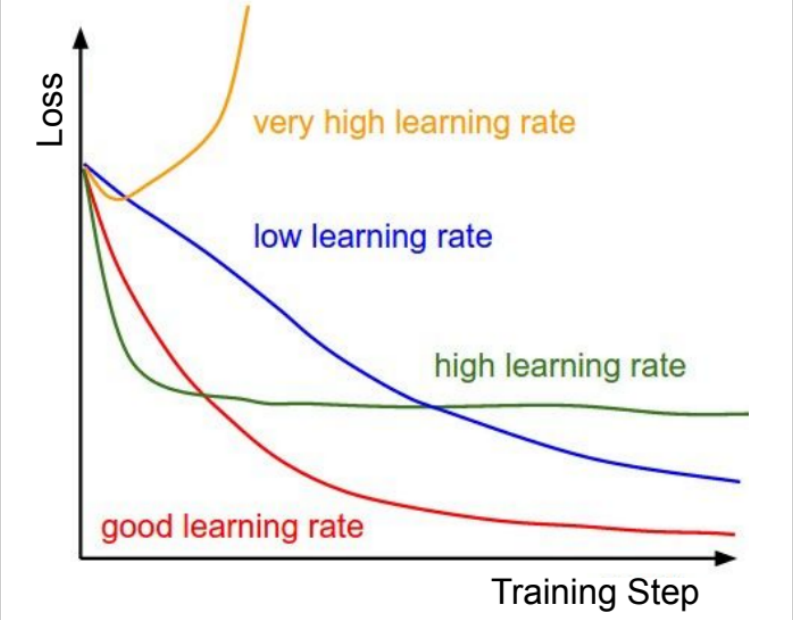


How Backpropagation Works

- Pass data forward
- Calculate error
- Pass error backward to update weights

Picture taken from here

Training a Neural Network: Updating Weights and Convergence



- **Goal:** Find minimum error (loss) as fast as possible:

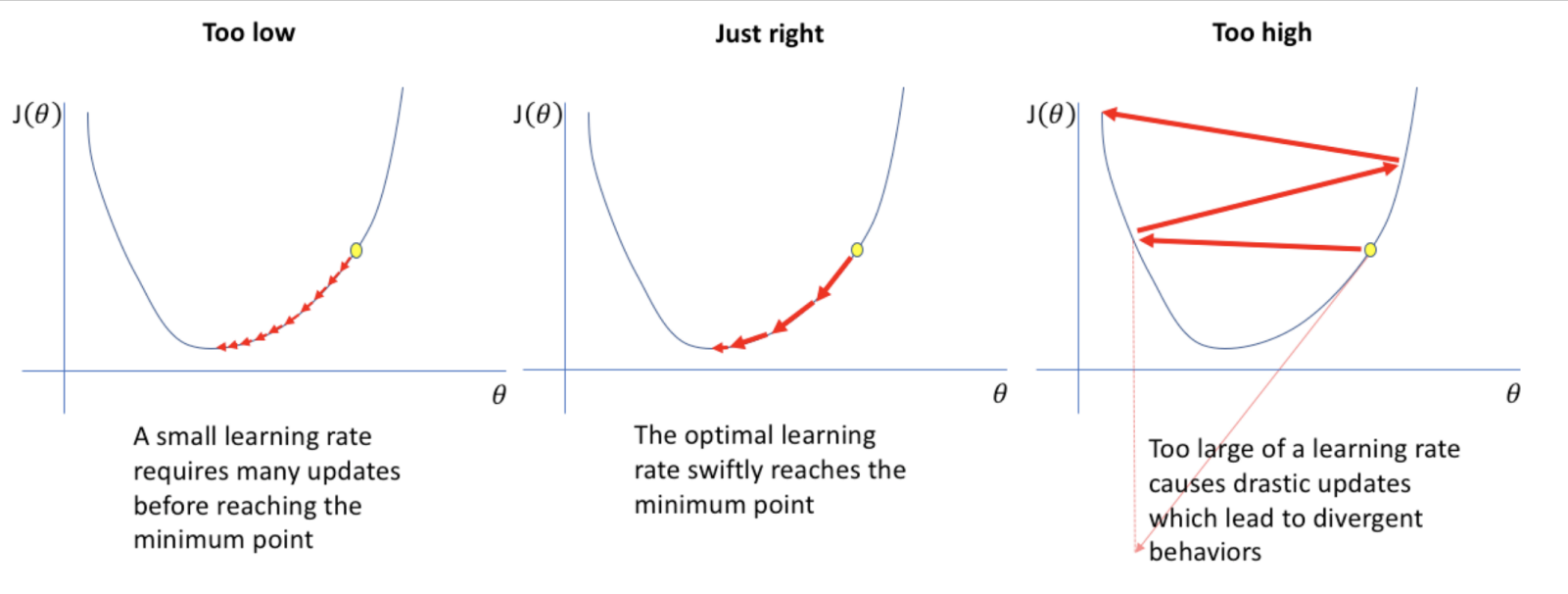
$$0 \stackrel{!}{=} d(Error) \propto \sum_i \sum_j \frac{\partial \text{Error}}{\partial w_{ij}} dw_{ij} \tag{1}$$

- Use:

$$\textbf{Gradient Descent: } \boldsymbol{w_{k+1} = w_k - \eta \nabla \text{Error}(w_k)} \tag{2}$$

- Error $\propto$ prediction - truth
- η : Learning rate

Training a Neural Network: Updating Weights and Convergence



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Validation Data and Generalizability

- Want to enable network to abstract / generalize on unknown data AND avoid overfitting (i.e. avoid that network reproduces features from training data only)

Picture taken from Brenda Ngs introductory talk at the: deep learning for science school 2019

Validation Data and Generalizability

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- **Validation Data:** Part of training data that is NOT used to update internal parameters[1], but used to determine when training is complete

[1] This data is "unseen" by the algorithm during the training stage

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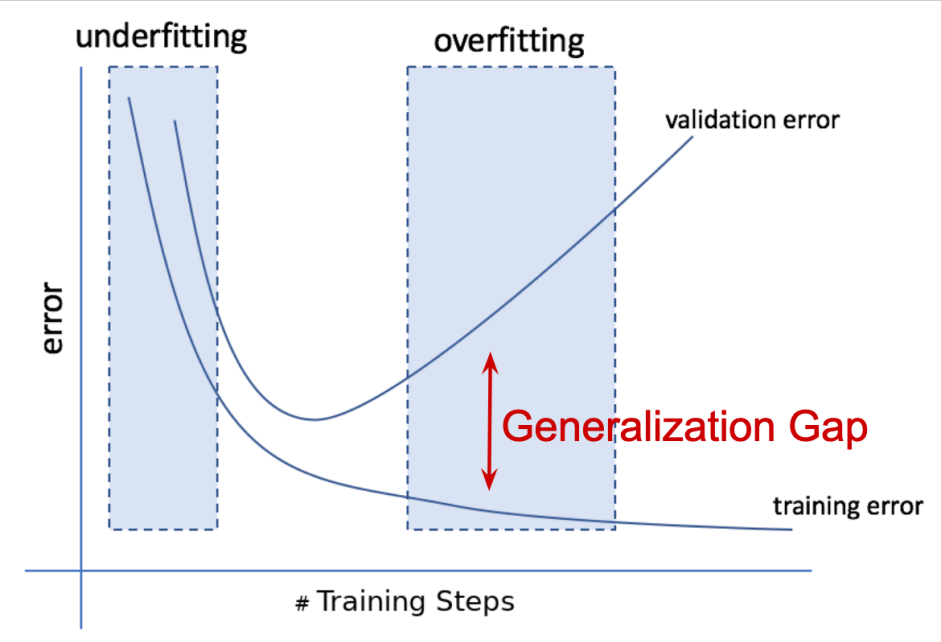

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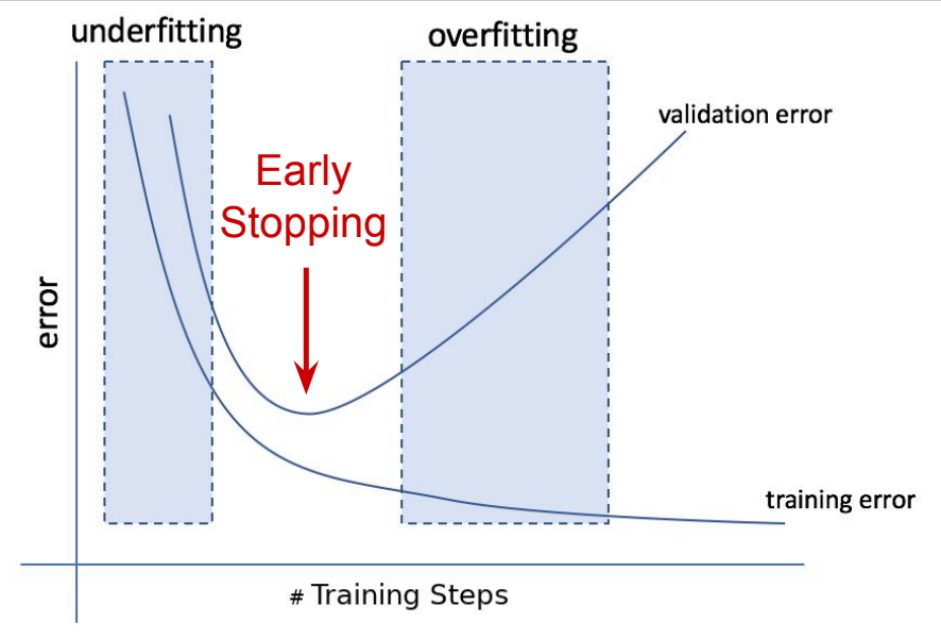

Picture taken from Mustafa Mustafas talk at the: deep learning for science school 2019

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Setting up and training a Neural Network in Scikit

```
from sklearn.neural_network import MLPClassifier

#Set up the network:
 my_mlp = MLPClassifier(
     hidden_layer_sizes=(8,5), #two hidden layers with 8/5 neurons
     activation='relu', #rectified linear unit function
     solver='sgd', #stochastic gradient descent optimizer #--> minimize error
     max_iter = 200, #maximum number of learning epochs
     validation_fraction=0.5, #--> Use 50$\%$ of data for validation
     early_stopping=True,#--> Use early stopping
     learning_rate_init = 0.05 #step size for the gradient
  )
```

Setting up and training a Neural Network in Scikit

```
#Train the network:
my_mlp.fit(X,Y)
#X = input data (energies, momenta,..)
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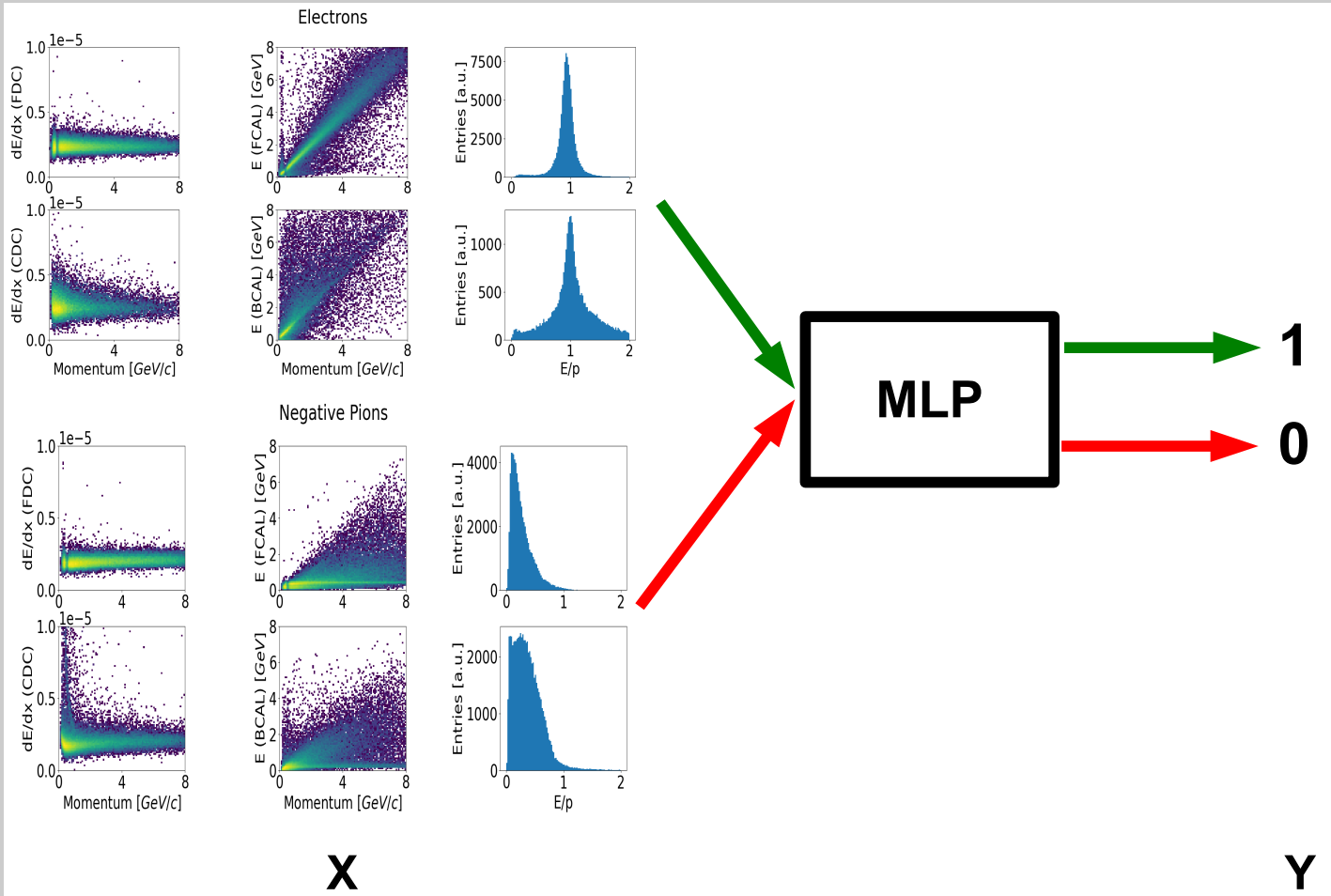

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  #Get the loss curve and validation score:
  loss_curve = my_mlp.loss_curve_
  val_score = my_mlp.validation_score_
```

Setting up a Neural Network in TF/Keras

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import tensorflow as tf

#1.) Set up the sequential model:
my_mlp = tf.keras.Sequential(name='keras_mlp')
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my_mlp = tf.keras.Sequential(name='keras_mlp')
#2.) Define the input layer:
input_layer = tf.keras.layers.Input(shape=(6,),name='input')
#3.) Define hidden layer(s):
dense_layer_1 = tf.keras.layers.Dense(8,'relu',name='dense_1')
dense_layer_2 = tf.keras.layers.Dense(5,'relu',name='dense_2')
#5.) Define the output layer:
output_layer = tf.keras.layers.Dense(1,'sigmoid',name='output')
#6.) Put the all the layers together:
my_mlp.add(input_layer)
my_mlp.add(dense_layer_1)
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my_mlp.add(output_layer)
#7.) Define the loss-function:
mlp_loss = tf.keras.losses.binary_crossentropy
#8.) Define the optimizer:
mlp_optimizer = tf.keras.optimizers.SGD(learning_rate=0.05)
#9.) Compile the model and get a summary:
my_mlp.compile(optimizer=mlp_optimizer,loss=mlp_loss,metrics=['accuracy'])
my_mlp.summary()
```

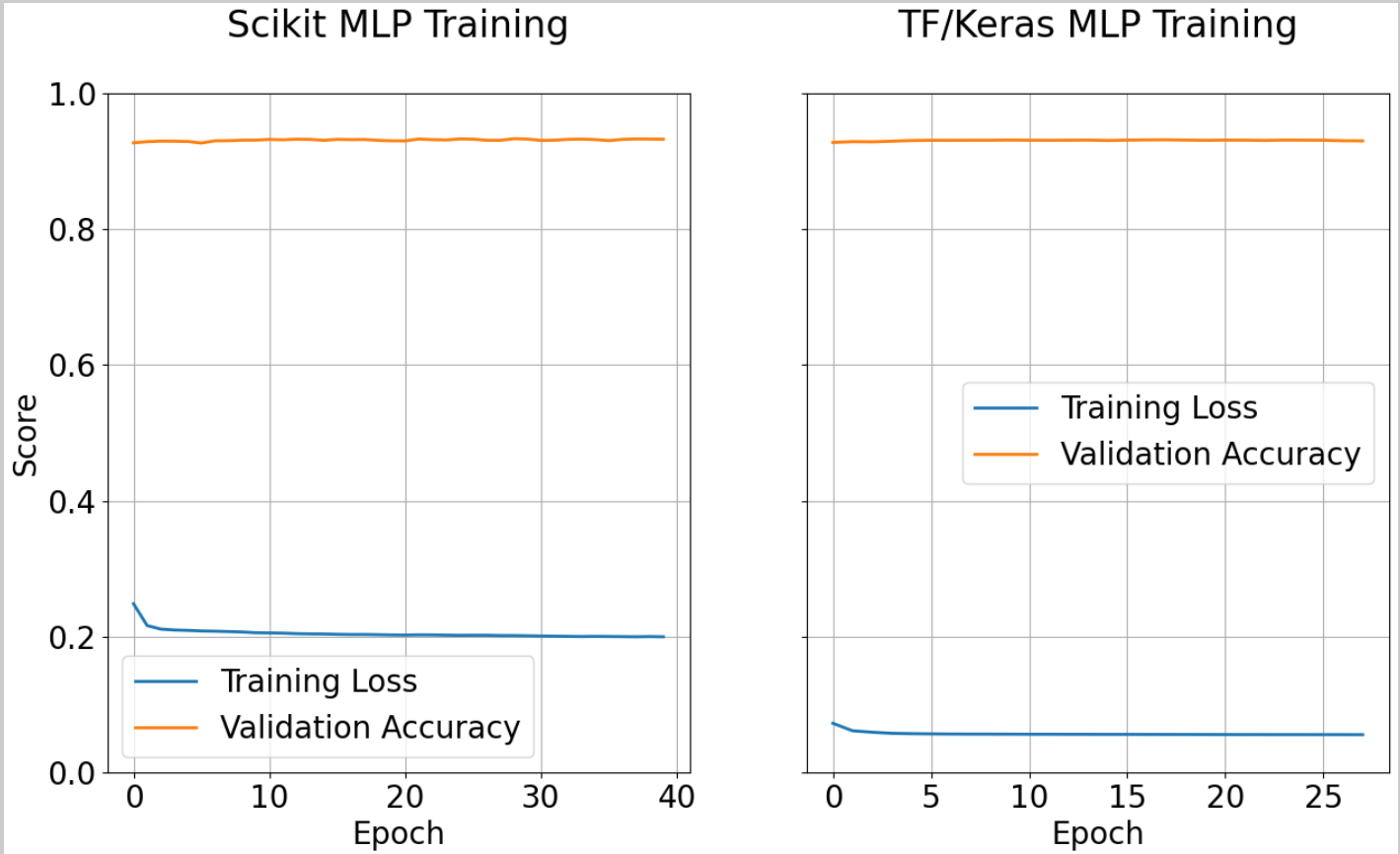
Training a Neural Network with TF/Keras

```
Model: "keras_mlp"
_________________________________________________________________
Layer (type)                 Output Shape              Param #
=================================================================
dense_0 (Dense)              (None, 8)                 56
_________________________________________________________________
dense_1 (Dense)              (None, 5)                 45
_________________________________________________________________
output (Dense)               (None, 1)                 6
=================================================================
Total params: 107
Trainable params: 107
Non-trainable params: 0
_________________________________________________________________
```

```
#Train the network
training_history = my_mlp.fit(
      x=X, #X = input data (energies, momenta,..)
      y=Y,  #Y = target labels (0: pions / 1: leptons)
      validation_slpit=0.5, #--> Use 50$\%$ of data for validation
      callbacks=tf.keras.EarlySopping() #--> Customize the
      #early stopping function
)

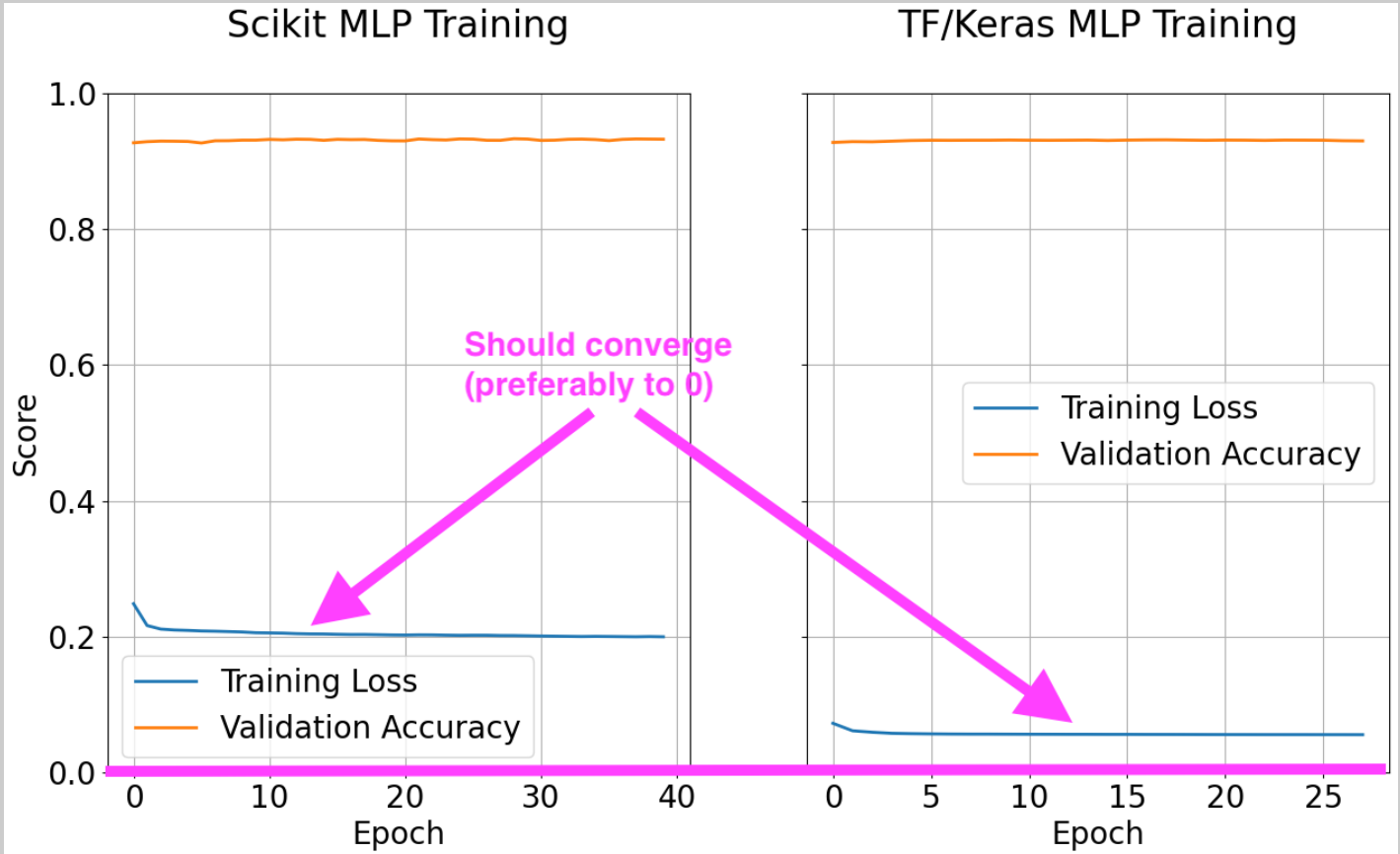
#Get the training loss and validation score:
loss_curve = training_history.history['loss']
val_score = training_history.history['val_accuracy']
```

Inspecting the learning Curves



- **NOTE(S):**
  - Most settings (e.g. architecture, loss,..) are similar for both networks
  - Did not tune individual parameters
- Both networks show similar accuracy

Inspecting the learning Curves



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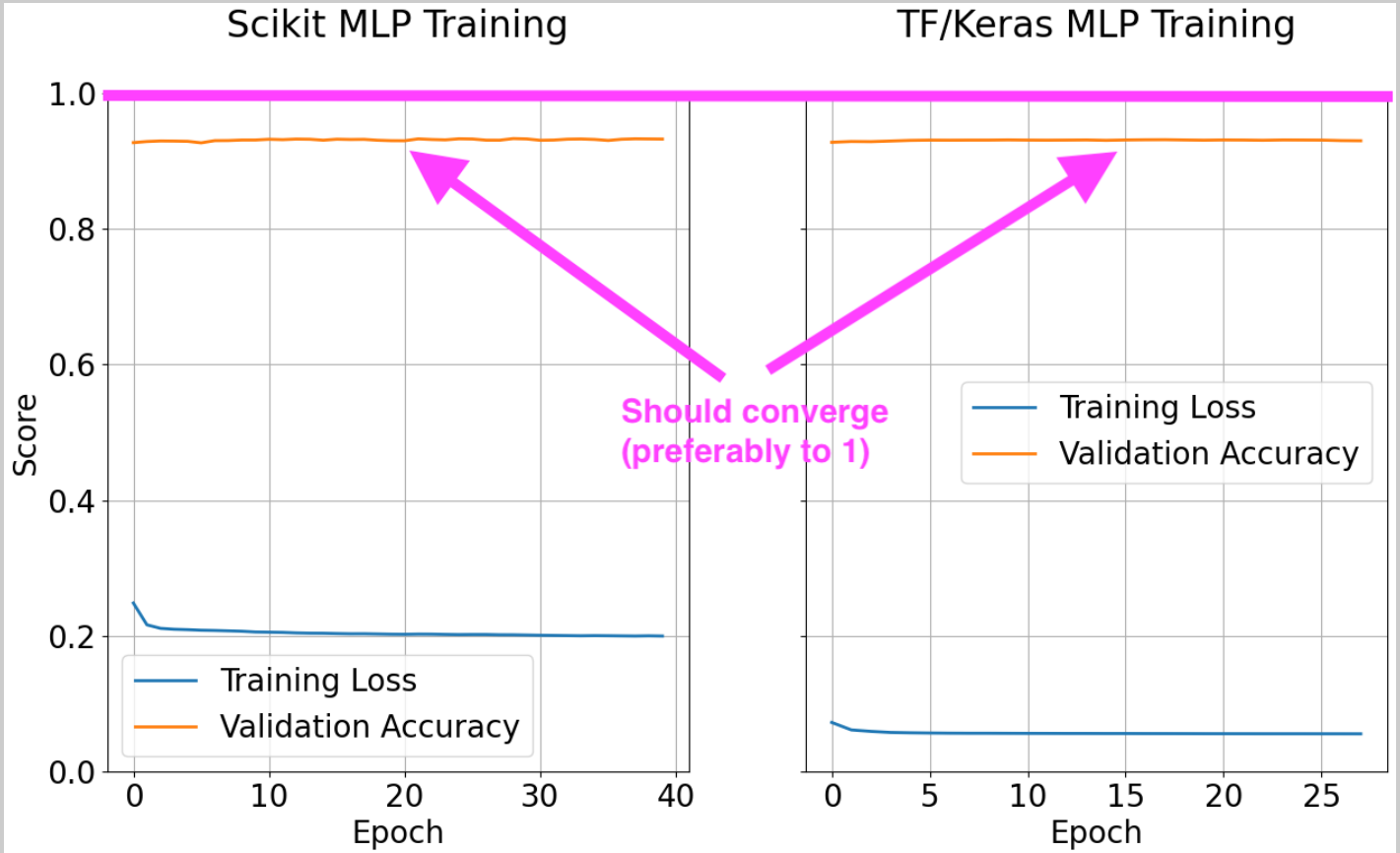

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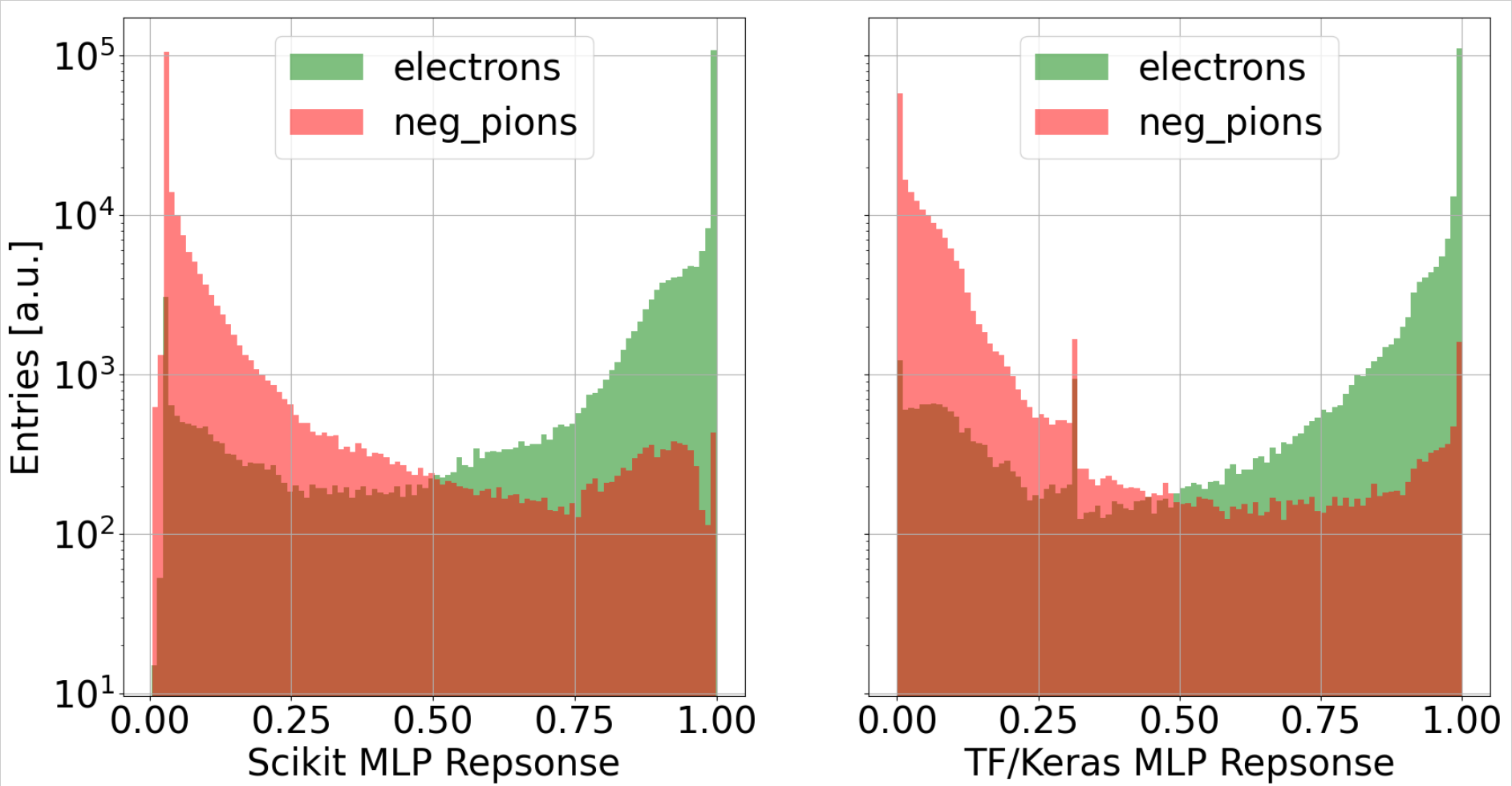
Network Responses

One of the very first things to check!



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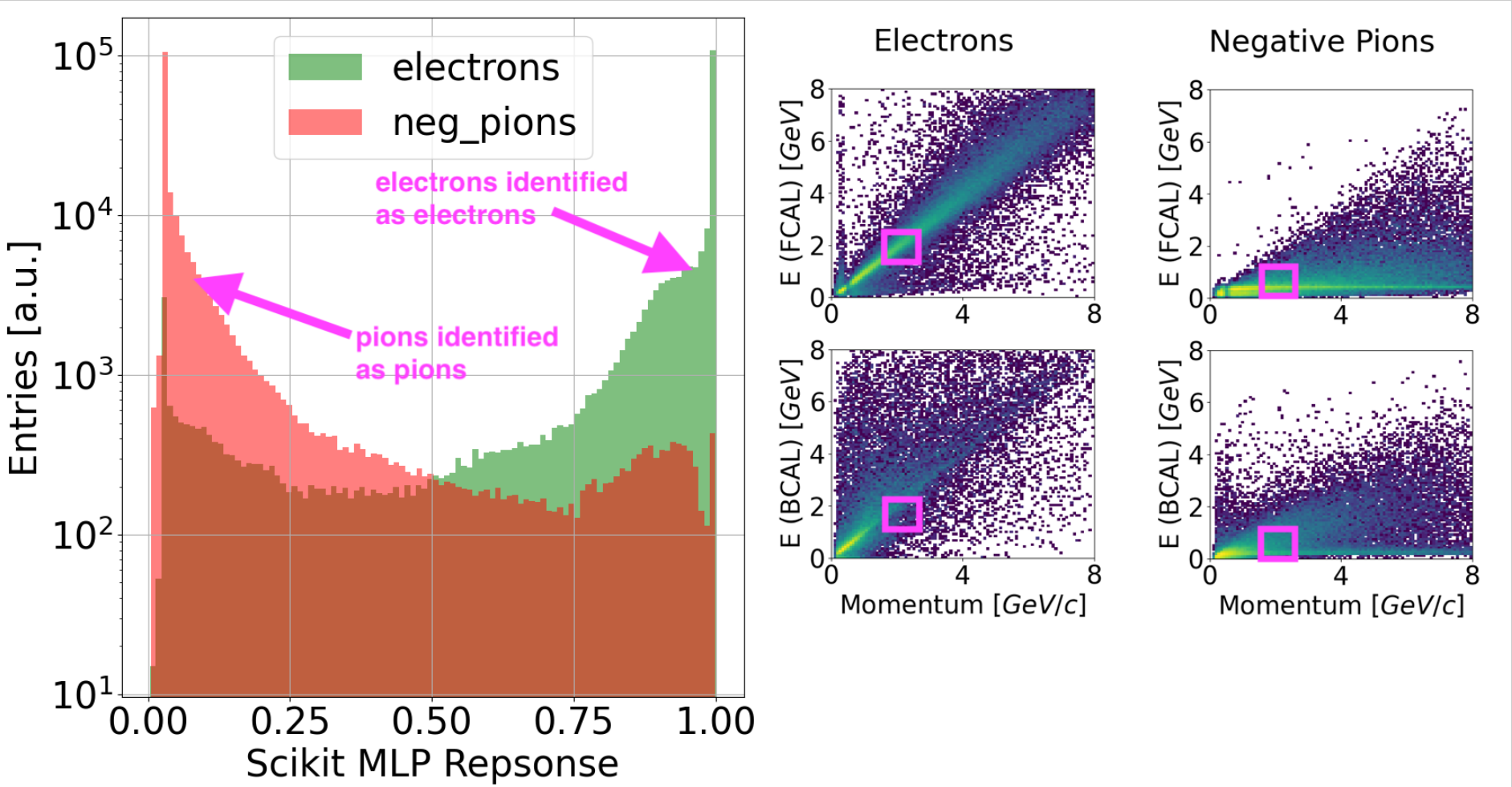

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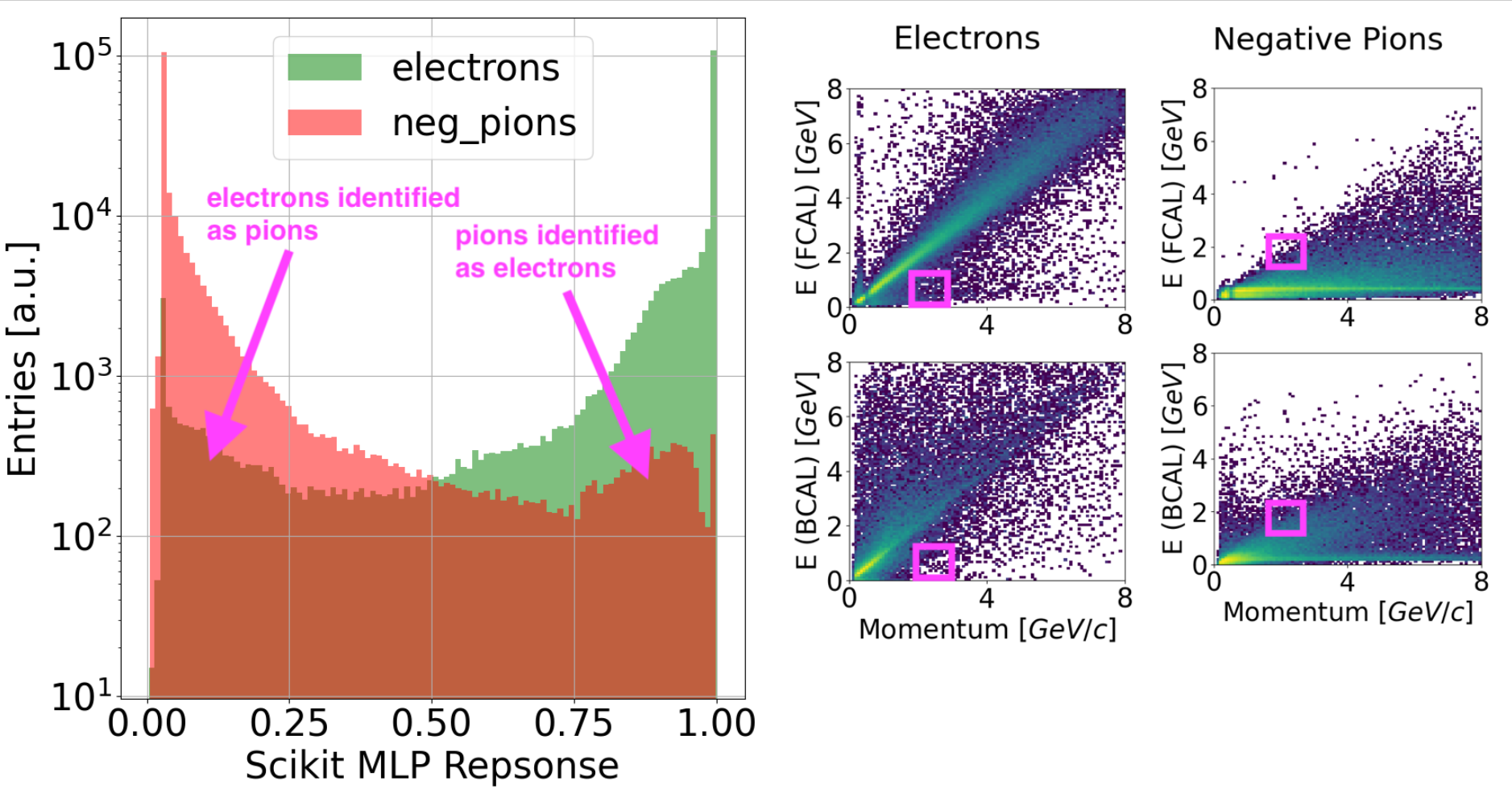

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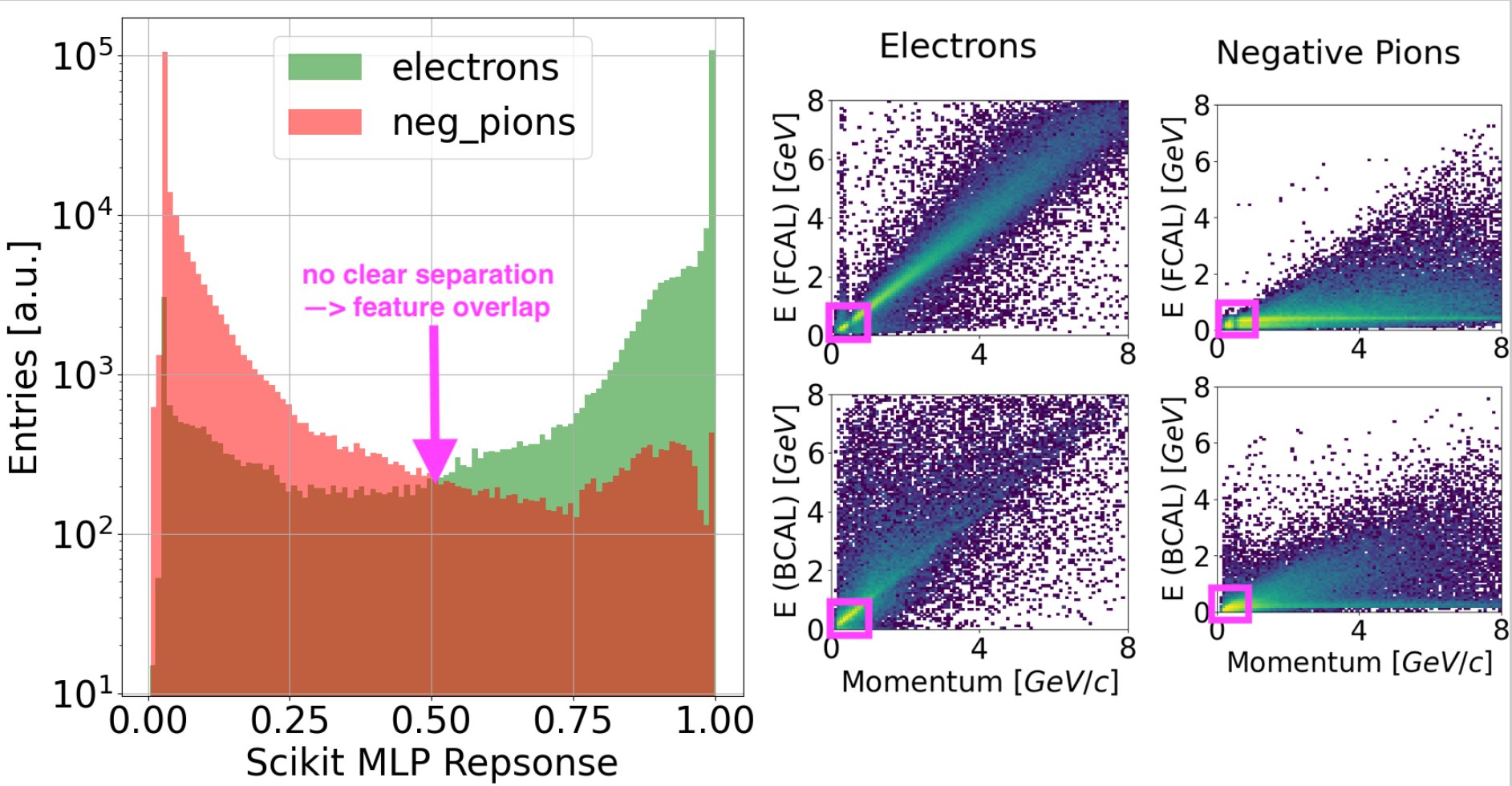

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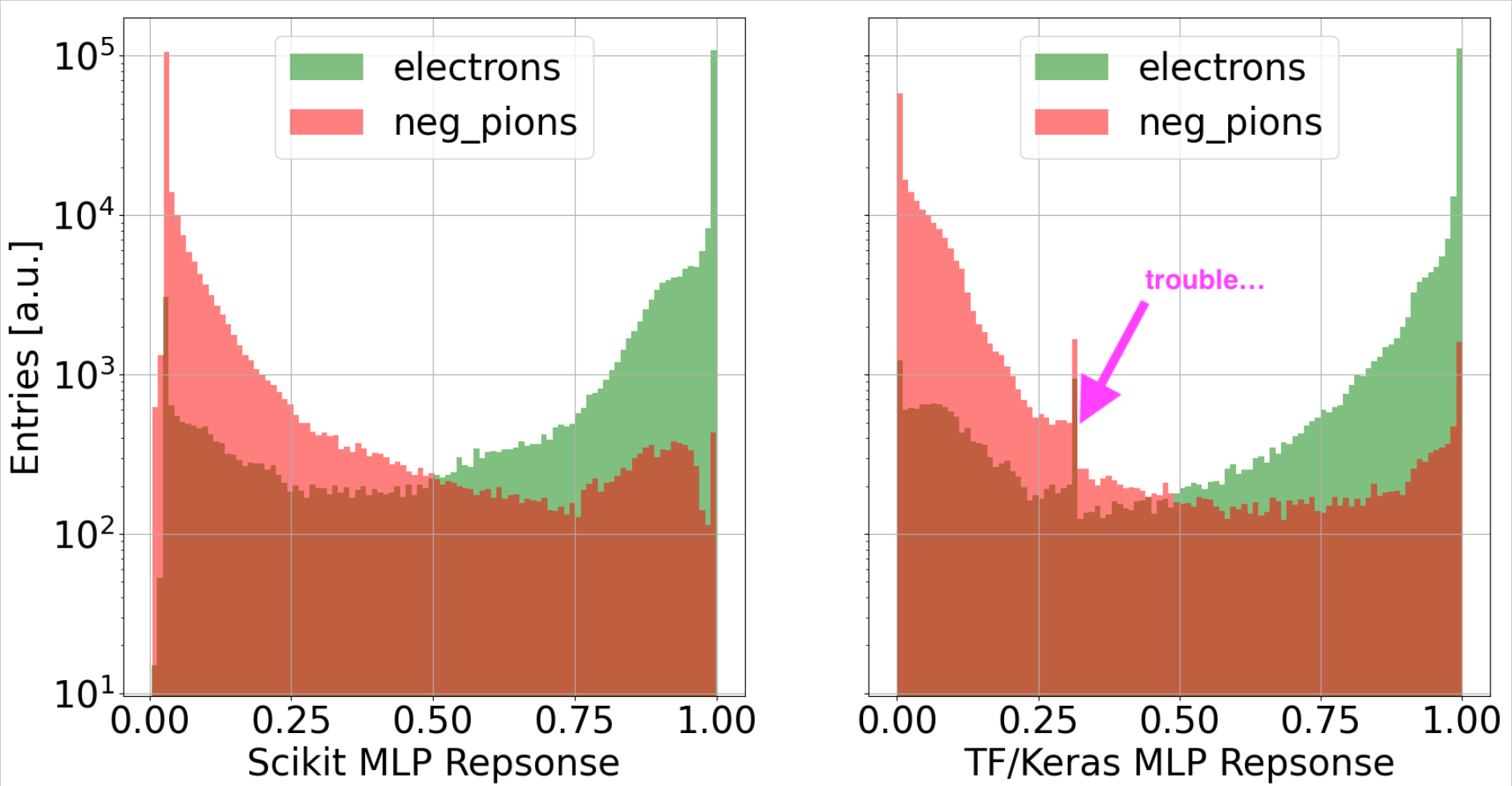
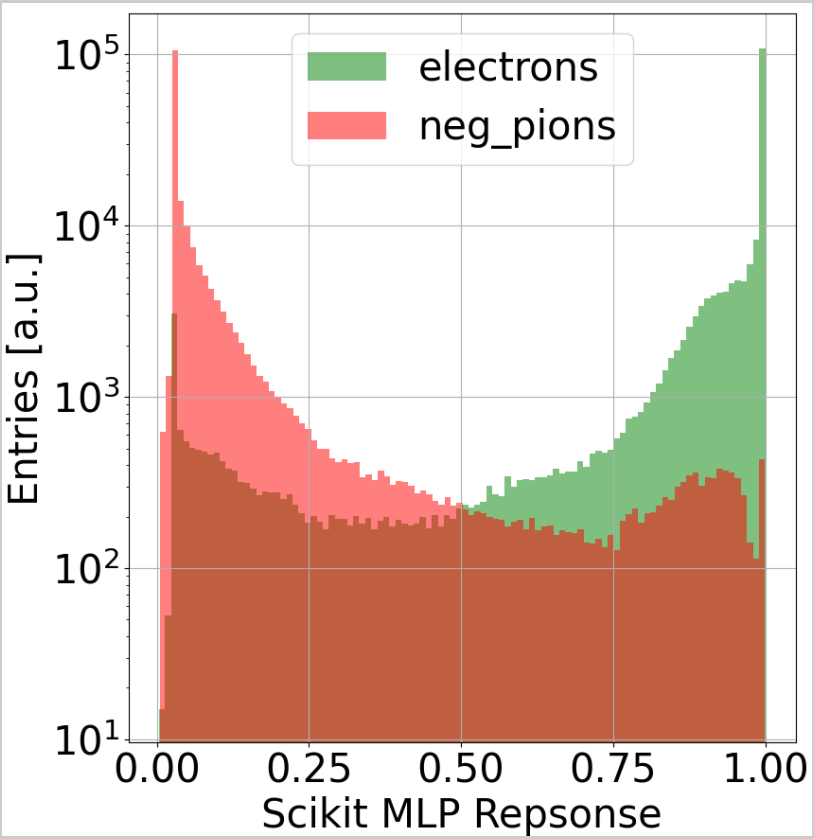
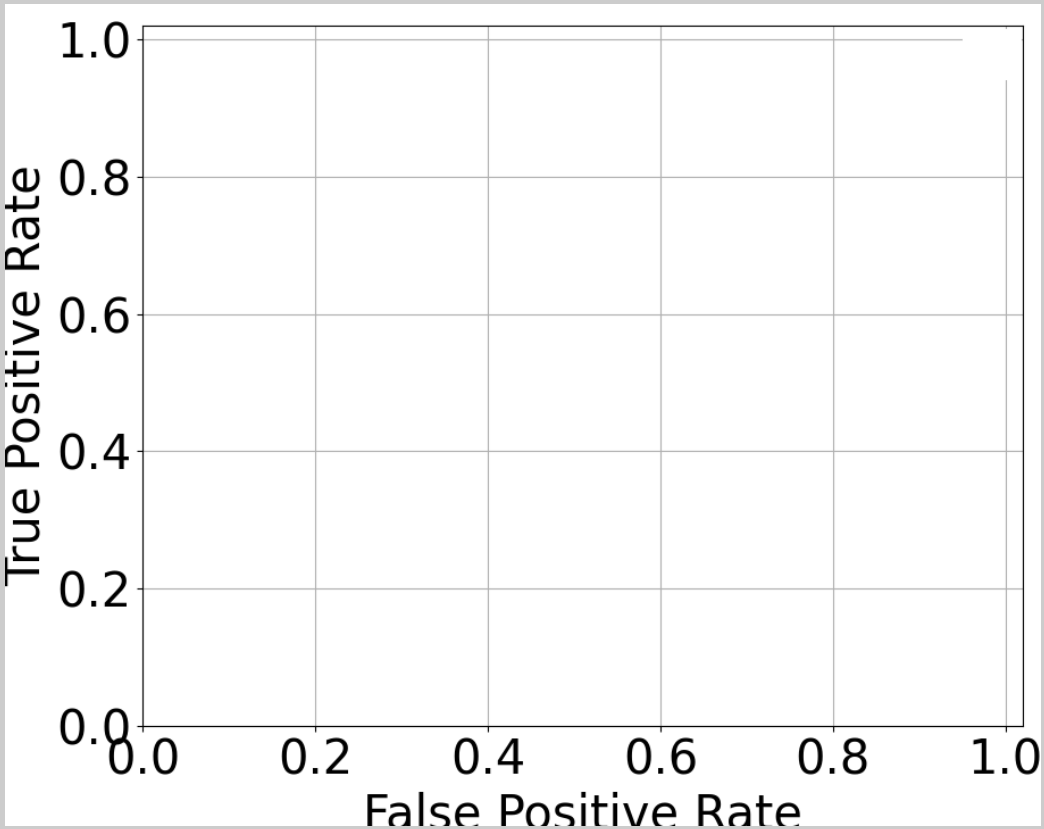


Threshold Scans





- Scan MLP responds distribution
- Calculate TPR / FPR and compare
- Find optimum threshold

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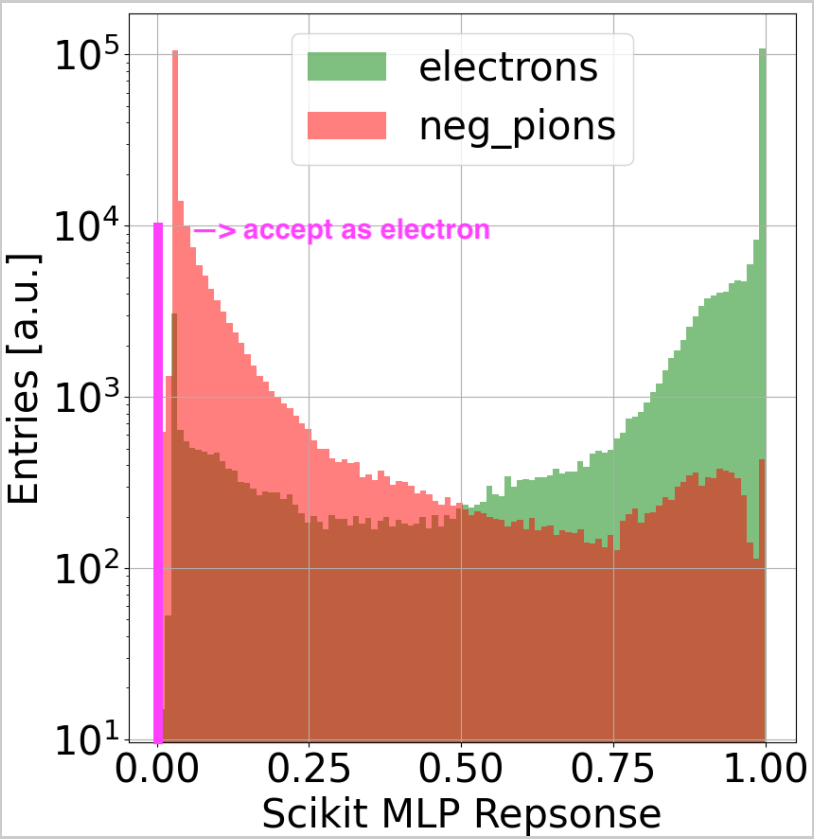

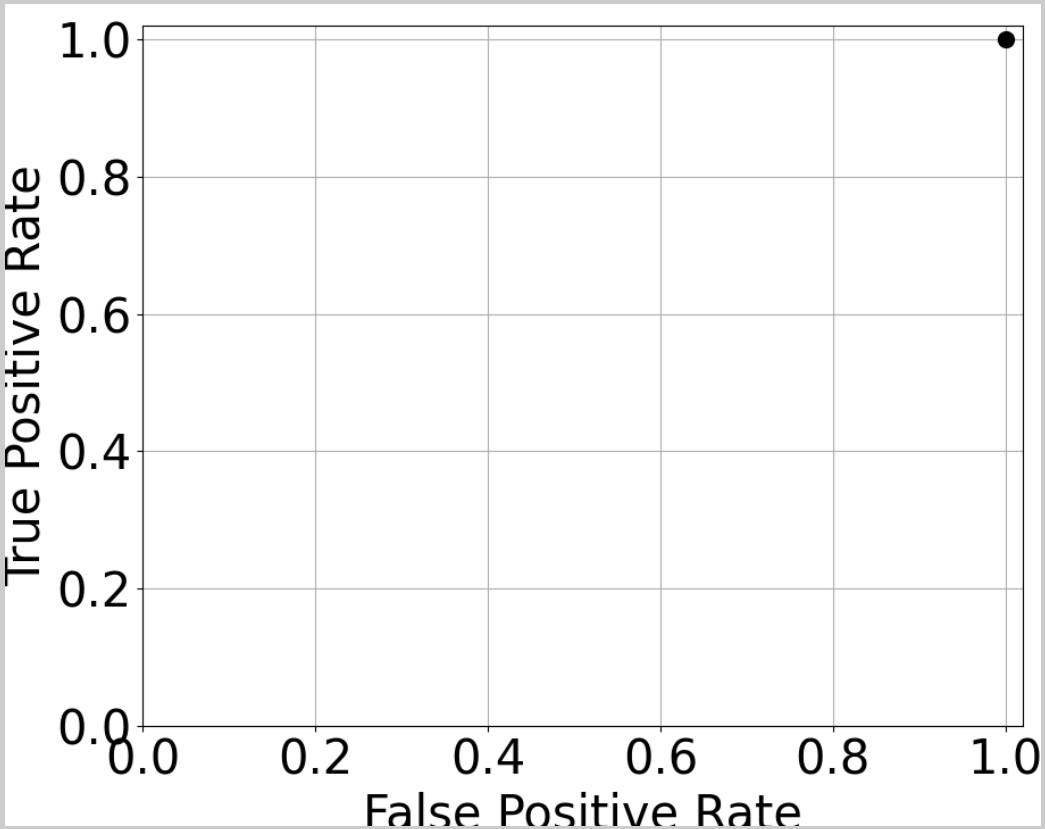

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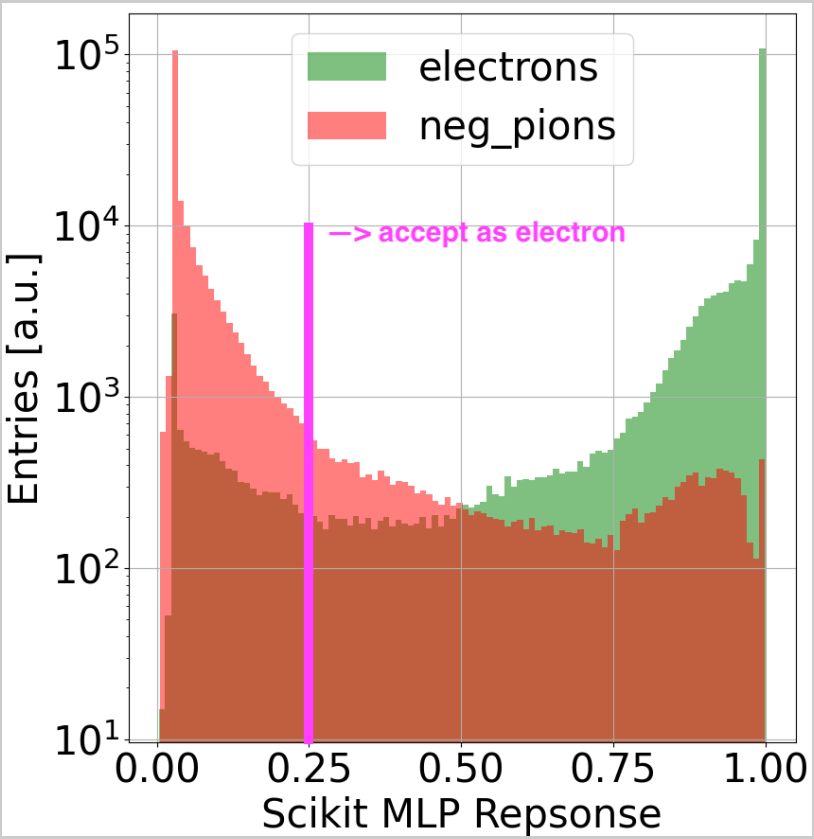

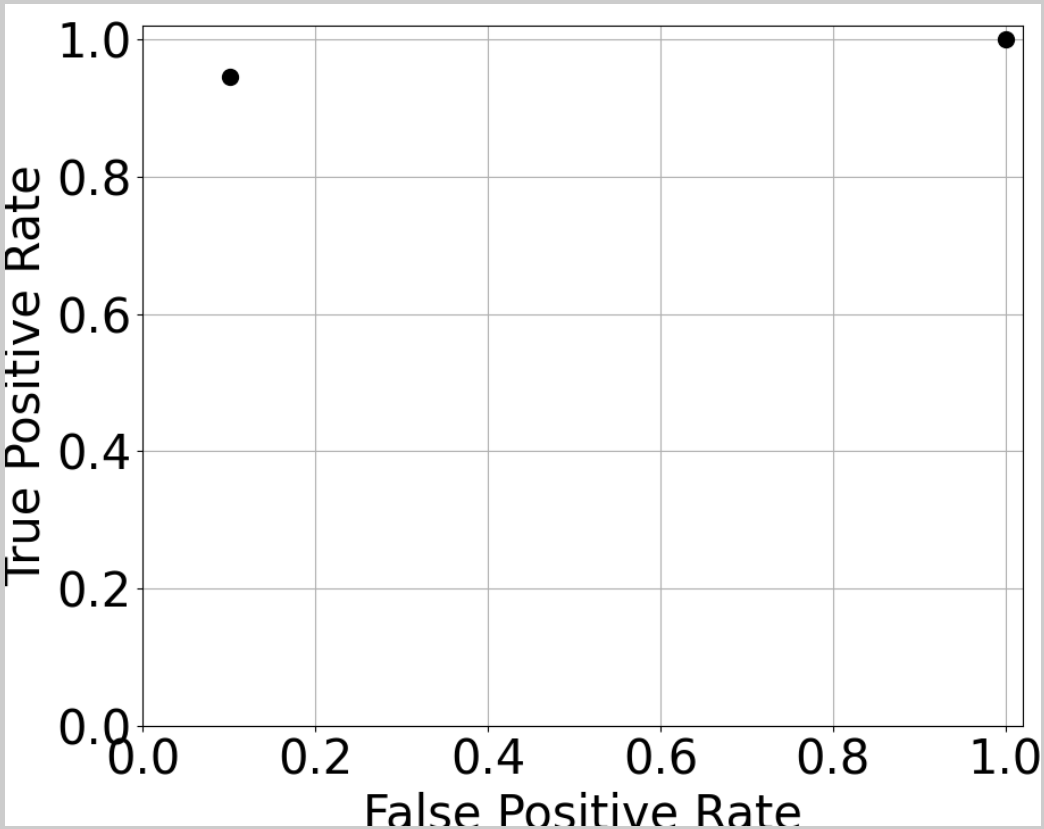

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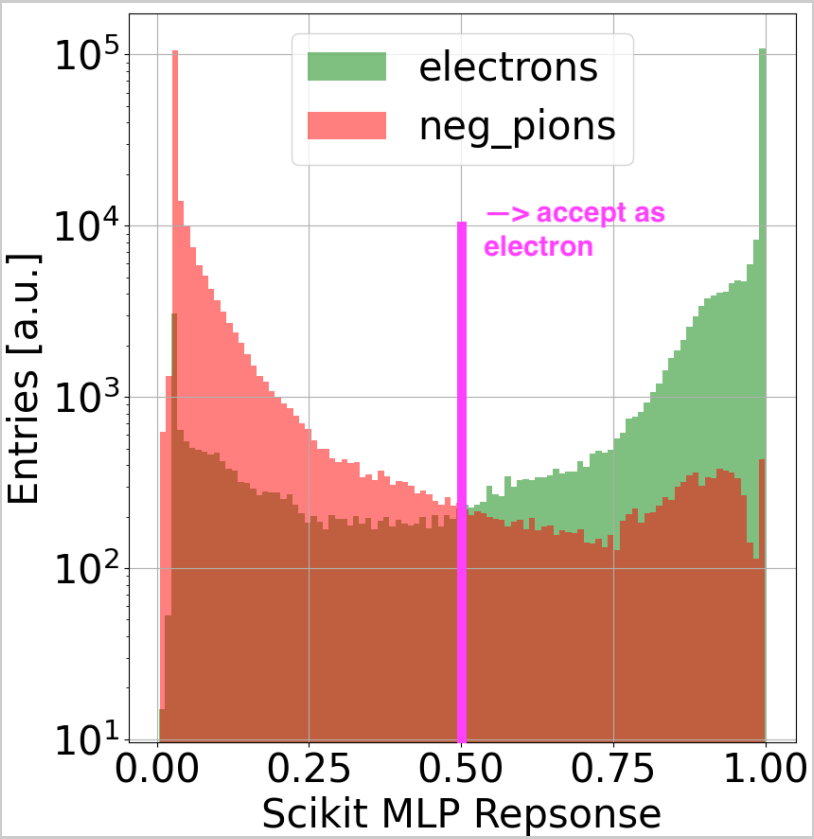

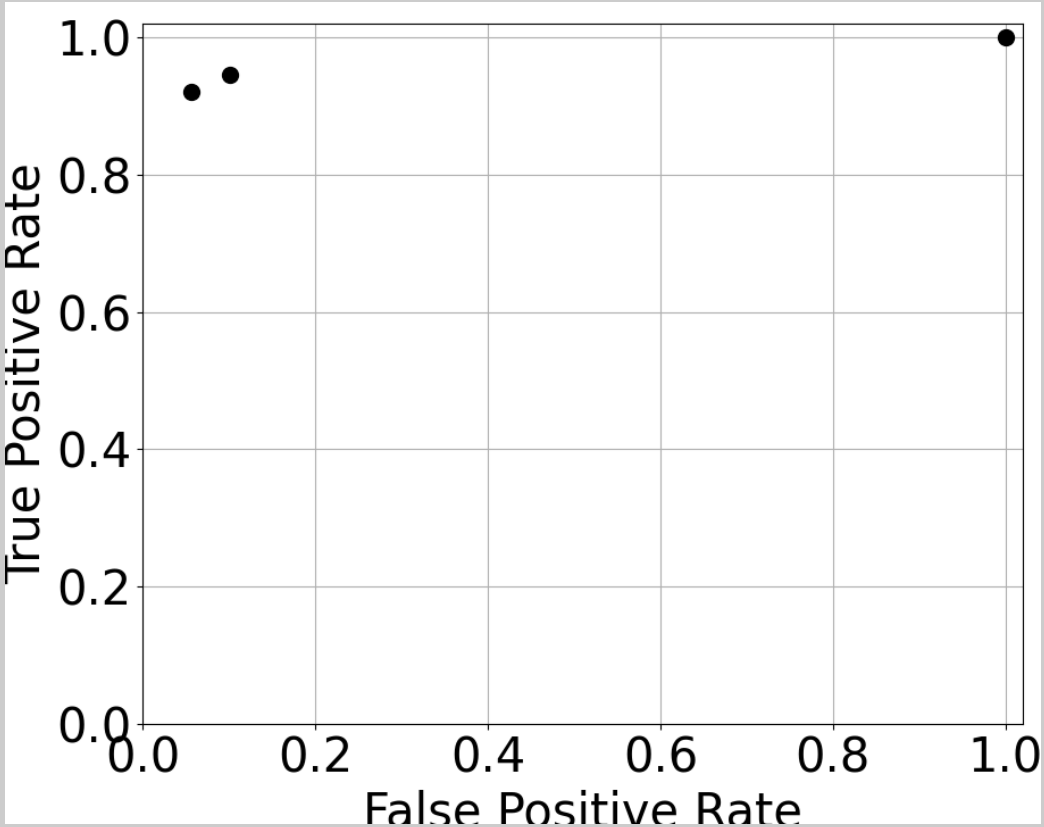

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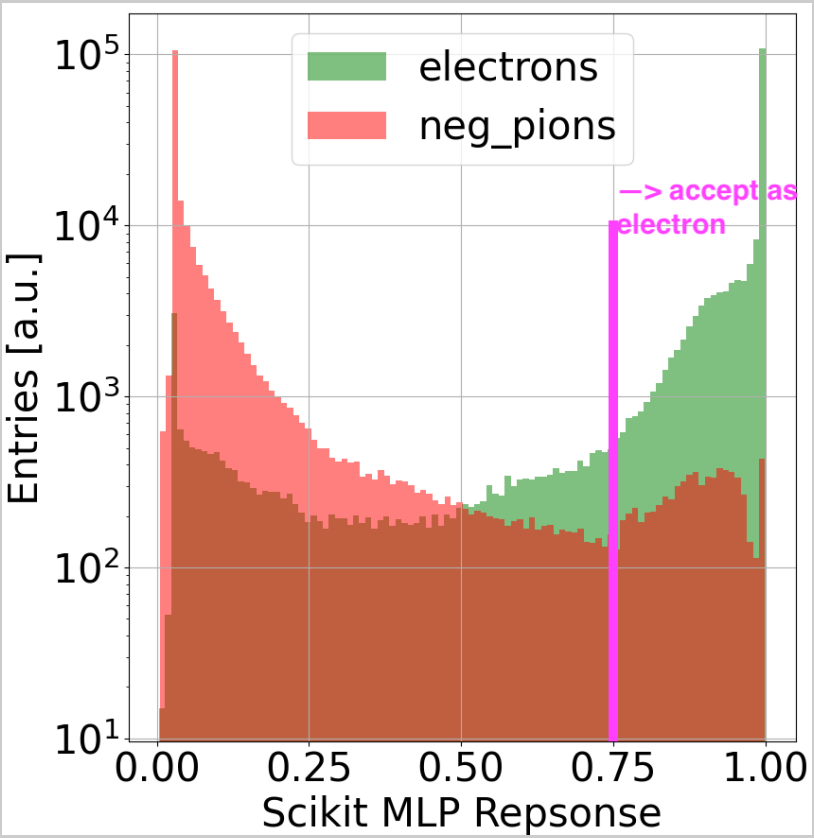

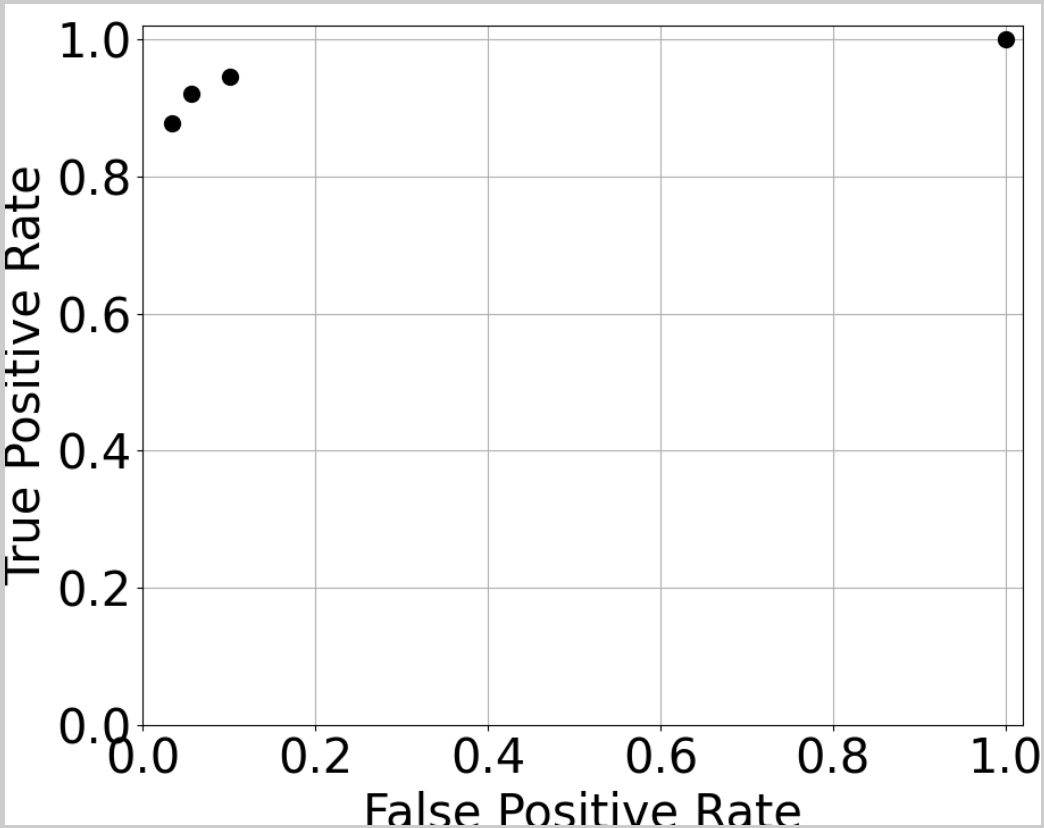

- Scan MLP responds distribution
- Calculate TPR / FPR and compare
- Find optimum threshold
- **ROC- (Receiver Operating Characteristic) curve**

The ROC-Curve

```
from sklearn.metrics import roc_curve

#Get the network response:
scikit_response = scikit_mlp.predict_proba(X)[:,1]
keras_response = keras_mlp.predict(X)

#Get the roc-curve:
fpr_scikit, tpr_scikit,_ = roc_curve(labels,scikit_response,pos_label=1)
fpr_keras, tpr_keras,_ = roc_curve(labels,kreas_response,pos_label=1)
```

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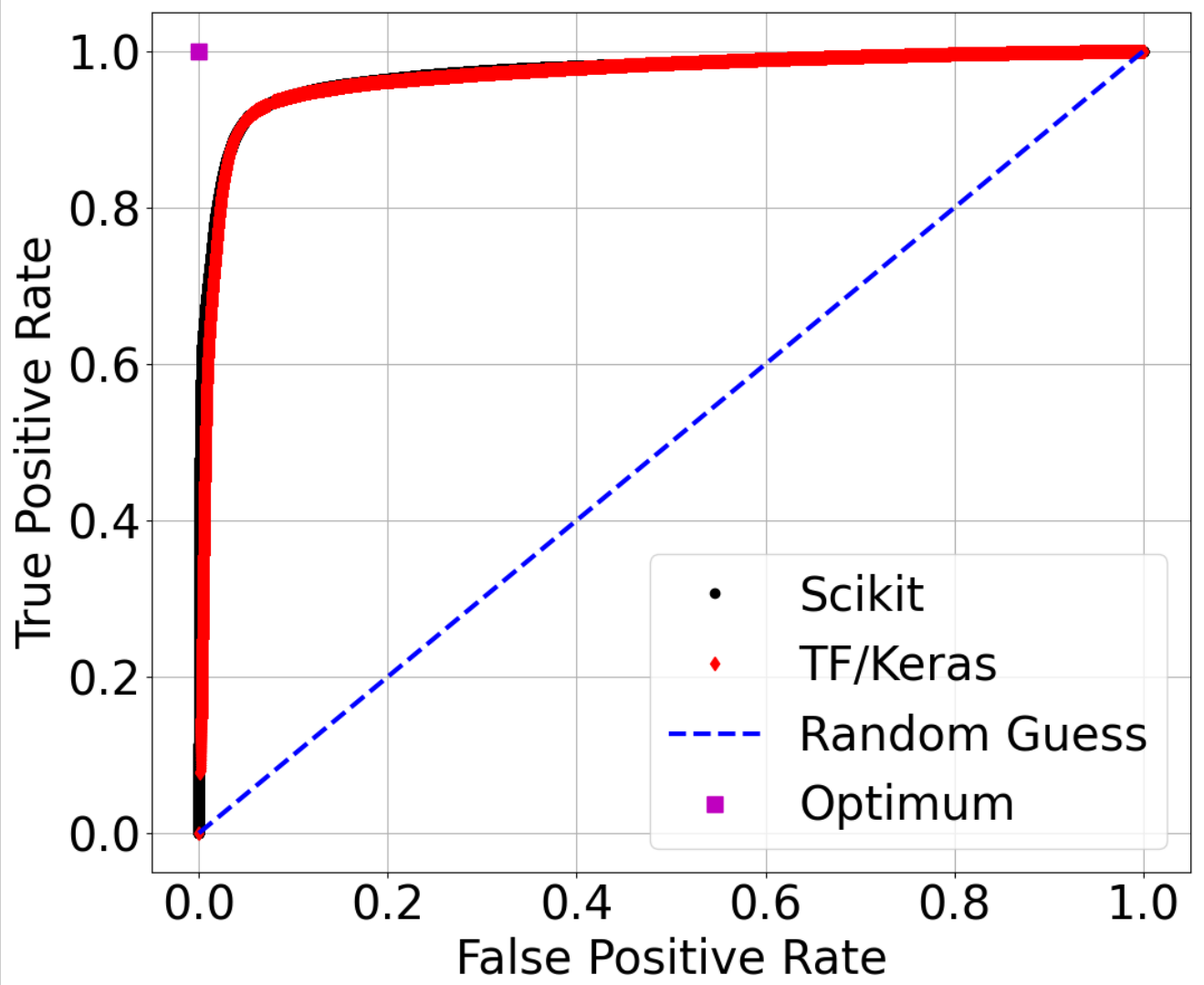

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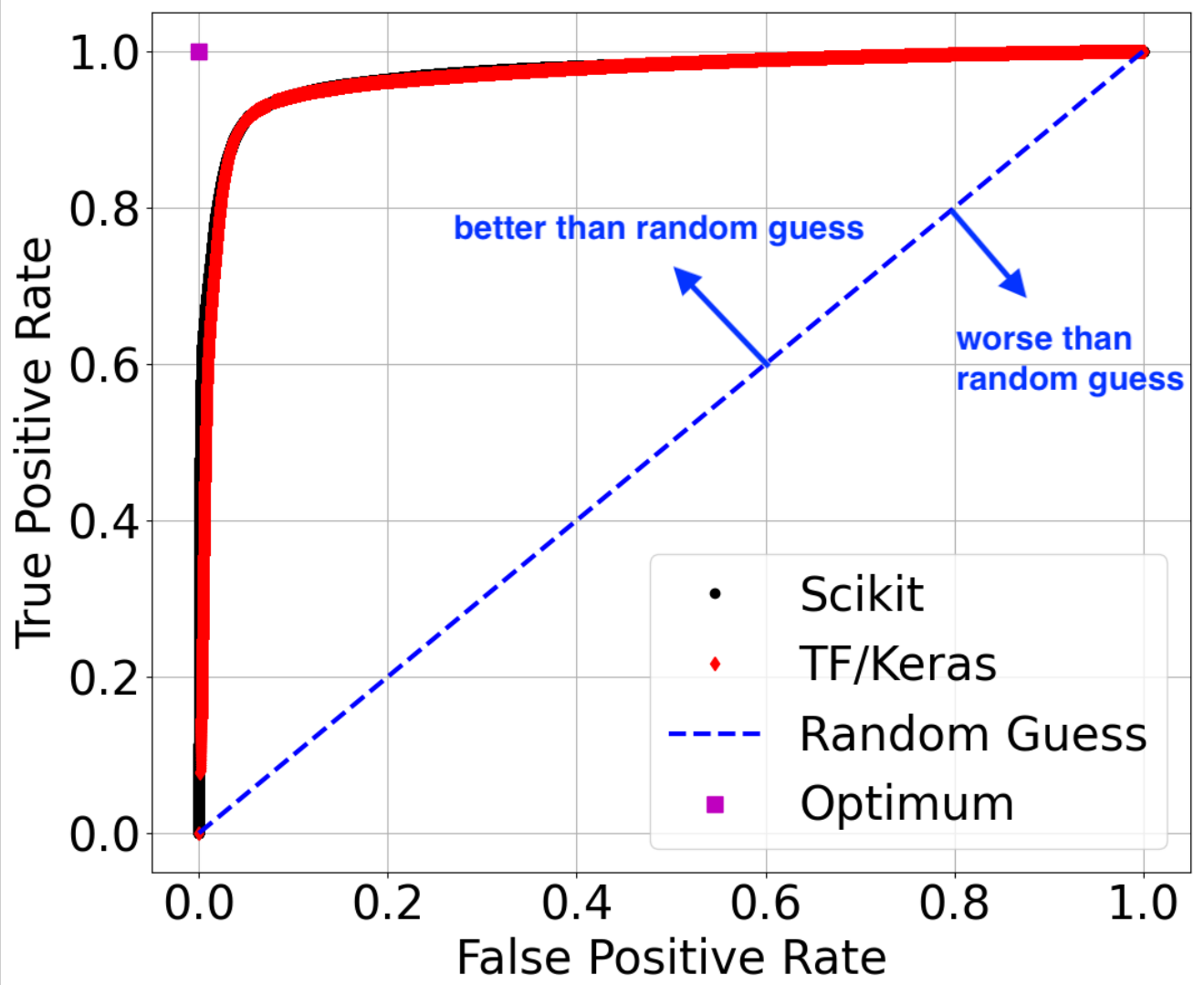

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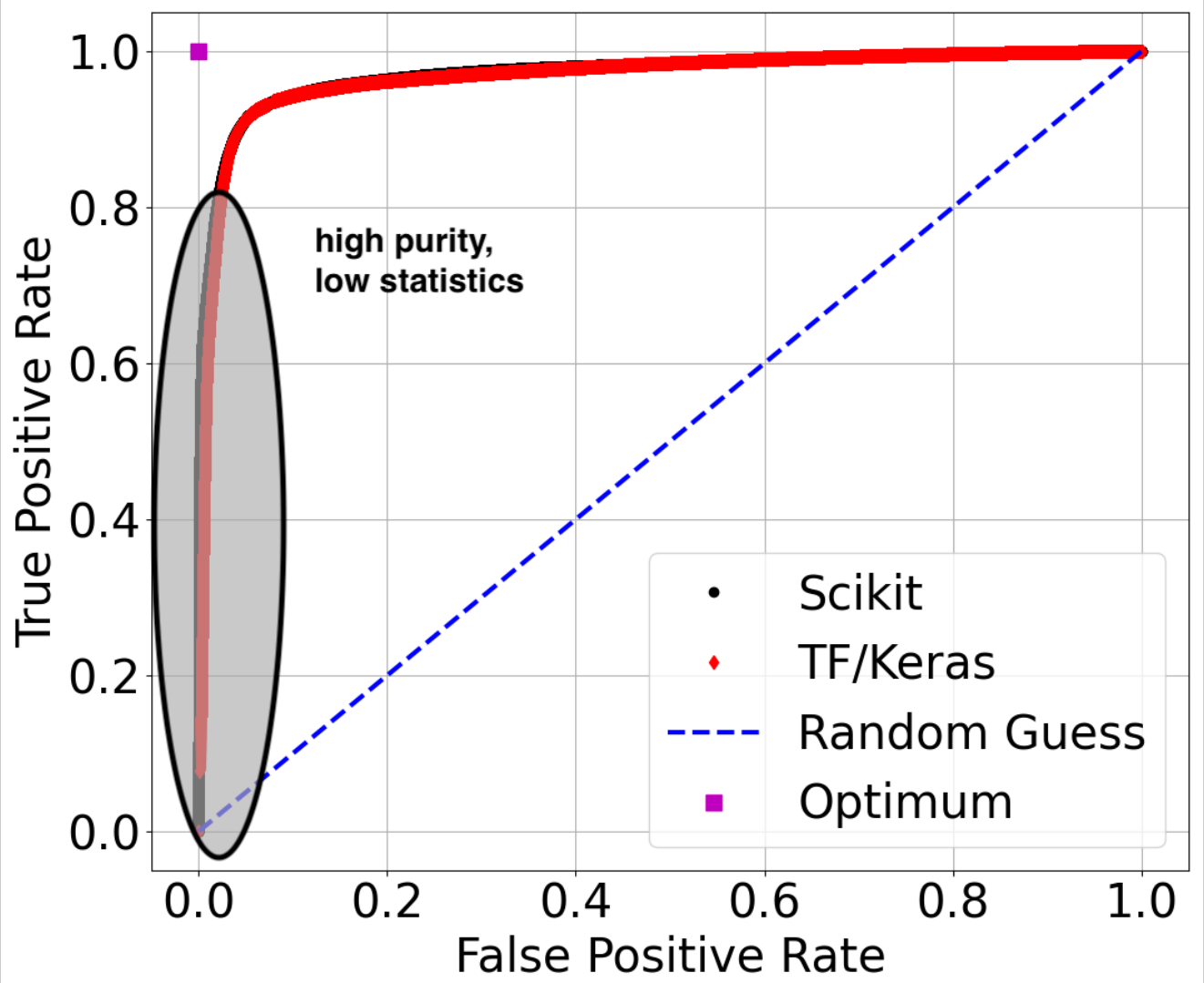

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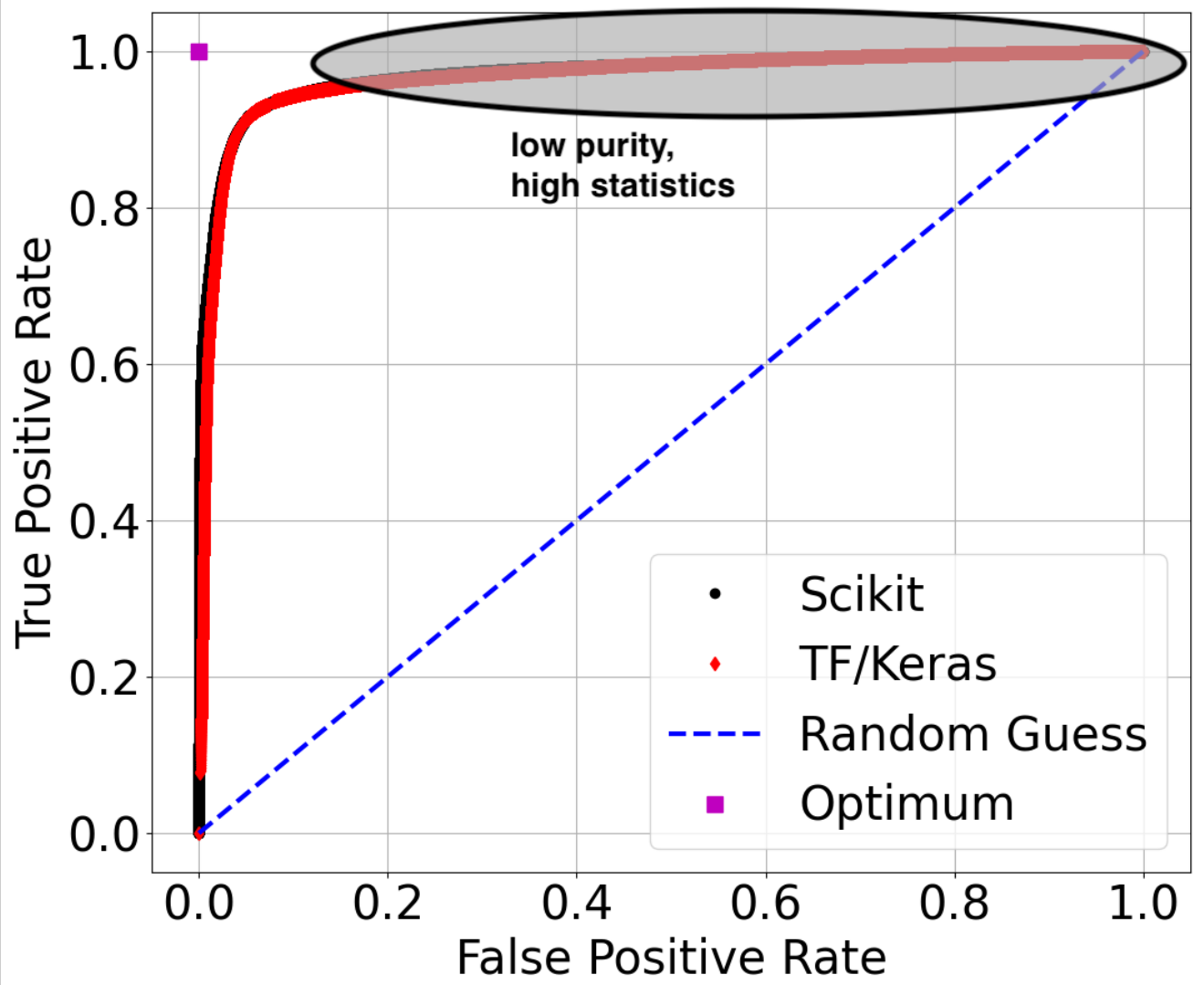

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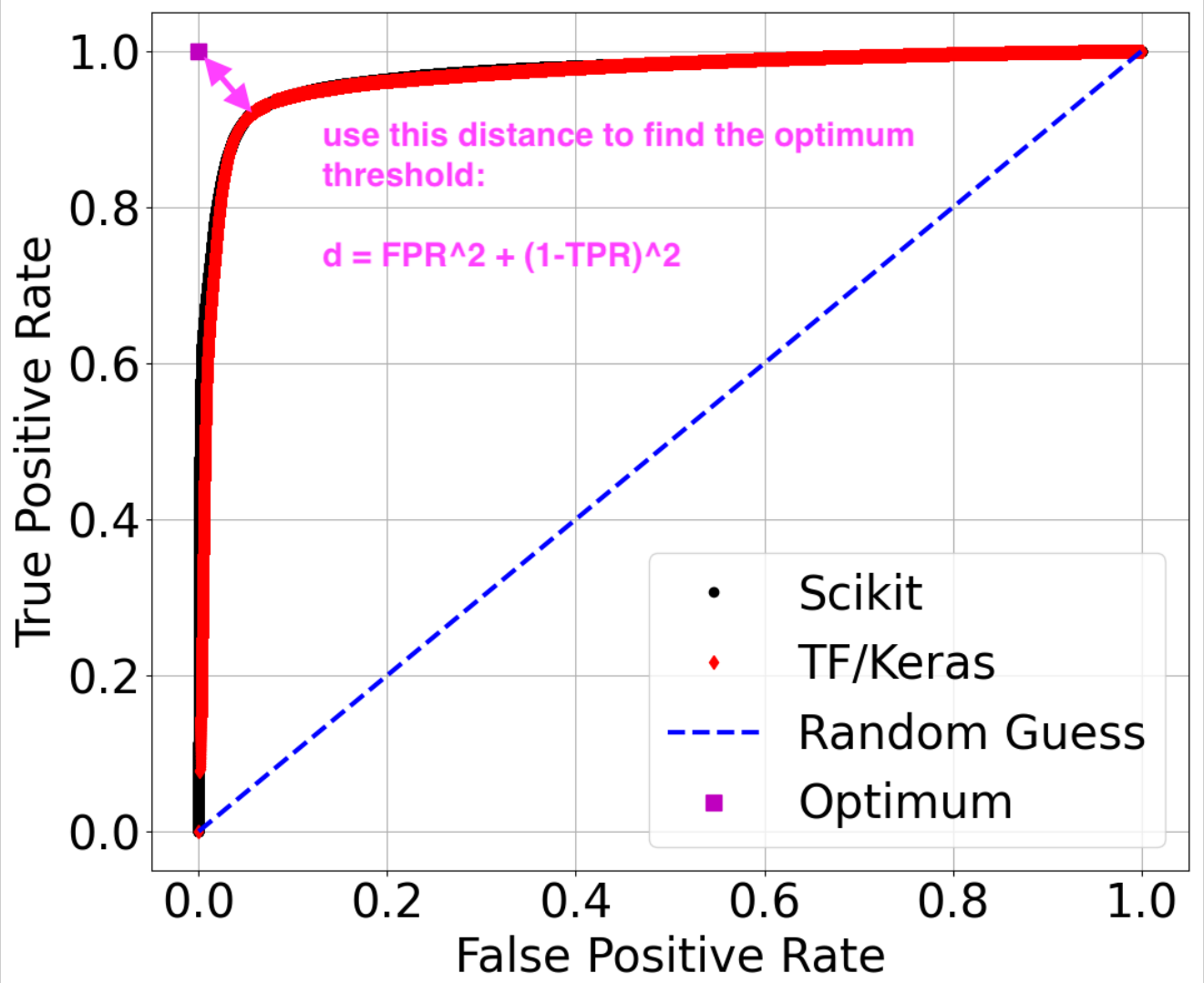
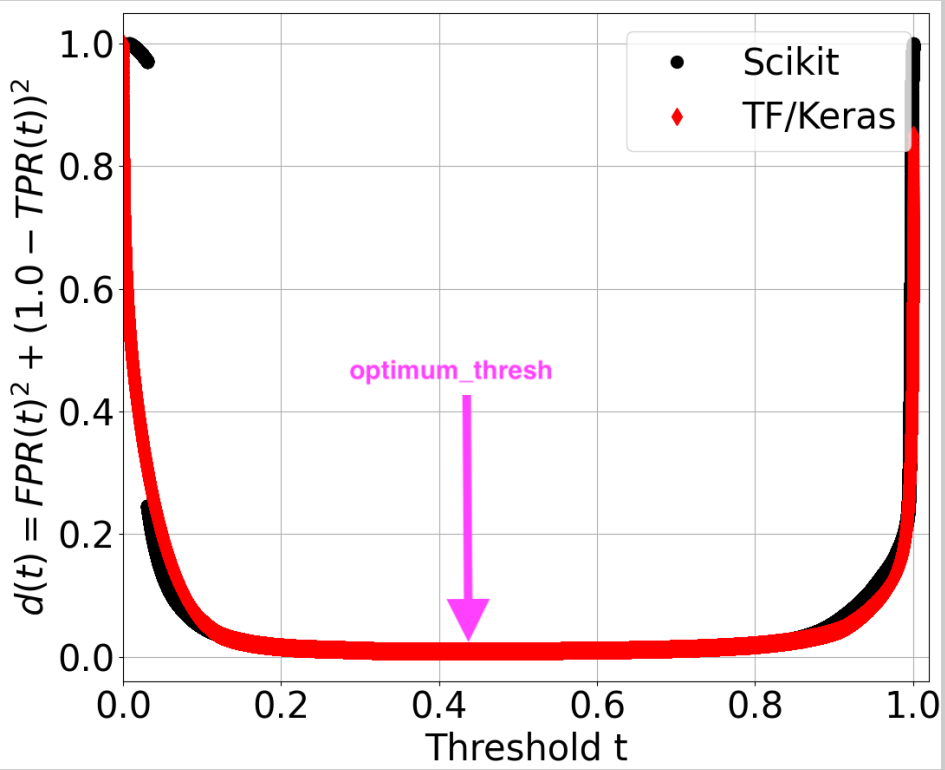


Optimum Thresholds and Labels

- Internally handled for scikit mlp
- Need to find threshold for keras mlp

```
#Labels from scikit:
scikit_labels = scikit_mlp.predict(X)

#Labels from keras:
keras_labels = np.where(keras_response>=optimum_thresh,1.0,0.0)
```



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```
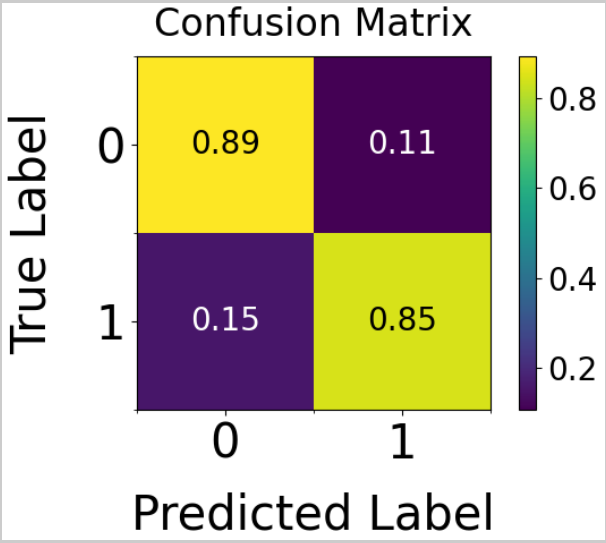
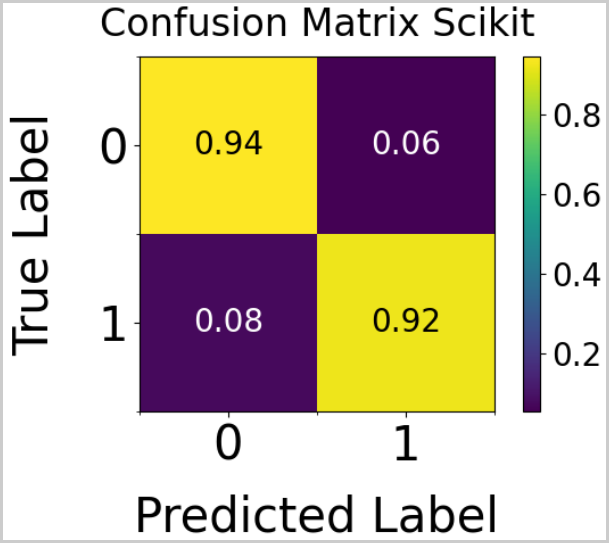
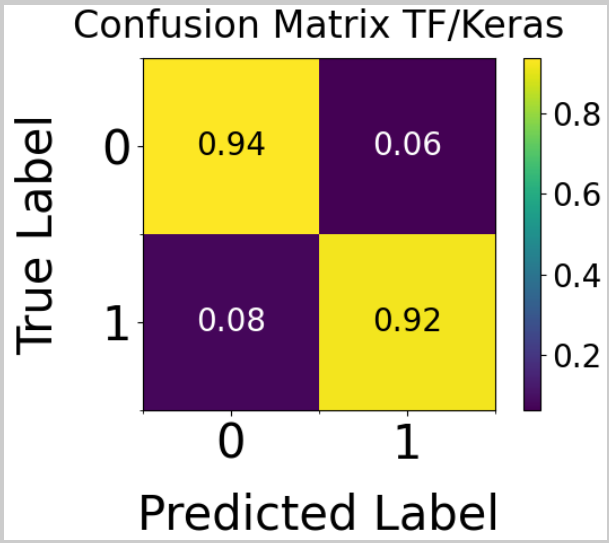

p	theta	phi	ddEdx_CDC	dE_BCAL_preshower	...	dE_FCAL	label	scikit_prob_lep	scikit_label	keras_prob_lep	keras_label
3.925110	0.166660	2.531556	0.000002	0.025954	...	0.000000	1.0	0.031089	0.0	0.000447	0.0
1.750640	0.206904	-2.695393	0.000003	0.916215	...	0.000000	1.0	0.787939	1.0	0.830379	1.0
2.336900	0.052576	2.885235	0.000000	0.000000	...	2.173967	1.0	0.996849	1.0	0.998797	1.0
5.825788	0.710650	-2.959795	0.000002	0.925353	...	0.000000	1.0	0.996104	1.0	0.998847	1.0
2.882963	0.143638	-0.763970	0.000002	0.000000	...	1.143092	0.0	0.101160	0.0	0.091617	0.0
0.661498	0.609131	3.100280	0.000002	0.086262	...	0.000000	0.0	0.451565	0.0	0.396868	0.0
0.443637	0.031602	2.455756	0.000000	0.000000	...	0.431946	1.0	0.951643	1.0	0.987271	1.0
2.020184	0.127360	0.079234	0.000002	0.000000	...	0.214426	0.0	0.031089	0.0	0.010049	0.0
1.827218	0.024664	2.837258	0.000000	0.000000	...	0.908476	0.0	0.168505	0.0	0.200512	0.0
6.215446	0.120326	-3.040930	0.000002	0.000000	...	0.436846	0.0	0.031089	0.0	0.000063	0.0

Electron Identification Performances

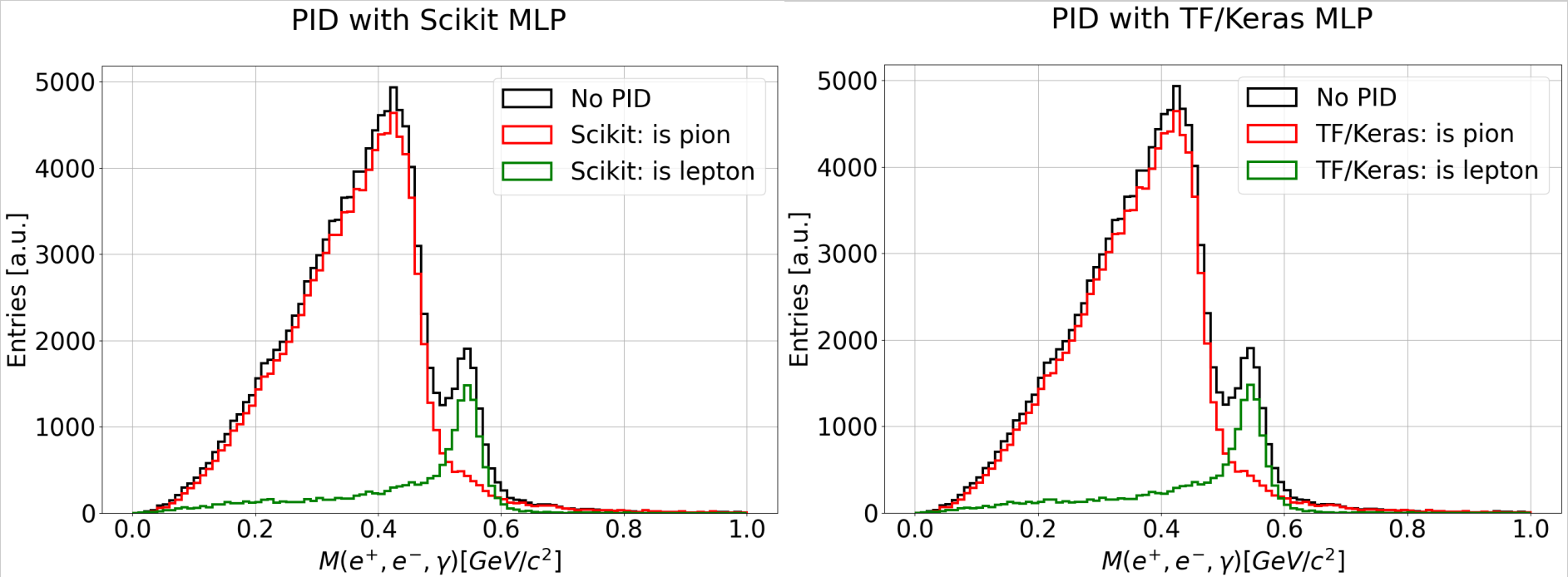






Method	TPR	FPR	min. $d(t)$	threshold t	Accuracy
Reference Analysis	0.85	0.11	na	na	0.87
Scikit MLP	0.92	0.06	0.0094	0.47	0.93
TF/Keras MLP	0.92	0.06	0.0094	0.43	0.93

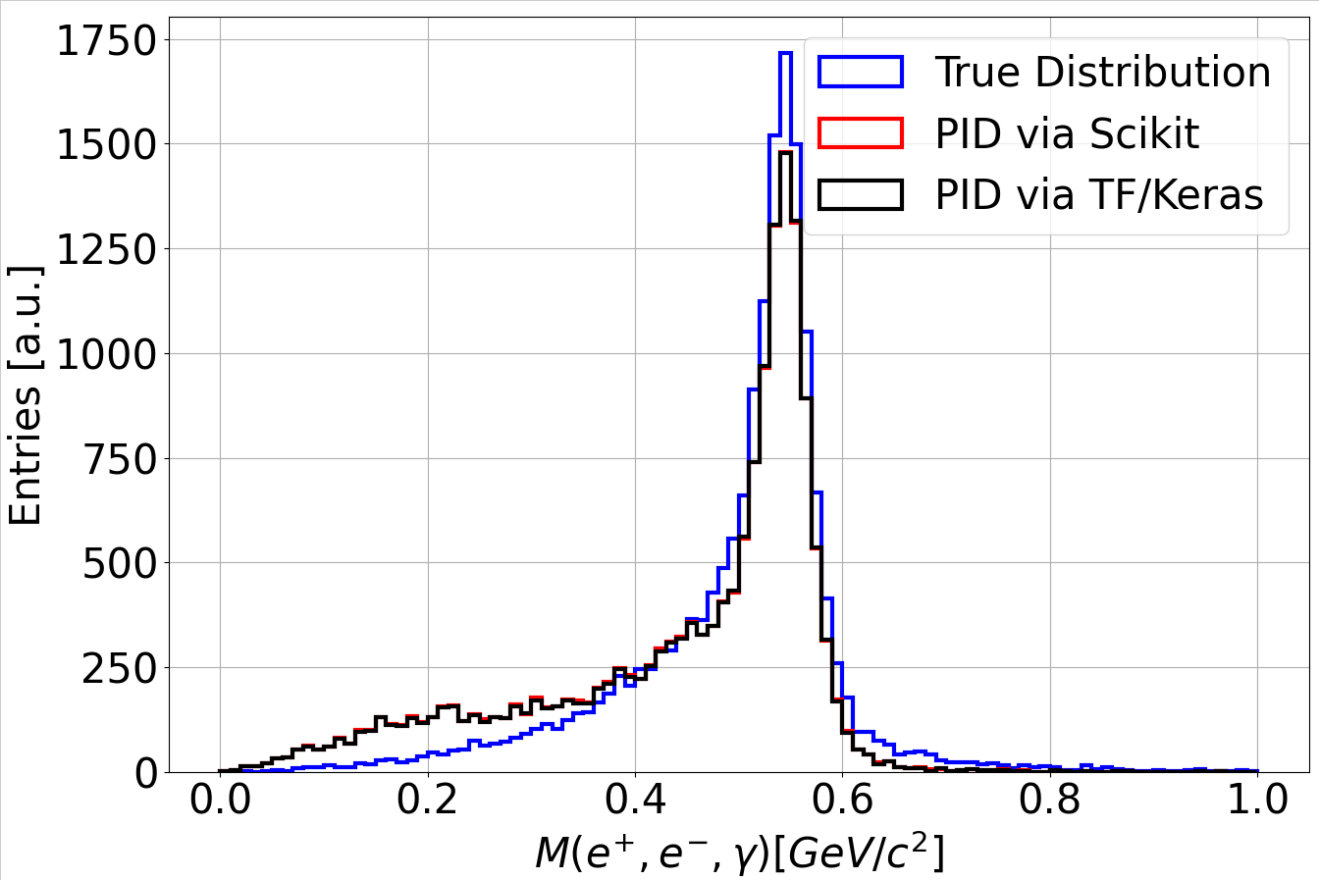
Reconstructing $\eta \to e^+e^-\gamma$ Events



- ☑ Networks separate $\eta \to \pi^+\pi^-\gamma$ from $\eta \to e^+e^-\gamma$
- ☑ $\eta \to e^+e^-\gamma$-signal shape is undisturbed (i.e. continuous and smooth)

Comparing Signal Shapes

- Networks do not significantly alter signal shape
- Reconstructed shapes are identical for both networks
- **NOTE:** Not always lucky to have true distribution



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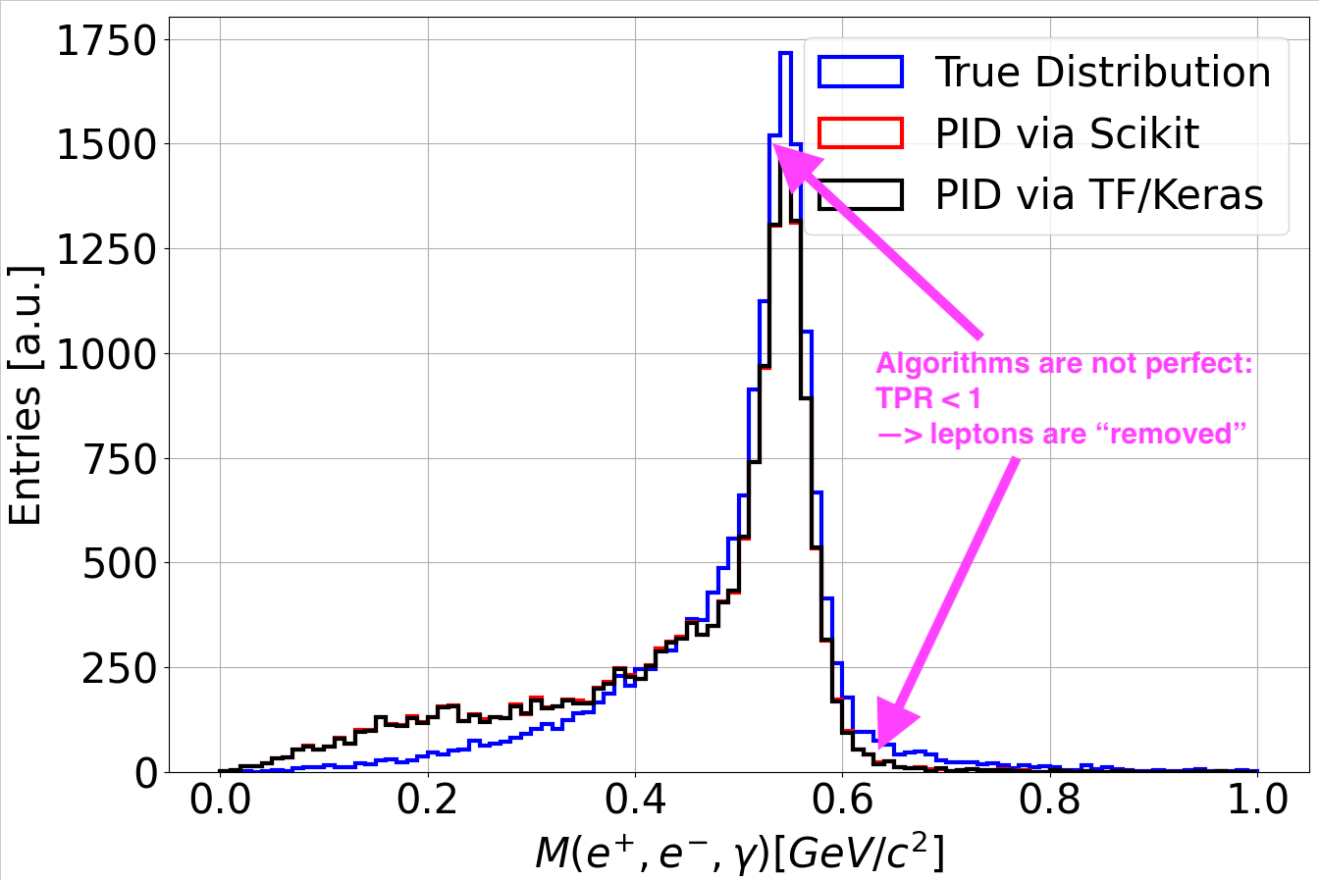

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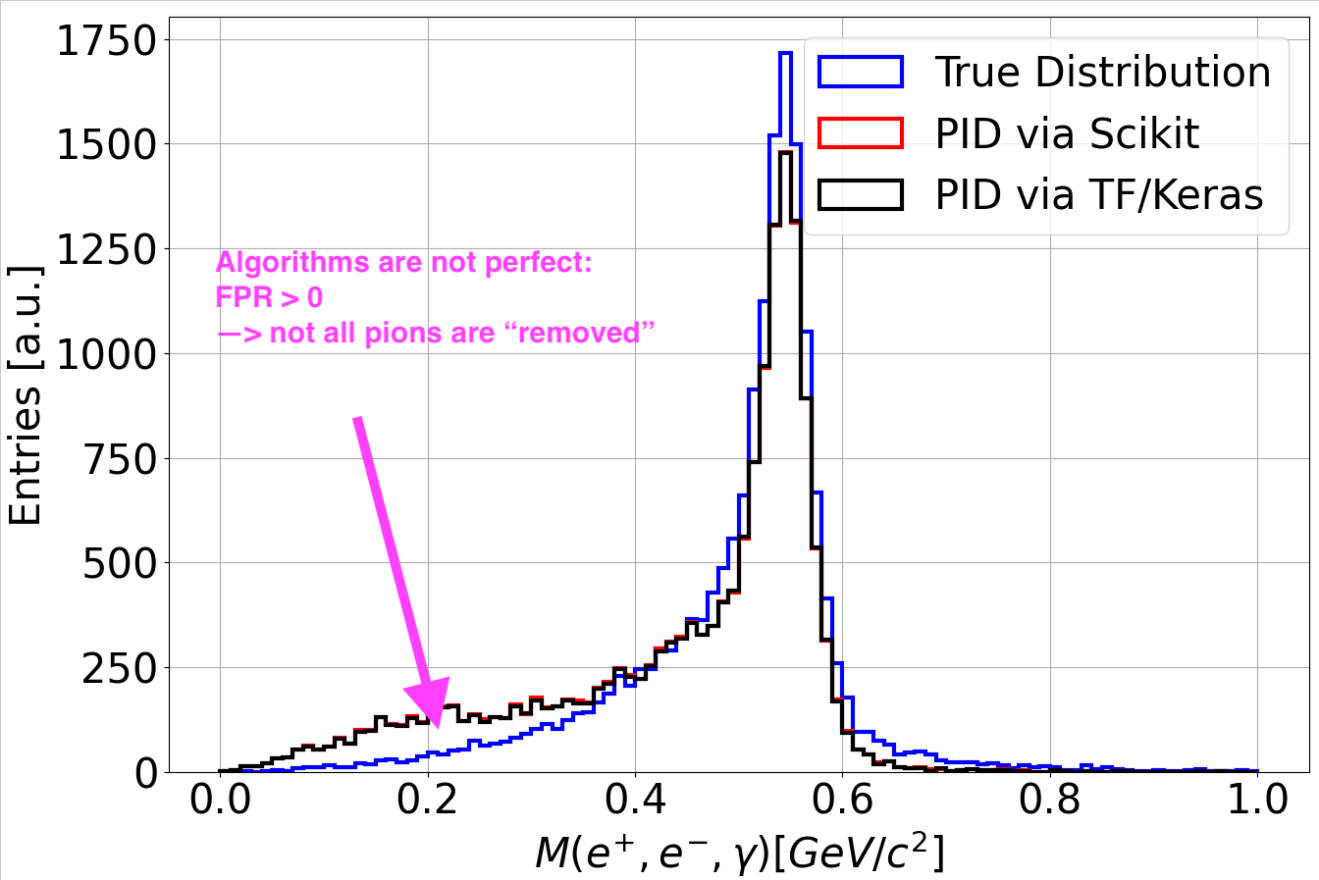


Where to go from here?

- Neural network classifiers show "reasonable" performance
  (Accuracy = 93% $\leftrightarrow$ current benchmark)
- **Legit question:** Can one do better?
- **Answer(s):**
  - Hopefully yes
  - Try different models and compare
    (i.e. random forest, Gaussian processes, likelihood estimator,...)
  - Tune network parameters $\rightarrow$ Hyper Parameter Optimization (HPO)

Hyper Parameters

- **Fit Parameters:** Model internal parameters → Set by optimization procedure → driven by data
- **Hyper Parameters:** Determine model architecture / performance → Set by user

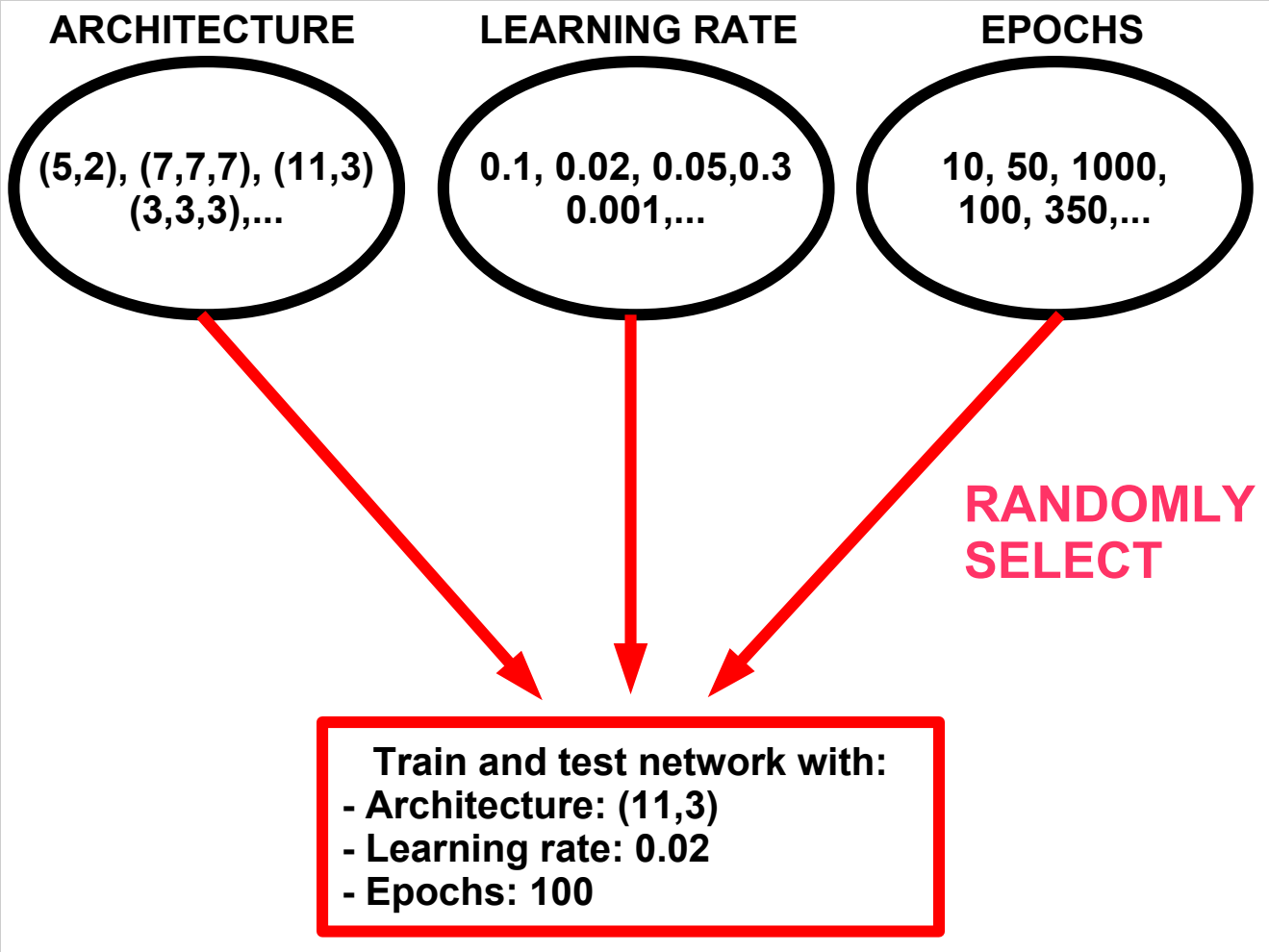
Model	Fit Parameters	Hyper Parameters
$pol(N) = p_N x^N + p_{N-1} x^{N-1} + ... + p_0$	$p_N, .., p_0$	N, minimizer,...
Multilayer Perceptron	weights, biases	#Hidden Layers, #Neurons, #Epochs,...

Hyper Parameter Optimization (HPO)

- **Goal:** Find set of hyper parameters which maximizes the prediction performance $\leftrightarrow$ Minimize prediction error
- **To consider:**
  - Use computational time efficiently
  - Generalizability $\leftrightarrow$ avoid overfitting $\rightarrow$ Use validation data!
  - Actually find optimum
- **How to: HPO?**
  - Test different settings manually $\rightarrow$ can be painful
  - Use algorithm
    - ★ Grid search: simple, but ineffective if parameter ranges are unknown $\#\text{Searches} = \prod_i \#\text{Settings[Parameter(i)]}$
    - ★ Random parameter search
    - ★ Bayesian optimization
    - ★ and many more...

Random Hyper Parameter Search

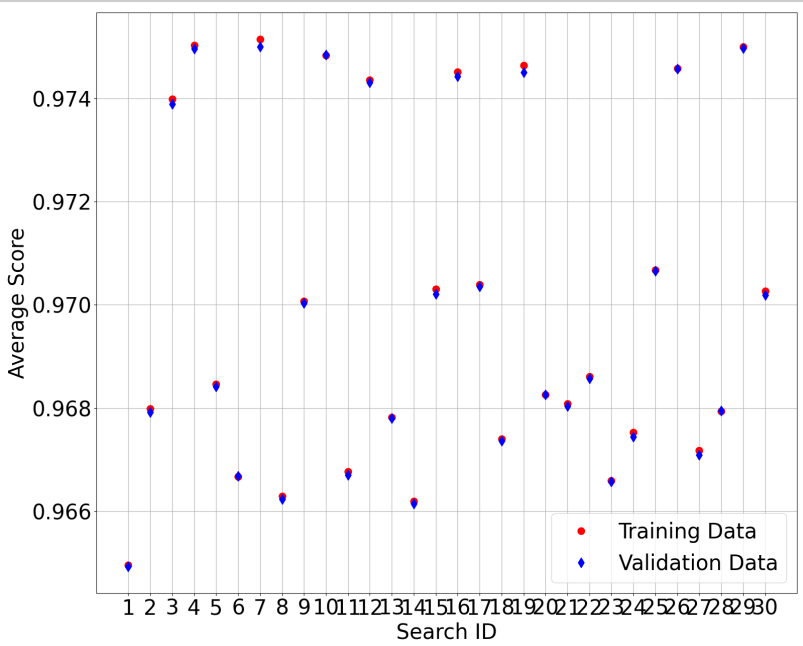
- Draw random parameter samples
- Use training and test data
- Select parameter sample with highest score on test data

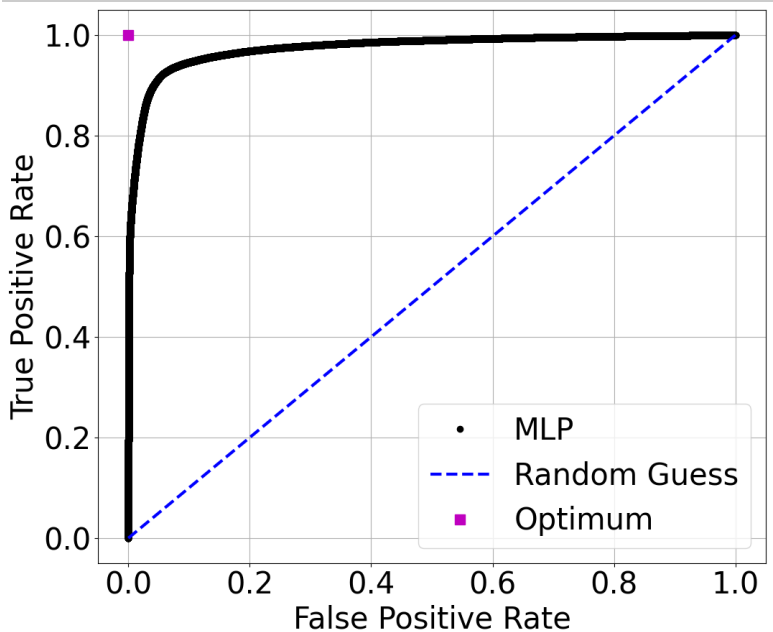


Random HPO in scikit

```
from sklearn.model_selection import RandomizedSearchCV
from sklearn.neural_network import MLPClassifier

#Which parameters do you want to tune?
parameters_to_tune_mlp = {
     'hidden_layer_sizes': [(5),(8,3),(3,3,3),...], #--> Architecture
     'learning_rate_init': stats.uniform(0.001,0.1), #--> Learning rate
     'max_iter': stats.randint(100,800) #Epochs
     #(number of training iterations
}

#Set up the search algorithm:
random_search = RandomizedSearchCV(
      MLPClassifier(), #--> The object you want to tune
      param_distributions=parameters_to_tune_mlp,
      n_iter=30, #--> Perform 30 random searches
      scoring='roc_auc' #--> Integral under the ROC-curve
 )

 #Run the search
 random_search.fit(X,Y)
```

And the Winner is...





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Reference Analysis	0.85	0.11	na	na	0.87
Scikit MLP	0.92	0.06	0.0094	0.47	0.93
TF/Keras MLP	0.92	0.06	0.0094	0.43	0.93
Scikit MLP (rnd search)	0.93	0.06	0.0092	0.44	0.933

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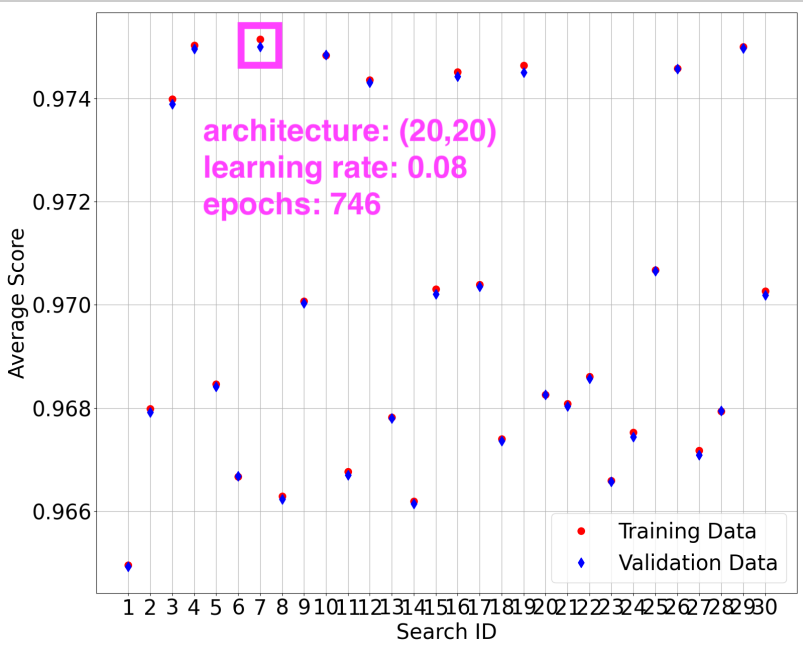

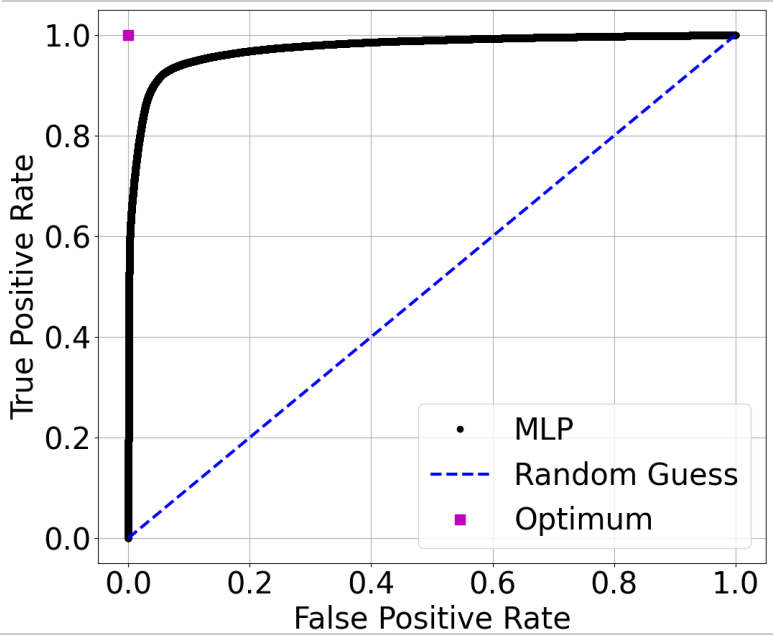

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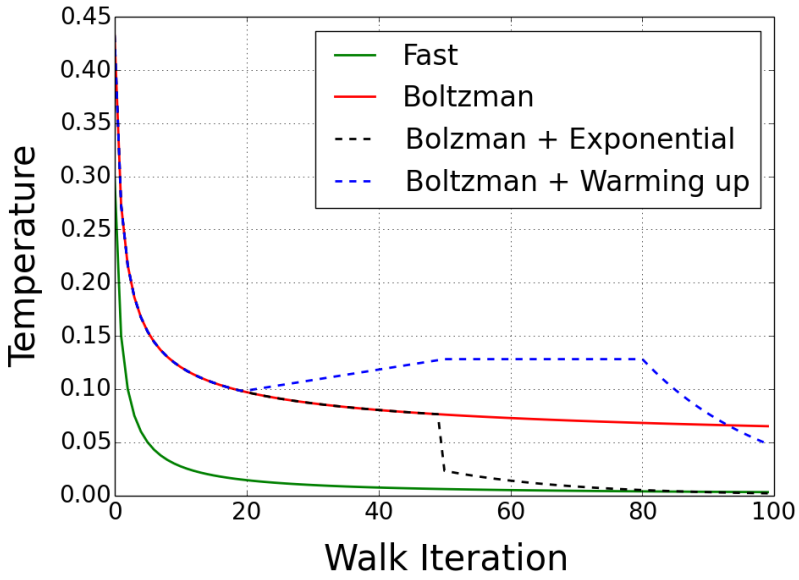
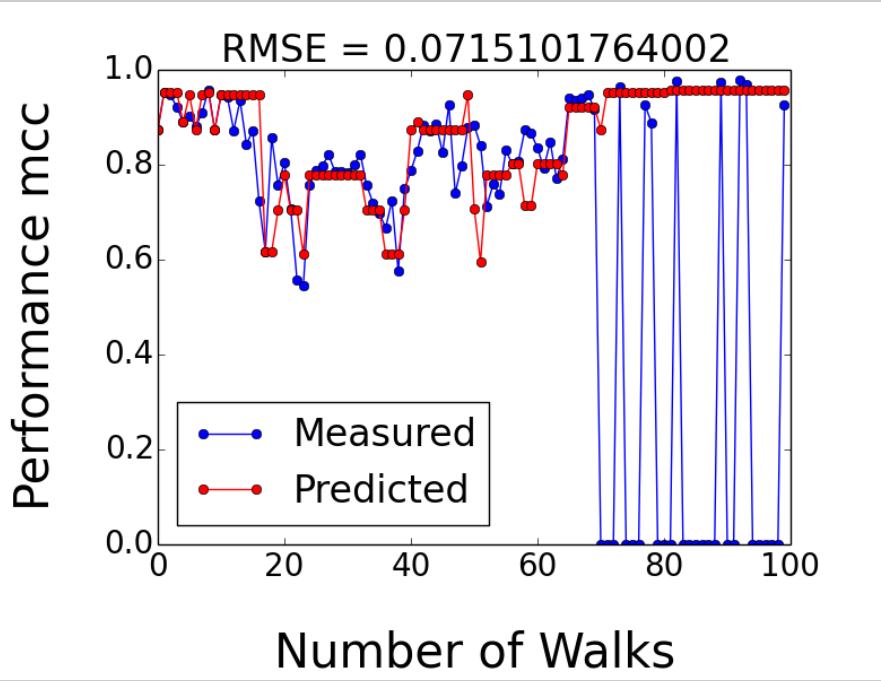
Conclusion

- Obtained minor improvement with HPO
  $\rightarrow$ This happens sometimes
- Use different (more efficient) HPO algorithm
  (Bayesian based optimizer)
- Try an other algorithm (e.g. random forest classifier)

R & D on Hyper Parameter Optimization (HPO)





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  - Only update if improvement in performance is found
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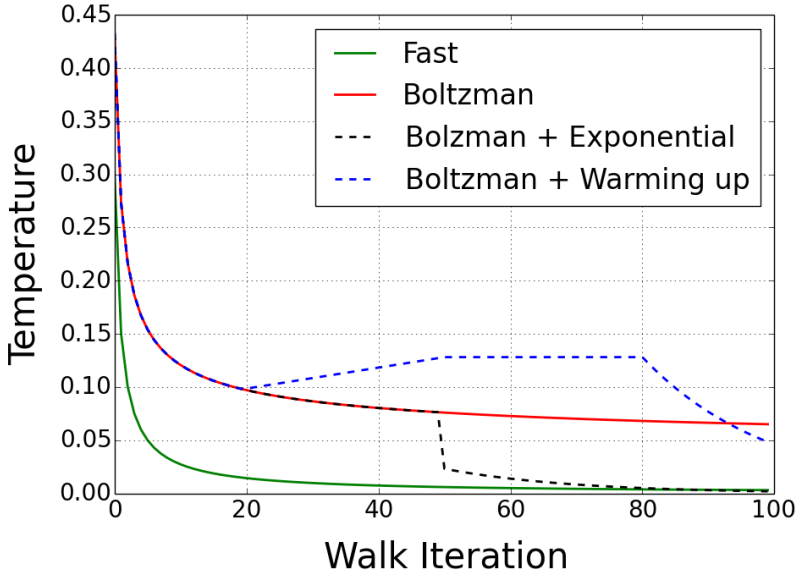

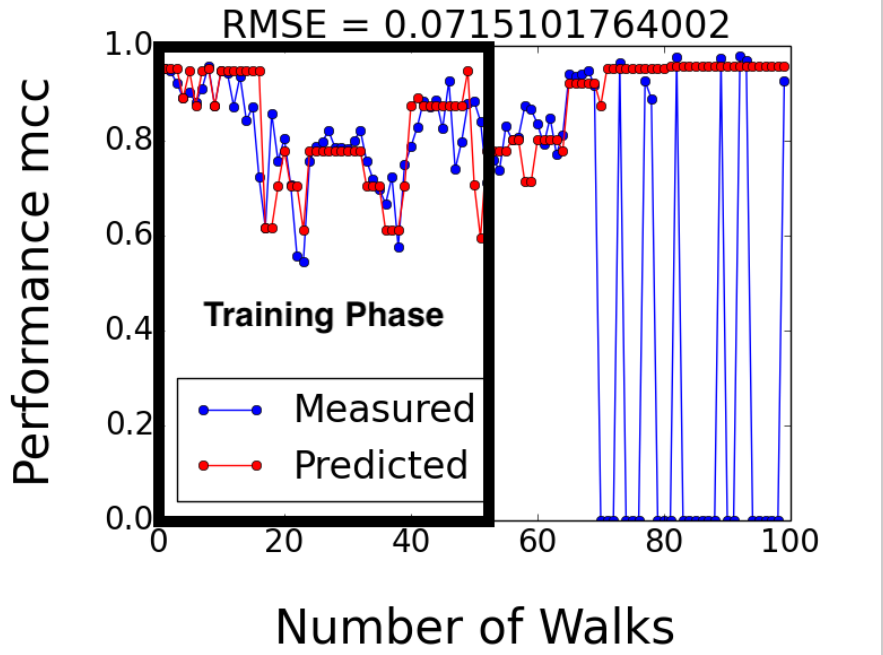

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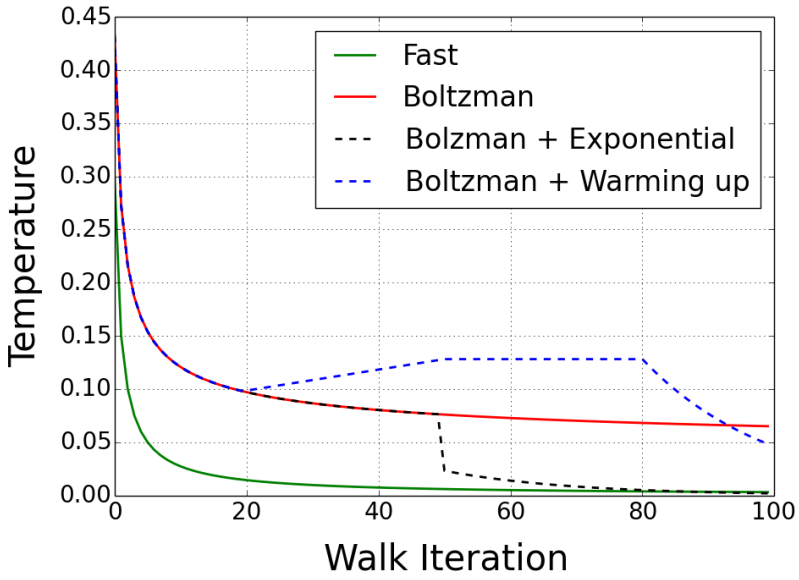

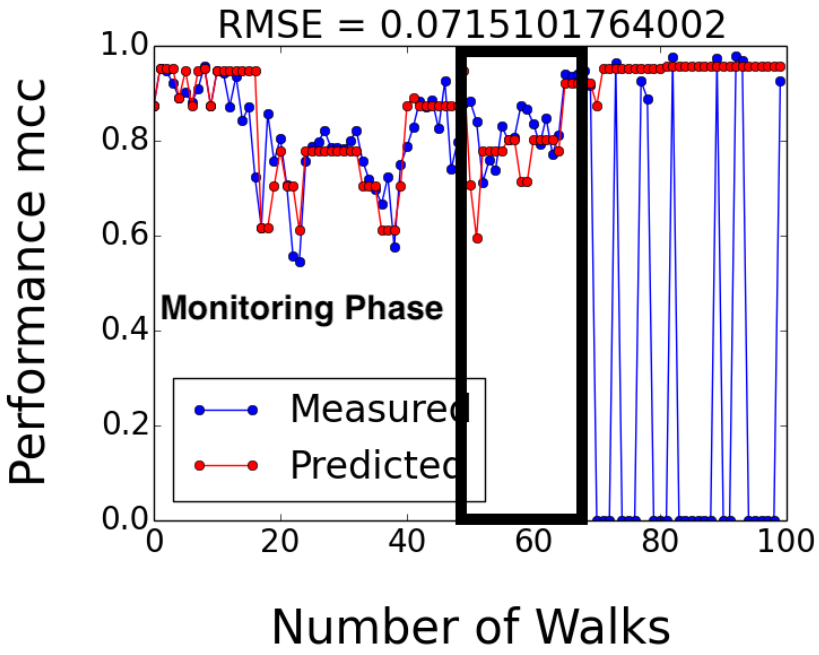

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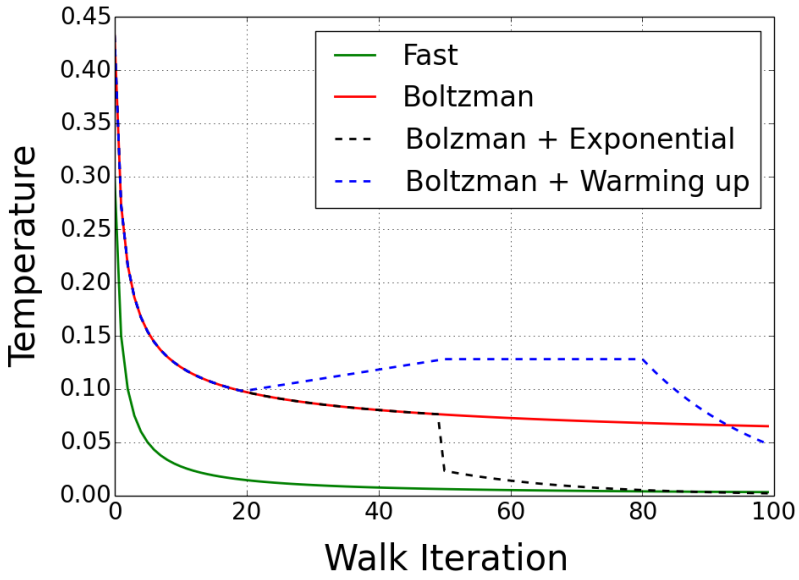

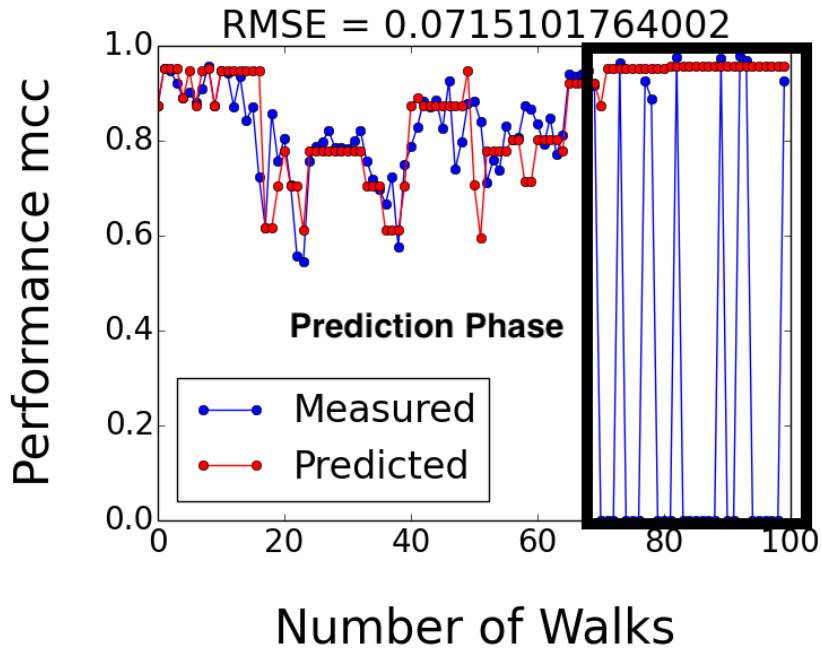

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