2018-07-17_TableTestingNotebook_Clean

July 17, 2018

1 Initialise

In [1]:
```
#! /usr/bin/env python

'''
Trains 7D QuaLiKiz-NN with a single output (efeETG_GB)
'''

from __future__ import print_function

import keras
from keras.models import Sequential, Model
from keras.layers import Dense, Dropout, BatchNormalization
from keras.optimizers import RMSprop, adam, Adam
from keras.initializers import TruncatedNormal
from keras import regularizers
from keras import backend as K
import pandas
import numpy
import sys
import os

import matplotlib.pyplot as plt
from matplotlib.colors import LogNorm

from copy import deepcopy
from keras.models import load_model
```

```
Using TensorFlow backend.
```

In [2]:
```
# Define new Metric: rmse = Root Mean Square Error
def rmse(y_true, y_pred):
    return K.sqrt(K.mean(K.square( y_true-y_pred )))

# Gets the current file name. Useful for procedurally generating output/log files.
file_name =  os.path.basename(sys.argv[0][:-3])
```

```
# Define neural network parameters
batch_size = 10
#num_classes = 1
epochs = 100

# Load Data (which is in HDF5 or .h5 format)
store = pandas.HDFStore("../unstable_training_gen2_7D_nions0_flat_filter7.h5")
target_df = store['efeETG_GB'].to_frame()  # This one is relatively easy to train
input_df = store['input']
```

In [3]:
```
# Puts inputs and outputs in the same pandas dataframe.
# Also only keeps overlapping entries.
joined_dataFrame = target_df.join(input_df)

# Make a copy of joined_dataFrame for late use
joined_dataFrame_original = deepcopy(joined_dataFrame)

# Normalize data by standard deviation and mean-centering the data
joined_dataFrame['efeETG_GB'] = (joined_dataFrame['efeETG_GB'] - joined_dataFrame['efeET
joined_dataFrame['Ati'] = (joined_dataFrame['Ati'] - joined_dataFrame['Ati'].mean()) / j
joined_dataFrame['Ate'] = (joined_dataFrame['Ate'] - joined_dataFrame['Ate'].mean()) / j
joined_dataFrame['An'] = (joined_dataFrame['An'] - joined_dataFrame['An'].mean()) / join
joined_dataFrame['qx'] = (joined_dataFrame['qx'] - joined_dataFrame['qx'].mean()) / join
joined_dataFrame['smag'] = (joined_dataFrame['smag'] - joined_dataFrame['smag'].mean())
joined_dataFrame['x'] = (joined_dataFrame['x'] - joined_dataFrame['x'].mean()) / joined_
joined_dataFrame['Ti_Te'] = (joined_dataFrame['Ti_Te'] - joined_dataFrame['Ti_Te'].mean(

# Shuffles dataset
shuffled_joined_dataFrame = joined_dataFrame.reindex(numpy.random.permutation(
                                                    joined_dataFrame.index))

# Creates a pandas dataframe for the outputs
shuffled_clean_output_df = shuffled_joined_dataFrame['efeETG_GB']

# Creates a pandas dataframe for the inputs
shuffled_clean_input_df = shuffled_joined_dataFrame.drop('efeETG_GB', axis=1)

# Creates training dataset (90% of total data) for outputs
y_train = shuffled_clean_output_df.iloc[:int(
    numpy.round(len(shuffled_clean_output_df)*0.9))]

# Creates training dataset (90% of total data) for inputs
x_train = shuffled_clean_input_df.iloc[:int(
    numpy.round(len(shuffled_clean_input_df)*0.9))]

# Creates testing dataset (10% of total data) for outputs
y_test = shuffled_clean_output_df.iloc[int(
```

```
    numpy.round(len(shuffled_clean_output_df)*0.9)):]

# Creates testing dataset (10% of total data) for inputs
x_test = shuffled_clean_input_df.iloc[int(
    numpy.round(len(shuffled_clean_input_df)*0.9)):]

# Deletes pandas dataframes that are no longer needed
del target_df, input_df

# Closes the HDFStore. This is good practice.
store.close()
```

DEBUGGING

In [4]:
```
joined_dataFrame.describe(include='all')
```

Out[4]:
```
          efeETG_GB           Ati           Ate            An            qx  \
count  638880.000000  6.388800e+05  6.388800e+05  6.388800e+05  6.388800e+05
mean        0.000011  3.921781e-13 -3.483536e-13  5.831676e-14  4.388160e-14
std         1.000114  1.000000e+00  1.000000e+00  1.000000e+00  1.000000e+00
min        -1.136391 -1.848058e+00 -2.151526e+00 -4.177720e+00 -8.735150e-01
25%        -0.802423 -6.589535e-01 -6.642361e-01 -6.349019e-01 -6.749461e-01
50%        -0.301873 -1.493374e-01 -1.684729e-01 -4.443218e-02 -4.385544e-01
75%         0.557895  6.150866e-01  4.925446e-01  5.460375e-01  1.524246e-01
max         3.965936  2.908359e+00  1.814580e+00  2.317447e+00  2.516341e+00

               smag             x         Ti_Te
count  6.388800e+05  6.388800e+05  6.388800e+05
mean   2.038081e-13 -3.500088e-14  1.390060e-13
std    1.000000e+00  1.000000e+00  1.000000e+00
min   -1.264894e+00 -1.375825e+00 -1.666559e+00
25%   -3.146967e-01 -9.567490e-01 -9.260135e-01
50%   -5.555202e-02 -1.185980e-01 -6.698017e-02
75%    4.627374e-01  7.195530e-01  4.217800e-01
max    3.918000e+00  1.767242e+00  1.665897e+00
```

In [5]:
```
joined_dataFrame_original.describe(include='all')
```

Out[5]:
```
          efeETG_GB           Ati            Ate             An  \
count  638880.000000  6.388800e+05  638880.000000  638880.000000
mean       26.038572  5.439559e+00       8.509738       2.075249
std        22.899494  2.943392e+00       3.025638       1.693567
min         0.015788  1.000000e-14       2.000000      -5.000000
25%         7.663502  3.500000e+00       6.500000       1.000000
50%        19.125839  5.000000e+00       8.000000       2.000000
75%        38.814079  7.250000e+00      10.000000       3.000000
max       116.856499  1.400000e+01      14.000000       6.000000
```

```
                  qx           smag              x          Ti_Te
count  638880.000000  638880.000000  638880.000000  638880.000000
mean        4.355203       0.464310       0.483960       1.375224
std         4.230269       1.157654       0.286345       0.675178
min         0.660000      -1.000000       0.090000       0.250000
25%         1.500000       0.100000       0.210000       0.750000
50%         2.500000       0.400000       0.450000       1.330000
75%         5.000000       1.000000       0.690000       1.660000
max        15.000000       5.000000       0.990000       2.500000
```

2 Load Model

```
In [6]: new_model = load_model('../Saved-Networks/2018-07-16_7D_Run0050d.h5', custom_objects={'r
```

Model information

```
In [7]: new_model.summary()
```

```
_________________________________________________________________
Layer (type)                 Output Shape              Param #
=================================================================
dense_1 (Dense)              (None, 30)                240
_________________________________________________________________
dense_2 (Dense)              (None, 30)                930
_________________________________________________________________
dense_3 (Dense)              (None, 30)                930
_________________________________________________________________
dense_4 (Dense)              (None, 1)                 31
=================================================================
Total params: 2,131
Trainable params: 2,131
Non-trainable params: 0
_________________________________________________________________
```

```
In [8]: new_model.get_weights()
```

```
Out[8]: [array([[-2.87334411e-03,  2.41862200e-02, -4.12066132e-02,
                 -1.34515027e-02,  9.28834919e-03,  1.93074974e-03,
                 -1.37387365e-02,  4.32844367e-03, -5.89680718e-03,
                  2.03450094e-03, -3.67641784e-02, -1.36629390e-02,
                  3.24408151e-03, -1.61009077e-02,  1.55328093e-02,
                 -5.37062017e-03,  2.79186517e-02,  1.23187387e-02,
                  5.63374674e-03,  1.52084474e-02,  5.09614870e-03,
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```

```
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 -7.73032486e-01,  6.38422847e-01, -6.03104711e-01,
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 -5.92427194e-01,  1.27917826e+00,  6.44989312e-02,
  9.25727010e-01, -8.36083233e-01, -7.87467599e-01,
 -9.92753729e-02, -8.13657269e-02, -9.42181349e-01,
  9.24308956e-01, -1.13008849e-01,  6.05998300e-02,
 -3.28860395e-02,  8.78981769e-01,  1.99197054e-01,
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  2.21149647e-03, -1.36668772e-01,  1.77159071e-01,
  3.52035493e-01,  2.74182153e+00,  2.96959970e-02,
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```

```
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```

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  8.01239684e-02,  2.27188095e-02, -6.81865036e-01,
 -6.57725567e-03,  7.14557409e-01,  1.02130103e+00,
  2.37337570e-03,  4.69690144e-01, -7.82996044e-03,
  1.10302828e-01, -1.87638495e-02,  4.54581203e-03,
  3.90936911e-01,  5.58428727e-02,  4.64445306e-03,
 -4.38056625e-02, -4.43072766e-01,  2.07188869e+00,
  1.28666925e+00,  4.46881391e-02,  1.13478637e+00],
[-3.38254124e-02,  1.84237158e+00, -6.96639001e-01,
  3.42306286e-01, -8.35664868e-02,  4.23246574e+00,
  5.95746748e-02,  1.22058237e+00, -1.61769938e+00,
  1.12840223e+00, -1.22274198e-02, -6.83897510e-02,
  6.60105720e-02,  1.08710080e-01,  5.85694849e-01,
 -2.67298315e-02,  1.52834833e-01, -1.69515777e-02,
  4.34023321e-01, -3.21768932e-02,  4.34057266e-02,
  6.73382103e-01,  4.28010616e-03, -2.01083273e-02,
 -1.71470027e-02,  2.89101839e-01,  2.45886624e-01,
 -1.98310185e-02,  1.00298040e-03, -6.03562951e-01],
[ 7.20714271e-01, -2.09795251e-01, -8.47141743e-02,
 -2.82501578e-01,  1.23694554e-01,  1.48467433e+00,
  1.03159295e-02, -2.25504923e+00, -7.25931525e-01,
 -1.23919487e+00, -6.58563618e-03, -5.42851448e-01,
 -1.86458770e-02,  4.79575396e-01,  6.06736958e-01,
  6.06722431e-04, -1.32022774e+00,  4.51993085e-02,
 -1.94127440e-01,  3.95609550e-02, -2.03085989e-02,
  8.47139239e-01,  6.53969720e-02,  2.33218465e-02,
  2.67347936e-02, -1.63809991e+00, -2.78170514e+00,
  6.83619022e-01, -7.10887909e-02,  1.14285922e+00],
[-5.96429169e-01,  6.39205217e-01, -6.58662081e-01,
  1.17396601e-01,  2.23911703e-01, -2.23790979e+00,
  6.85726777e-02,  3.42500061e-01,  6.81941509e-01,
  2.34271741e+00,  2.45838854e-02,  2.41839468e-01,
  4.37811650e-02, -1.27655312e-01,  3.70694369e-01,
  5.06829210e-02, -2.12187052e-01, -8.53935704e-02,
  3.30974877e-01, -1.71830729e-02,  3.85299250e-02,
  6.31709769e-02,  1.86524559e-02, -2.85049137e-02,
 -8.86198133e-03, -2.07771659e-01, -2.94297755e-01,
```

```
        -1.34284186e+00, -3.86409052e-02, -2.85674661e-01]], dtype=float32),
array([ 1.8225375 , -2.4948206 ,  2.0260894 , -2.5787468 , -2.837735  ,
        1.6059943 ,  0.07396222, -1.9054754 , -1.9716415 , -3.121214  ,
       -0.02978724, -2.1414735 ,  0.06670253,  0.2886331 ,  2.3389769 ,
        0.00541568, -0.2198047 , -0.01787575, -1.0289241 ,  0.00486385,
        0.00845327,  0.91894853, -0.08716204,  0.06282846, -0.04619095,
        0.9383229 ,  0.4835131 ,  2.0221548 ,  0.04195892,  0.1033548 ],
      dtype=float32),
array([[-3.4717968e-01],
       [-2.6527724e-01],
       [ 3.6765152e-01],
       [ 2.1935374e-01],
       [ 1.8445426e-01],
       [ 6.5788761e-02],
       [-5.0895205e-03],
       [-8.3981164e-02],
       [ 9.6544378e-02],
       [ 2.4194971e-01],
       [ 1.9571478e-03],
       [-9.2007920e-02],
       [-1.5618777e-03],
       [-1.6256732e-01],
       [-2.5405091e-01],
       [-2.8014879e-03],
       [ 1.8248655e-01],
       [ 1.8508438e-03],
       [ 4.7898191e-01],
       [ 2.4726149e-04],
       [ 2.9022794e-04],
       [ 1.9850802e-01],
       [ 2.9635595e-03],
       [ 4.0588146e-03],
       [-4.7782147e-03],
       [-7.6923266e-02],
       [ 5.0785702e-02],
       [-1.5145859e-01],
       [ 4.7635529e-03],
       [-9.9846974e-02]], dtype=float32),
array([-0.26492894], dtype=float32)]
```

```
In [9]: new_model.optimizer
```

```
Out[9]: <keras.optimizers.Adam at 0x223800cbb70>
```

3 Predictions (Global)

"Global" in this sense means that I've fed model.predict() with all the possible parameters. This gives a good overview of the overall performance of the network. This can be useful to spot largescale phenomena like network overfitting but is not so great at looking at say individual data slices. This is done later.

Nota Bene: all data here is NORMALIZED at this stage.

```
In [10]: y_test_np_array = y_test.values
         print(y_test_np_array)
```

```
[-0.02230498  0.55885508 -0.65827708 ...  3.20071806  0.9469378
 -0.74114729]
```

```
In [11]: x_test_np_array = x_test.values
         print(x_test_np_array)
```

```
[[ 0.3602786  -0.41635451 -0.63490191 ...  0.20359267 -0.53767346
  -0.9260135 ]
 [-0.40414545 -0.41635451  0.25080268 ... -1.26489399  0.30047748
   0.42178003]
 [-0.91376148 -0.41635451  0.25080268 ... -1.26489399  0.30047748
   1.66589724]
 ...
 [-1.1685695   0.49254462  0.54603754 ...  0.89464524 -1.37582451
   1.66589724]
 [-0.14933743  1.81457971 -2.99678081 ... -0.05555202 -1.37582451
  -1.29628647]
 [ 0.10547058  1.81457971 -2.99678081 ... -1.26489399 -0.53767346
   0.42178003]]
```

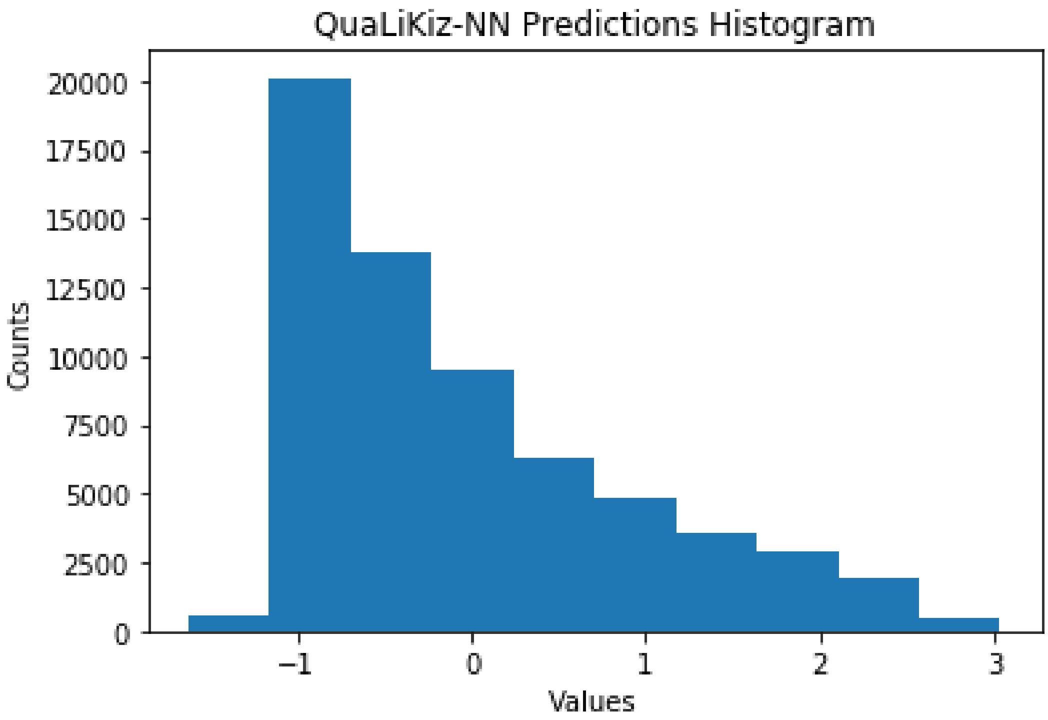
```
In [12]: predictions_global = new_model.predict(x_test_np_array, batch_size = 10, verbose=0)
         print(type(predictions_global))

         predictions_global = predictions_global.flatten()
         print(predictions_global.shape)
         print(type(predictions_global))
```

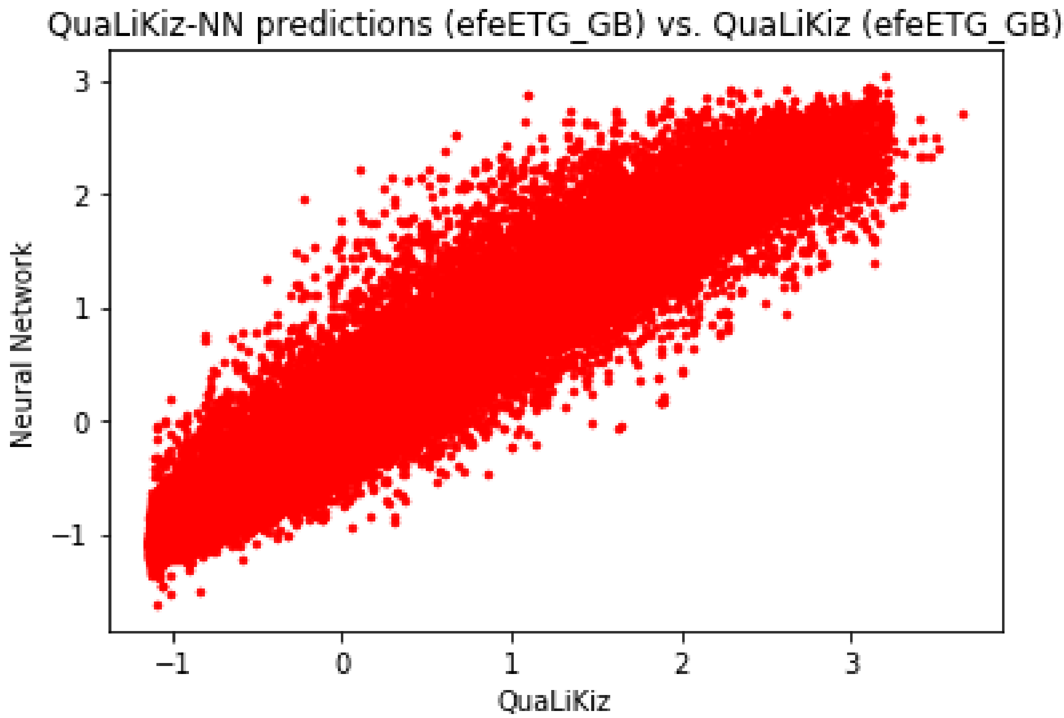
```
<class 'numpy.ndarray'>
(63888,)
<class 'numpy.ndarray'>
```

3.0.1 Predictions (Global) review - Normalized

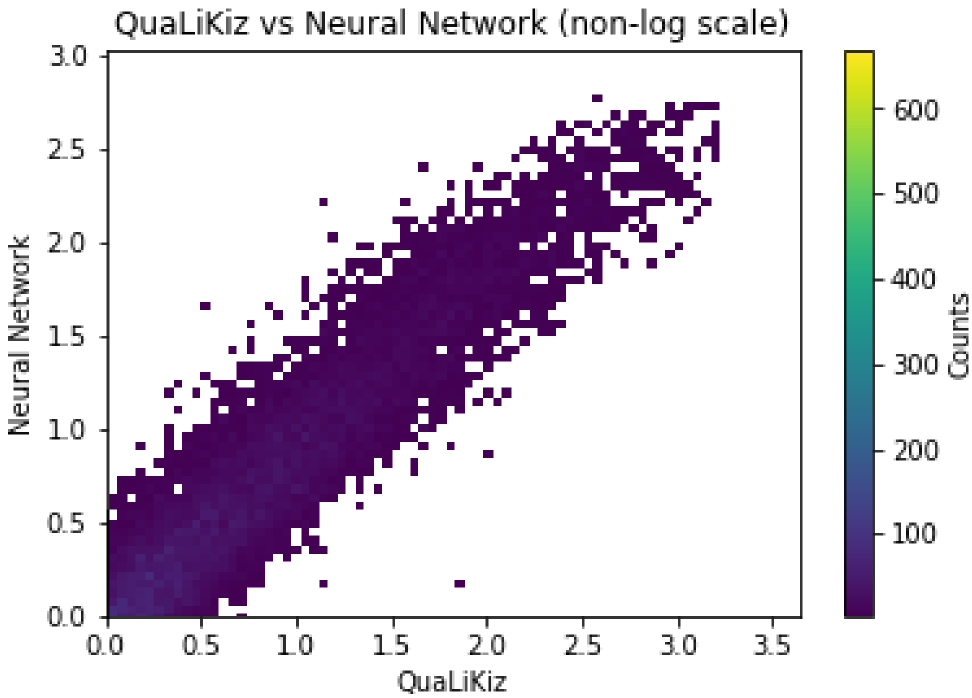
```
In [13]: plt.hist(predictions_global)
         plt.title('QuaLiKiz-NN Predictions Histogram')
         plt.xlabel('Values')
         plt.ylabel('Counts')
         # plt.savefig('./2018-07-10_Run0050b_DataSlicerPlot/NN_Predictions.png', dpi = 100)
         plt.show()
```




```
In [14]: plt.plot(y_test_np_array, predictions_global, 'r.', ms = 5, label = 'QuaLiKiz-NN')
         plt.title('QuaLiKiz-NN predictions (efeETG_GB) vs. QuaLiKiz (efeETG_GB)')
         plt.xlabel('QuaLiKiz')
         plt.ylabel('Neural Network')
         plt.show()
```

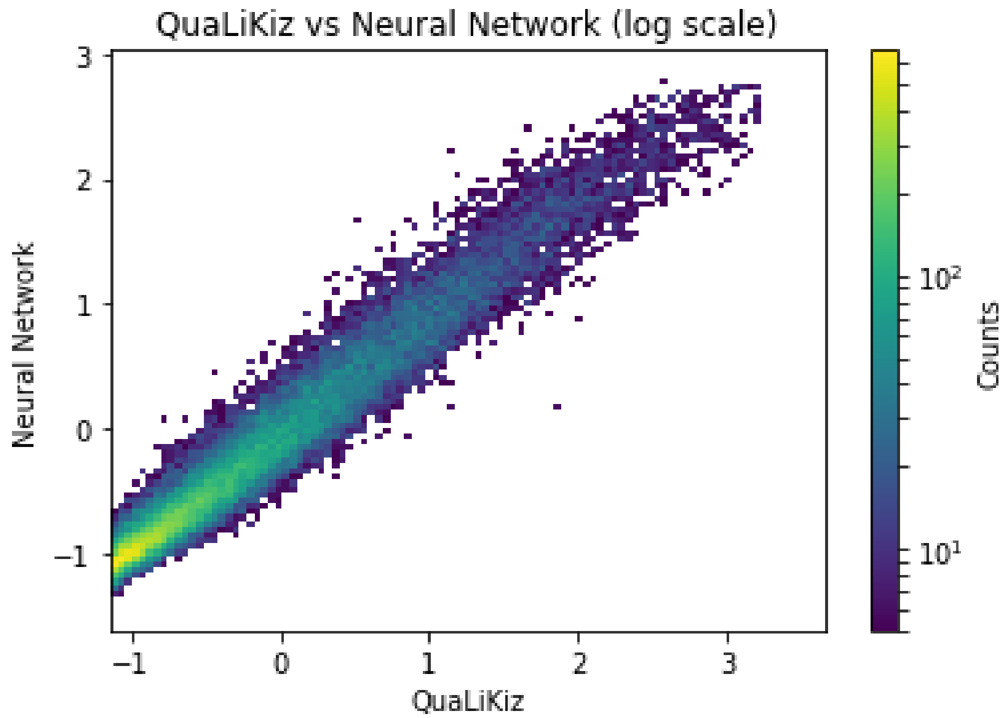



```
In [15]: plt.hist2d(y_test_np_array, predictions_global, bins=100, cmin=5)
         # plt.plot( [0,1],[0,1] )
         plt.title('QuaLiKiz vs Neural Network (non-log scale)')
         plt.xlabel('QuaLiKiz')
         plt.ylabel('Neural Network')
         plt.ylim(0)
         plt.xlim(0)
         cbar = plt.colorbar()
         cbar.ax.set_ylabel('Counts')
         # plt.savefig('./2018-07-10_Run0050b_DataSlicerPlot/QuaLiKiz-vs-NN_nonLogScale_bins100.
         plt.show()
```




```
In [16]: plt.hist2d(y_test_np_array, predictions_global, bins=100, norm=LogNorm(), cmin=5)
         # plt.plot( [0,1],[0,1] )
         plt.title('QuaLiKiz vs Neural Network (log scale)')
         plt.xlabel('QuaLiKiz')
         plt.ylabel('Neural Network')
         # plt.ylim(0)
         # plt.xlim(0)
         cbar = plt.colorbar()
         cbar.ax.set_ylabel('Counts')
         plt.show()

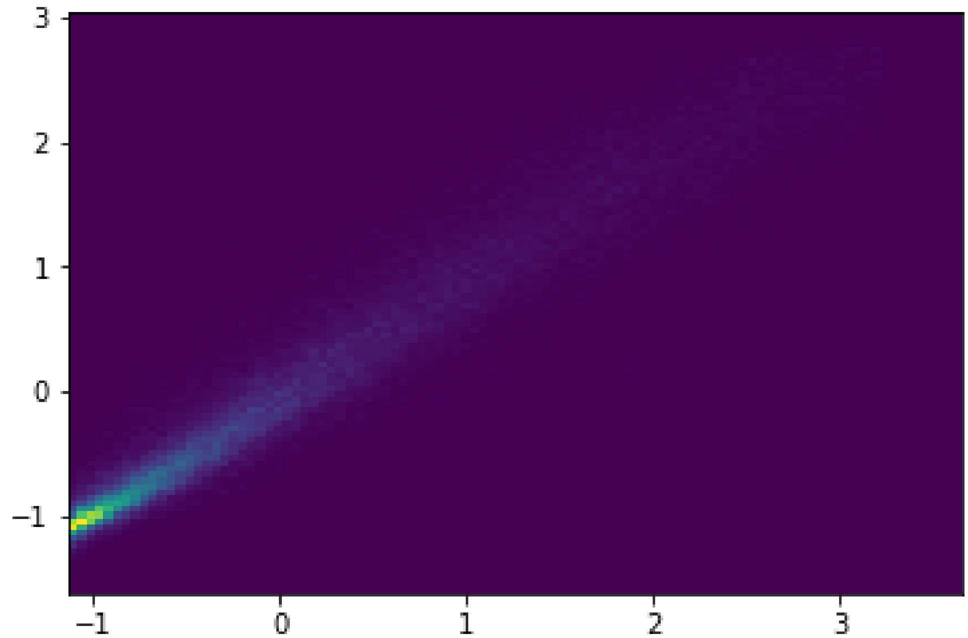
C:\Users\danie\Anaconda3\lib\site-packages\matplotlib\colors.py:1031: RuntimeWarning: invalid va
  mask |= resdat <= 0
```



3.0.2 Sigmas (Normalized)

These plots show how spread out the datapoints in the earlier Neural Network vs. QuaLiKiz plots are.

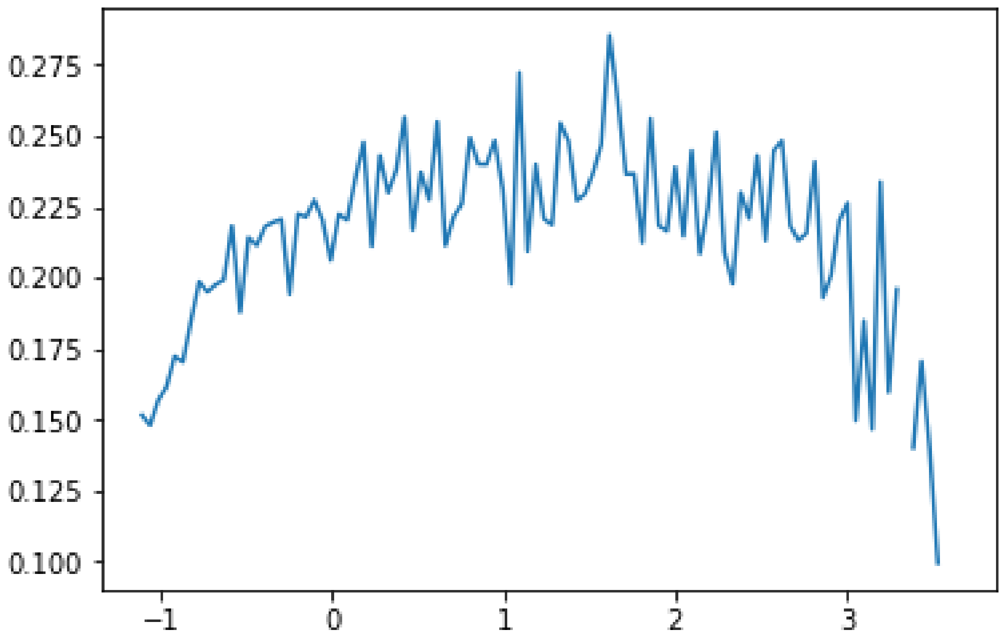
```
In [17]: h = plt.hist2d(y_test_np_array, predictions_global,bins = 100)
```



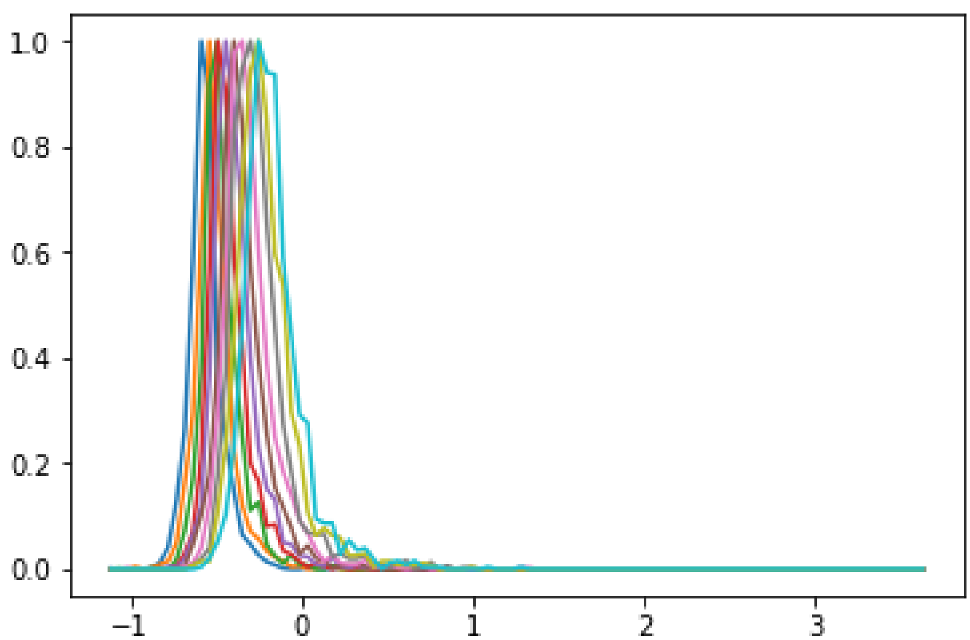

```
In [18]: sigmas = []
         Qualikiz = y_test_np_array
         for i in range(len(h[0])):
             sigmas.append(numpy.std(h[0][i] / numpy.max(h[0][i])))

C:\Users\danie\Anaconda3\lib\site-packages\ipykernel_launcher.py:4: RuntimeWarning: invalid valu
  after removing the cwd from sys.path.
```

```
In [19]: plt.plot((numpy.array(h[1][1:]) + numpy.array(h[1][:-1]))/2.,sigmas)
         plt.show()
```




```
In [20]: for i in range(10):
             plt.plot((h[1][1:] + h[1][:-1])/2., h[0][i]/numpy.max(h[0][i]) )
```

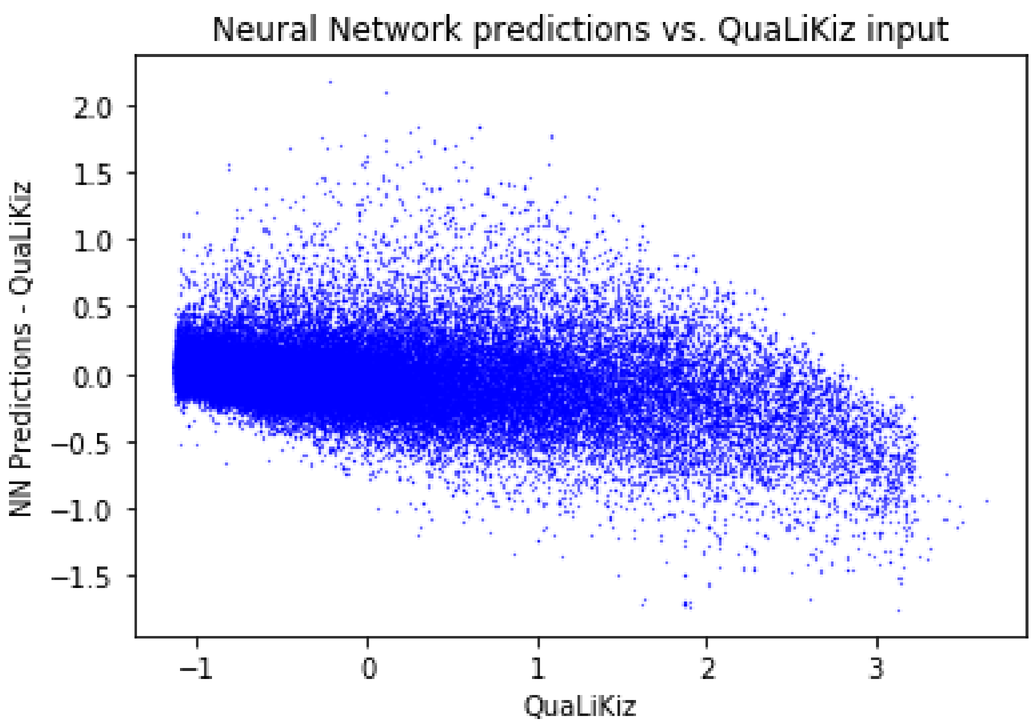


3.0.3 Exploring the spread of the predictions vs. original QuaLiKiz inputs

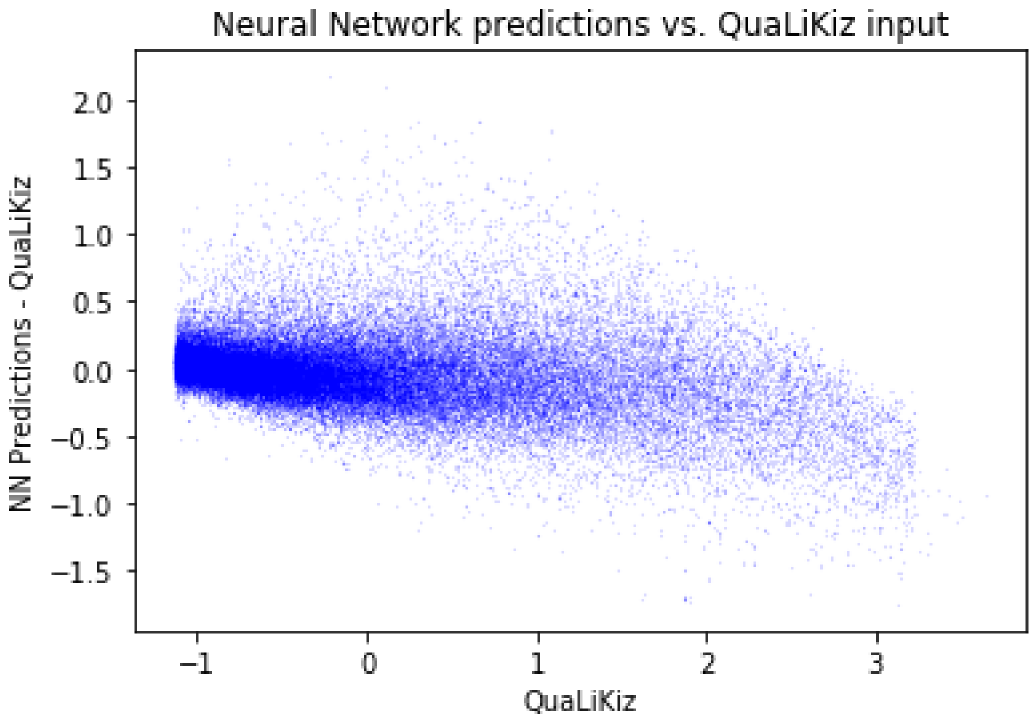
Here we explore the difference between our neural network predictions (of efeETG_GB) vs. the values of the original dataset (unstable_training_gen2_7D_nions0_flat_filter7.h5). The two graphs merely show different dot sizes.

In a perfect case we would have a single line at y = 0 signaling zero disagreement.

In [21]:
```
plt.plot(y_test_np_array, predictions_global - y_test_np_array, 'b.', ms = 0.5)
plt.title('Neural Network predictions vs. QuaLiKiz input')
plt.xlabel('QuaLiKiz')
plt.ylabel('NN Predictions - QuaLiKiz')
plt.show()
```



In [22]:
```
plt.plot(y_test_np_array, predictions_global - y_test_np_array, 'b.', ms = 0.1)
plt.title('Neural Network predictions vs. QuaLiKiz input')
plt.xlabel('QuaLiKiz')
plt.ylabel('NN Predictions - QuaLiKiz')
plt.show()
```



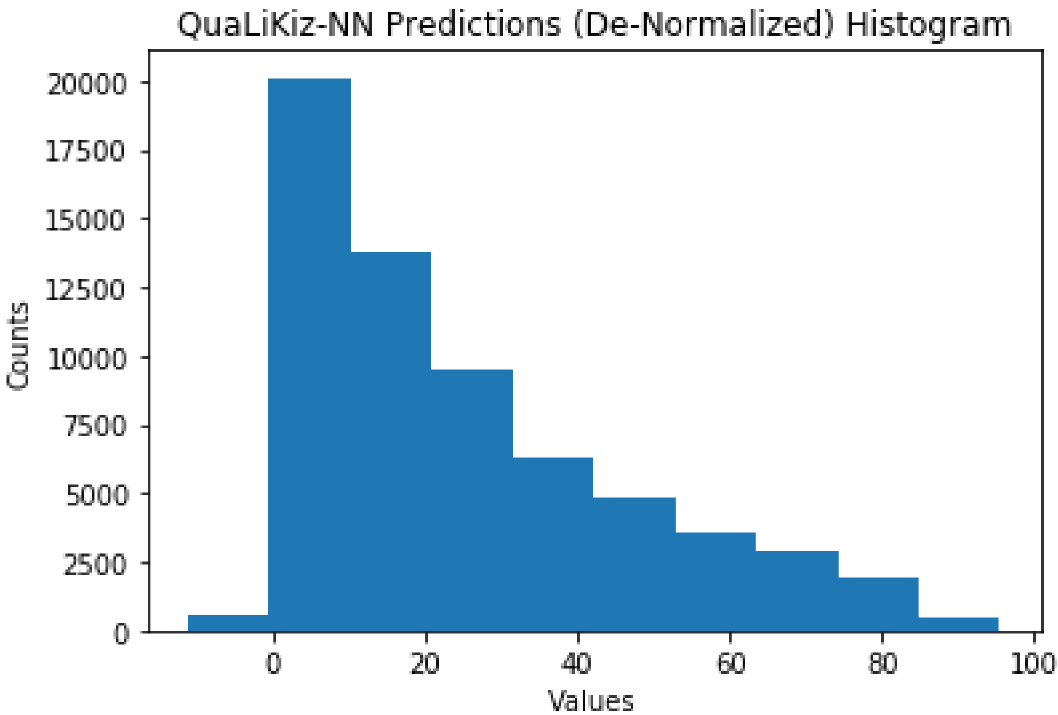
3.0.4 Predictions (Global) review - De-Normalized

```
In [23]: predictions_global_deNormalized = (predictions_global * joined_dataFrame_original['efeE
```

```
In [24]: y_test_deNormalized = (y_test * joined_dataFrame_original['efeETG_GB'].std()) + joined_
```

```
In [25]: y_test_deNormalized_np_array = y_test_deNormalized.values
```

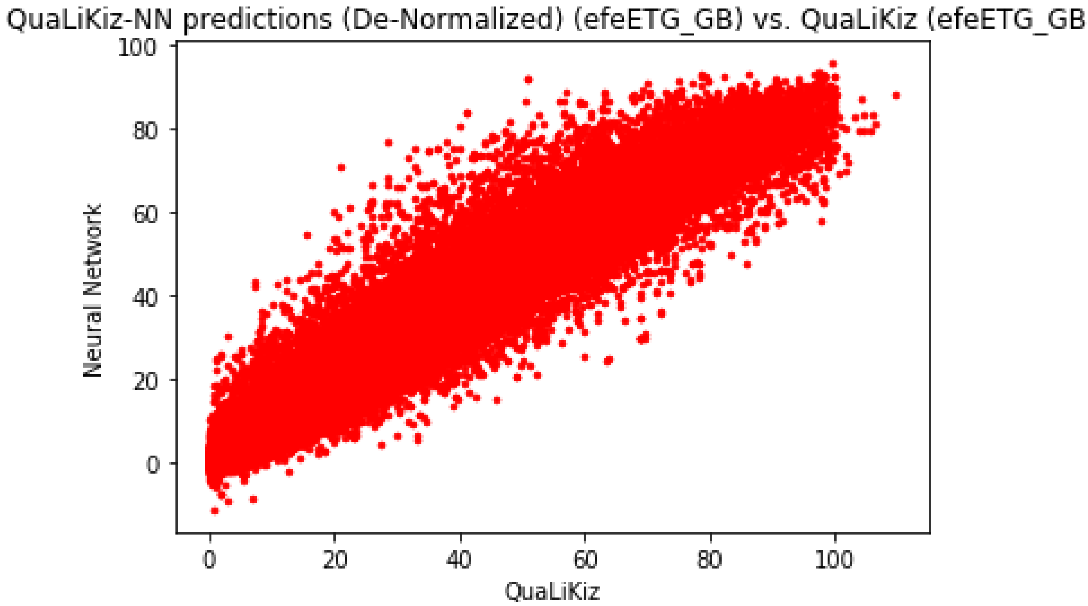
```
In [26]: plt.hist(predictions_global_deNormalized)
         plt.title('QuaLiKiz-NN Predictions (De-Normalized) Histogram')
         plt.xlabel('Values')
         plt.ylabel('Counts')
         # plt.savefig('./2018-07-10_Run0050b_DataSlicerPlot/NN_Predictions.png', dpi = 100)
         plt.show()
```



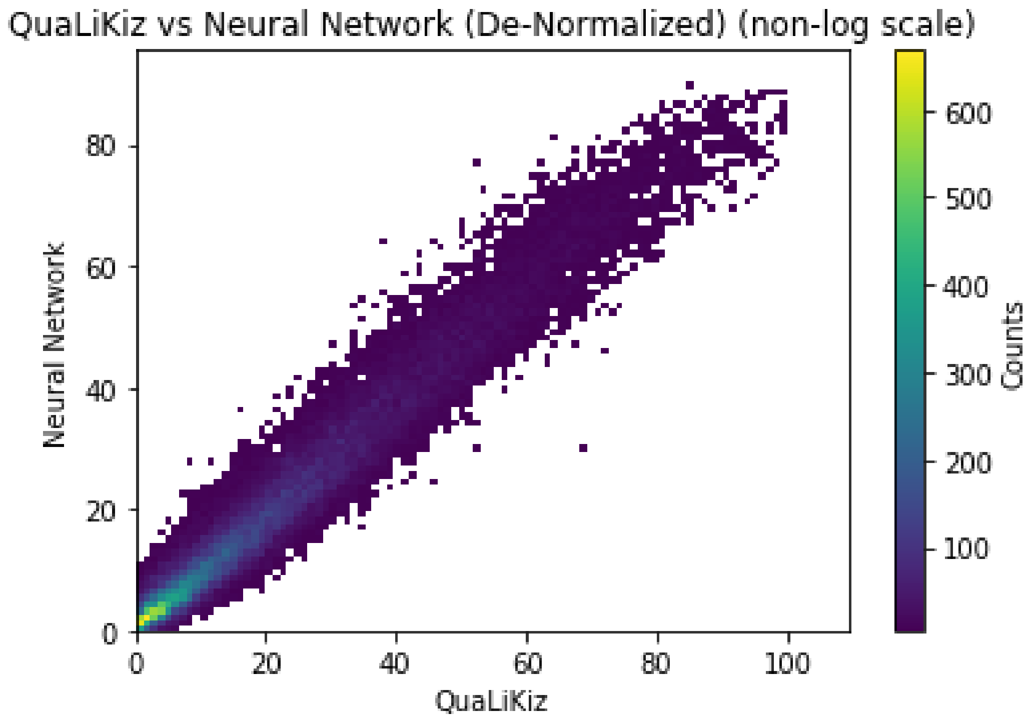

```
In [27]: print(predictions_global.shape)
```

```
(63888,)
```

```
In [28]: plt.plot(y_test_deNormalized_np_array, predictions_global_deNormalized, 'r.', ms = 5, l
         plt.title('QuaLiKiz-NN predictions (De-Normalized) (efeETG_GB) vs. QuaLiKiz (efeETG_GB)
         plt.xlabel('QuaLiKiz')
         plt.ylabel('Neural Network')
         plt.show()
```

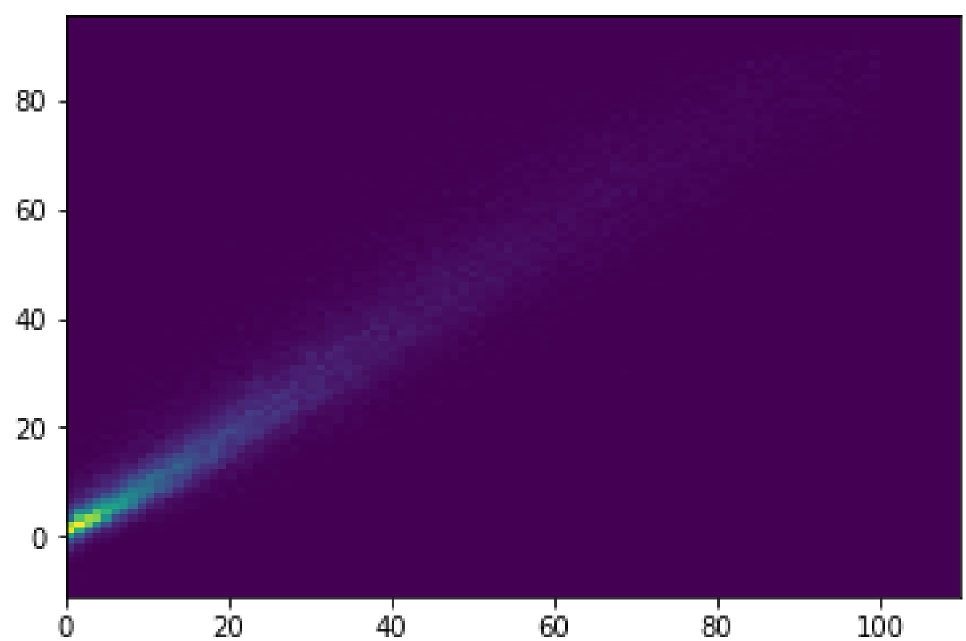



```
In [29]: plt.hist2d(y_test_deNormalized_np_array, predictions_global_deNormalized, bins=100, cmi
         # plt.plot( [0,1],[0,1] )
         plt.title('QuaLiKiz vs Neural Network (De-Normalized) (non-log scale)')
         plt.xlabel('QuaLiKiz')
         plt.ylabel('Neural Network')
         plt.ylim(0)
         plt.xlim(0)
         cbar = plt.colorbar()
         cbar.ax.set_ylabel('Counts')
         # plt.savefig('./2018-07-10_Run0050b_DataSlicerPlot/QuaLiKiz-vs-NN_nonLogScale_bins100.
         plt.show()
```



3.0.5 Sigmas (De-Normalized)

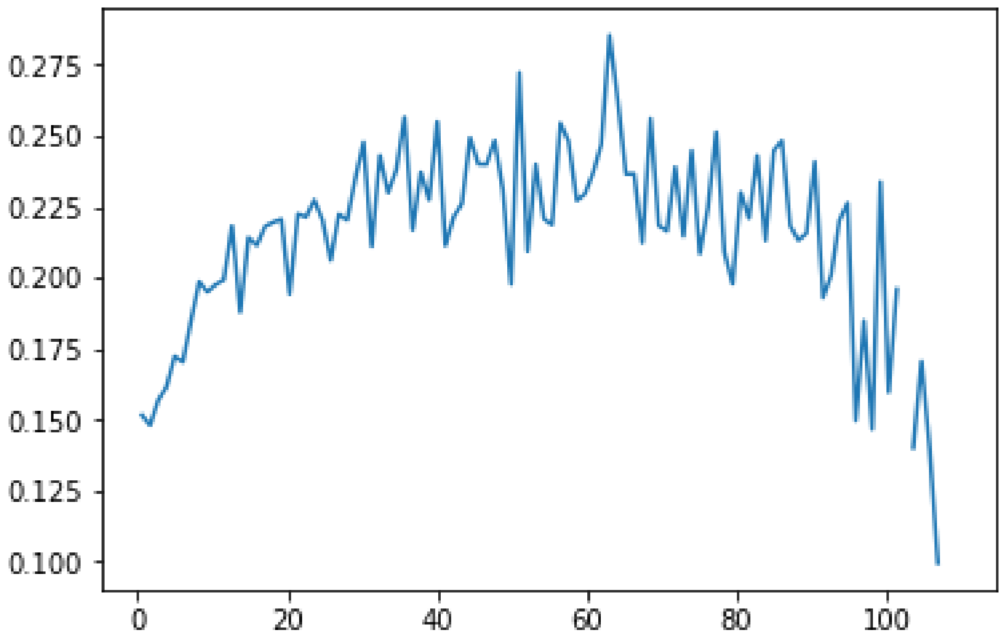
```
In [30]: h_deNormalized = plt.hist2d(y_test_deNormalized_np_array, predictions_global_deNormaliz
```



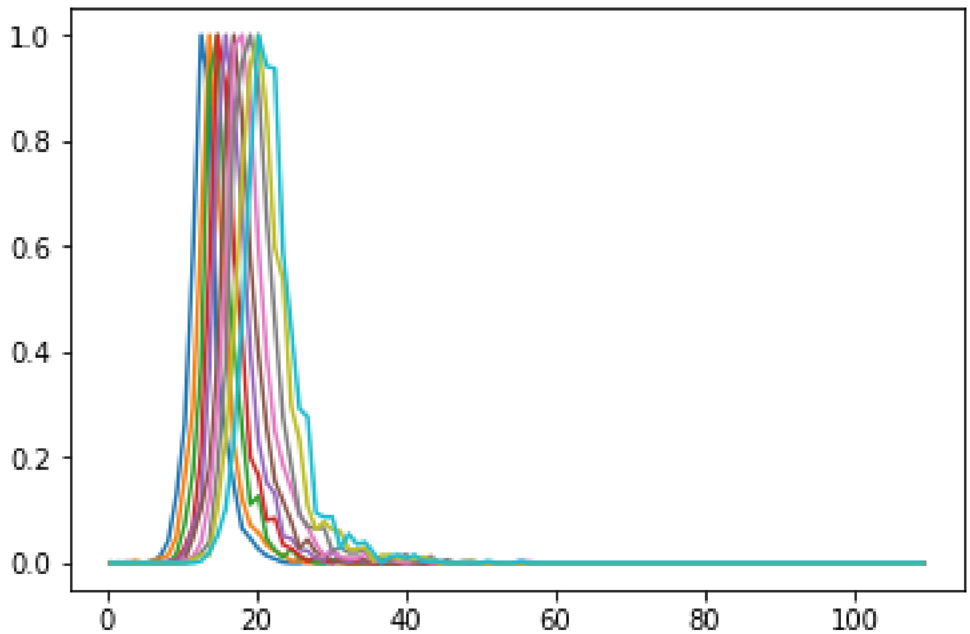
```
In [31]: sigmas_deNormalized = []
         Qualikiz_deNormalized = y_test_deNormalized_np_array
         for i in range(len(h[0])):
             sigmas_deNormalized.append(numpy.std(h_deNormalized[0][i] / numpy.max(h_deNormalize

C:\Users\danie\Anaconda3\lib\site-packages\ipykernel_launcher.py:4: RuntimeWarning: invalid valu
  after removing the cwd from sys.path.
```

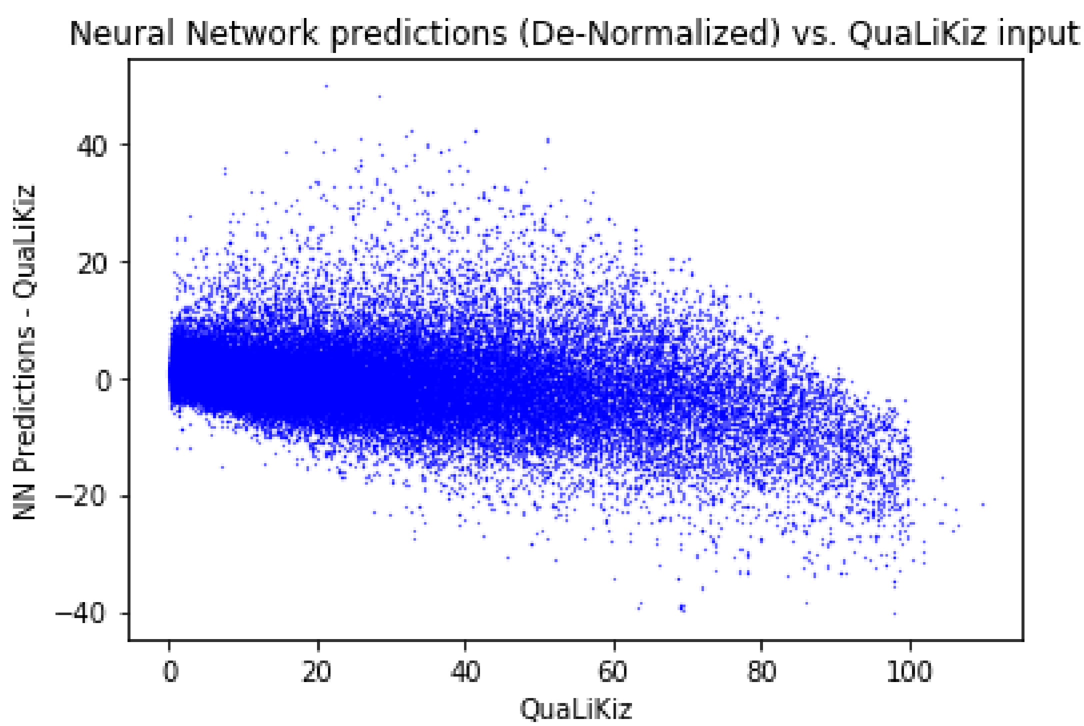
```
In [32]: plt.plot((numpy.array(h_deNormalized[1][1:]) + numpy.array(h_deNormalized[1][:-1]))/2.,
         plt.show()
```



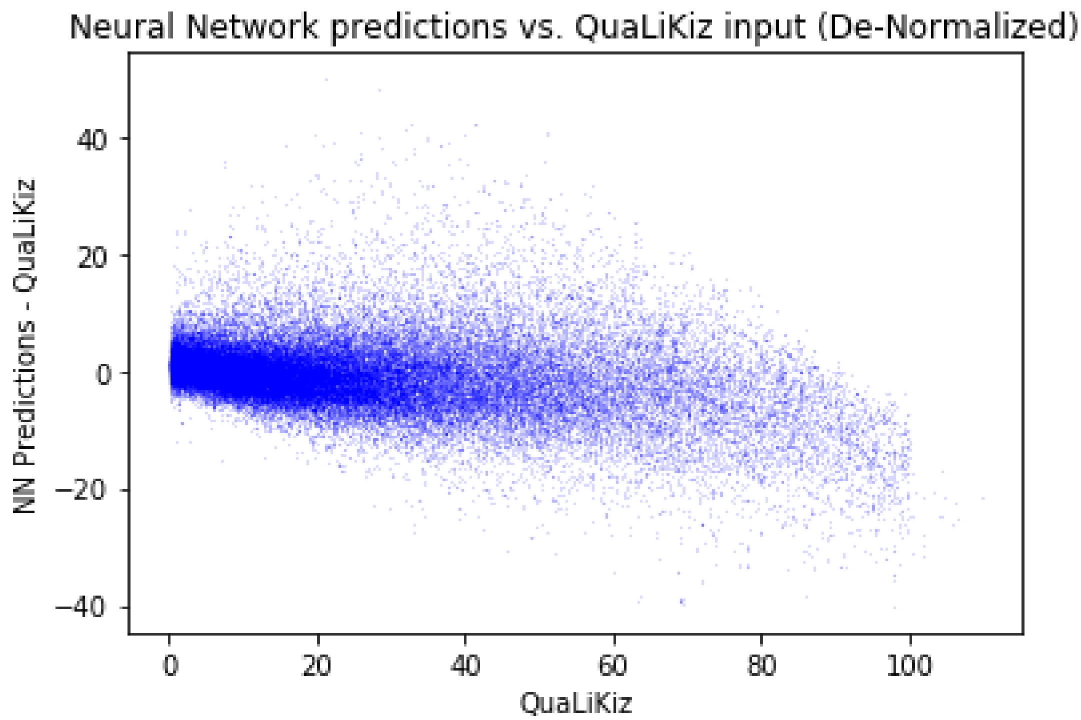

```
In [33]: for i in range(10):
             plt.plot((h_deNormalized[1][1:] + h_deNormalized[1][:-1])/2., h_deNormalized[0][i]/
```




```
In [34]: plt.plot(y_test_deNormalized_np_array, predictions_global_deNormalized - y_test_deNorma
         plt.title('Neural Network predictions (De-Normalized) vs. QuaLiKiz input')
         plt.xlabel('QuaLiKiz')
         plt.ylabel('NN Predictions - QuaLiKiz')
         plt.show()
```



```
In [35]: plt.plot(y_test_deNormalized_np_array, predictions_global_deNormalized - y_test_deNorma
         plt.title('Neural Network predictions vs. QuaLiKiz input (De-Normalized)')
         plt.xlabel('QuaLiKiz')
         plt.ylabel('NN Predictions - QuaLiKiz')
         plt.show()
```



4 Predictions (single Data Slice)

4.0.1 Predictions - Initialise table to feed predictions

```
In [36]: # table (Original values from input file unstable_training_gen2_7D_nions0_flat_filter7.
         # Hard-coded variables for the data slice

         table = numpy.zeros((200,7))

         table[:,0] = 5.75     # Ati
         table[:,1] = numpy.linspace(2,14,200)   # Ate
         table[:,2] = 3        # An
         table[:,3] = 3        # qx
         table[:,4] = 0.7      # smag
```

```
table[:,5] = 0.45    # x
table[:,6] = 1.33    # Ti_Te

table
```

```
Out[36]: array([[ 5.75      ,  2.        ,  3.        , ...,  0.7       ,
                  0.45      ,  1.33      ],
                [ 5.75      ,  2.06030151,  3.        , ...,  0.7       ,
                  0.45      ,  1.33      ],
                [ 5.75      ,  2.12060302,  3.        , ...,  0.7       ,
                  0.45      ,  1.33      ],
                ...,
                [ 5.75      , 13.87939698,  3.        , ...,  0.7       ,
                  0.45      ,  1.33      ],
                [ 5.75      , 13.93969849,  3.        , ...,  0.7       ,
                  0.45      ,  1.33      ],
                [ 5.75      , 14.        ,  3.        , ...,  0.7       ,
                  0.45      ,  1.33      ]])
```

```
In [37]: # Normalized table (inputs for model.predict())
         table_normalized = numpy.zeros((200,7))

         DataSlice_Ati = 5.75
         DataSlice_Ate = numpy.linspace(2,14,200)
         DataSlice_An = 3
         DataSlice_qx = 3
         DataSlice_smag = 0.7
         DataSlice_x = 0.45
         DataSlice_Ti_Te = 1.33

         # Normalize data by standard deviation and mean-centering the data
         table_normalized[:,0] = (DataSlice_Ati - joined_dataFrame_original['Ati'].mean()) / joi
         table_normalized[:,1] = (DataSlice_Ate - joined_dataFrame_original['Ate'].mean()) / joi
         table_normalized[:,2] = (DataSlice_An - joined_dataFrame_original['An'].mean()) / joine
         table_normalized[:,3] = (DataSlice_qx - joined_dataFrame_original['qx'].mean()) / joine
         table_normalized[:,4] = (DataSlice_smag - joined_dataFrame_original['smag'].mean()) / j
         table_normalized[:,5] = (DataSlice_x - joined_dataFrame_original['x'].mean()) / joined_
         table_normalized[:,6] = (DataSlice_Ti_Te - joined_dataFrame_original['Ti_Te'].mean()) /
```

```
In [38]: table_normalized
```

```
Out[38]: array([[ 0.10547058, -2.15152557,  0.54603754, ...,  0.20359268,
                 -0.118598  , -0.06698023],
                [ 0.10547058, -2.13159539,  0.54603754, ...,  0.20359268,
                 -0.118598  , -0.06698023],
                [ 0.10547058, -2.11166521,  0.54603754, ...,  0.20359268,
                 -0.118598  , -0.06698023],
                ...,
                [ 0.10547058,  1.77471936,  0.54603754, ...,  0.20359268,
```

```
        -0.118598  , -0.06698023],
       [ 0.10547058,  1.79464954,  0.54603754, ...,  0.20359268,
        -0.118598  , -0.06698023],
       [ 0.10547058,  1.81457971,  0.54603754, ...,  0.20359268,
        -0.118598  , -0.06698023]])
```

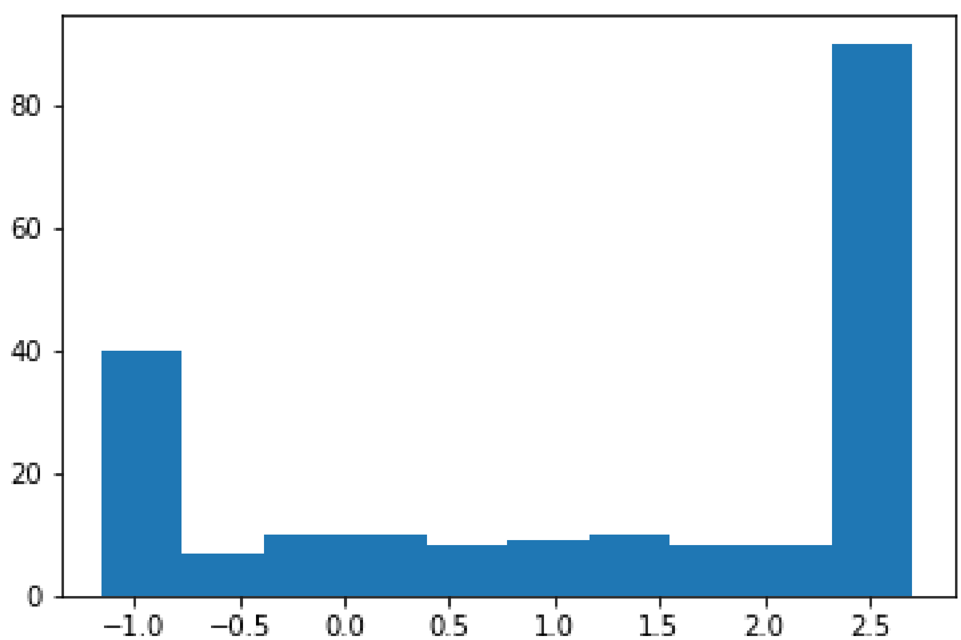
In [39]:
```
# joined_dataFrame.to_csv('./out_joined_dataFrame.csv', encoding='utf-8')
```

In [40]:
```
predictions = new_model.predict(table_normalized, batch_size = 10, verbose=0)
print(type(predictions))

predictions = predictions.flatten()
print(predictions.shape)
print(type(predictions))
```

```
<class 'numpy.ndarray'>
(200,)
<class 'numpy.ndarray'>
```

In [41]:
```
plt.hist(predictions)
plt.show()
```



5 Masks

These are used to rapidly select which parameters to look at (for a given data slice).

Ate

```
In [42]: Ate_mask1 = joined_dataFrame_original.Ate == 2
         Ate_mask2 = joined_dataFrame_original.Ate == 2.75
         Ate_mask3 = joined_dataFrame_original.Ate == 3.5
         Ate_mask4 = joined_dataFrame_original.Ate == 4.25
         Ate_mask5 = joined_dataFrame_original.Ate == 5
         Ate_mask6 = joined_dataFrame_original.Ate == 5.75
         Ate_mask7 = joined_dataFrame_original.Ate == 6.5
         Ate_mask8 = joined_dataFrame_original.Ate == 7.25
         Ate_mask9 = joined_dataFrame_original.Ate == 8
         Ate_mask10 = joined_dataFrame_original.Ate == 10
         Ate_mask11 = joined_dataFrame_original.Ate == 14

         Ate_anti_mask1 = joined_dataFrame_original.Ate != 2
         Ate_anti_mask2 = joined_dataFrame_original.Ate != 2.75
         Ate_anti_mask3 = joined_dataFrame_original.Ate != 3.5
         Ate_anti_mask4 = joined_dataFrame_original.Ate != 4.25
         Ate_anti_mask5 = joined_dataFrame_original.Ate != 5
         Ate_anti_mask6 = joined_dataFrame_original.Ate != 5.75
         Ate_anti_mask7 = joined_dataFrame_original.Ate != 6.5
         Ate_anti_mask8 = joined_dataFrame_original.Ate != 7.25
         Ate_anti_mask9 = joined_dataFrame_original.Ate != 8
         Ate_anti_mask10 = joined_dataFrame_original.Ate != 10
         Ate_anti_mask11 = joined_dataFrame_original.Ate != 14
```

An

```
In [43]: An_mask1 = joined_dataFrame_original.An == -5
         An_mask2 = joined_dataFrame_original.An == -3
         An_mask3 = joined_dataFrame_original.An == -1
         An_mask4 = numpy.array(joined_dataFrame_original.An <= 1.1e-14) * numpy.array(joined_da
         An_mask5 = joined_dataFrame_original.An == 0.5
         An_mask6 = joined_dataFrame_original.An == 1.0
         An_mask7 = joined_dataFrame_original.An == 1.5
         An_mask8 = joined_dataFrame_original.An == 2.0
         An_mask9 = joined_dataFrame_original.An == 2.5
         An_mask10 = joined_dataFrame_original.An == 3.0
         An_mask11 = joined_dataFrame_original.An == 4.0
         An_mask12 = joined_dataFrame_original.An == 6.0

         An_anti_mask1 = joined_dataFrame_original.An != -5
         An_anti_mask2 = joined_dataFrame_original.An != -3
         An_anti_mask3 = joined_dataFrame_original.An != -1
         An_anti_mask4 = numpy.array(joined_dataFrame_original.An >= 1.1e-14) * numpy.array(join
         An_anti_mask5 = joined_dataFrame_original.An != 0.5
         An_anti_mask6 = joined_dataFrame_original.An != 1.0
         An_anti_mask7 = joined_dataFrame_original.An != 1.5
```

```
An_anti_mask8 = joined_dataFrame_original.An != 2.0
An_anti_mask9 = joined_dataFrame_original.An != 2.5
An_anti_mask10 = joined_dataFrame_original.An != 3.0
An_anti_mask11 = joined_dataFrame_original.An != 4.0
An_anti_mask12 = joined_dataFrame_original.An != 6.0
```

Ati

```
In [44]: Ati_mask1 = numpy.array(joined_dataFrame_original.Ati <= 1.1e-14) * numpy.array(joined_
         Ati_mask2 = joined_dataFrame_original.Ati == 2
         Ati_mask3 = joined_dataFrame_original.Ati == 2.75
         Ati_mask4 = joined_dataFrame_original.Ati == 3.5
         Ati_mask5 = joined_dataFrame_original.Ati == 4.25
         Ati_mask6 = joined_dataFrame_original.Ati == 5
         Ati_mask7 = joined_dataFrame_original.Ati == 5.75
         Ati_mask8 = joined_dataFrame_original.Ati == 6.5
         Ati_mask9 = joined_dataFrame_original.Ati == 7.25
         Ati_mask10 = joined_dataFrame_original.Ati == 8
         Ati_mask11 = joined_dataFrame_original.Ati == 10
         Ati_mask12 = joined_dataFrame_original.Ati == 14
```

qx

```
In [45]: qx_mask0 = numpy.array(joined_dataFrame_original.qx <= 0.67) * numpy.array(joined_dataF
         qx_mask1 = joined_dataFrame_original.qx == 1.0
         qx_mask2 = joined_dataFrame_original.qx == 1.5
         qx_mask3 = joined_dataFrame_original.qx == 2.0
         qx_mask4 = joined_dataFrame_original.qx == 2.5
         qx_mask5 = joined_dataFrame_original.qx == 3.0
         qx_mask6 = joined_dataFrame_original.qx == 4.0
         qx_mask7 = joined_dataFrame_original.qx == 5.0
         qx_mask8 = joined_dataFrame_original.qx == 10.00
         qx_mask9 = joined_dataFrame_original.qx == 15.00

         qx_anti_mask0 = numpy.array(joined_dataFrame_original.qx >= 0.67) * numpy.array(joined_
         qx_anti_mask1 = joined_dataFrame_original.qx != 1.0
         qx_anti_mask2 = joined_dataFrame_original.qx != 1.5
         qx_anti_mask3 = joined_dataFrame_original.qx != 2.0
         qx_anti_mask4 = joined_dataFrame_original.qx != 2.5
         qx_anti_mask5 = joined_dataFrame_original.qx != 3.0
         qx_anti_mask6 = joined_dataFrame_original.qx != 4.0
         qx_anti_mask7 = joined_dataFrame_original.qx != 5.0
         qx_anti_mask8 = joined_dataFrame_original.qx != 10.00
         qx_anti_mask9 = joined_dataFrame_original.qx != 15.00
```

smag

```
In [46]: smag_mask1 = joined_dataFrame_original.smag == -1.0
         smag_mask2 = numpy.array(joined_dataFrame_original.smag <= 0.11) * numpy.array(joined_d
```

```
smag_mask3 = numpy.array(joined_dataFrame_original.smag <= 0.41) * numpy.array(joined_d
smag_mask4 = numpy.array(joined_dataFrame_original.smag <= 0.71) * numpy.array(joined_d
smag_mask5 = joined_dataFrame_original.smag == 1
smag_mask6 = joined_dataFrame_original.smag == 1.5
smag_mask7 = joined_dataFrame_original.smag == 2.0
smag_mask8 = joined_dataFrame_original.smag == 2.75
smag_mask9 = joined_dataFrame_original.smag == 3.5
smag_mask10 = joined_dataFrame_original.smag == 5.0

smag_anti_mask1 = joined_dataFrame_original.smag != -1.0
smag_anti_mask2 = numpy.array(joined_dataFrame_original.smag >= 0.11) * numpy.array(joi
smag_anti_mask3 = numpy.array(joined_dataFrame_original.smag >= 0.41) * numpy.array(joi
smag_anti_mask4 = numpy.array(joined_dataFrame_original.smag >= 0.71) * numpy.array(joi
smag_anti_mask5 = joined_dataFrame_original.smag != 1
smag_anti_mask6 = joined_dataFrame_original.smag != 1.5
smag_anti_mask7 = joined_dataFrame_original.smag != 2.0
smag_anti_mask8 = joined_dataFrame_original.smag != 2.75
smag_anti_mask9 = joined_dataFrame_original.smag != 3.5
smag_anti_mask10 = joined_dataFrame_original.smag != 5.0
```

x

```
In [47]: x_mask1 = numpy.array(joined_dataFrame_original.x <= 0.10) * numpy.array(joined_dataFra
         x_mask2 = numpy.array(joined_dataFrame_original.x <= 0.22) * numpy.array(joined_dataFra
         x_mask3 = numpy.array(joined_dataFrame_original.x <= 0.34) * numpy.array(joined_dataFra
         x_mask4 = numpy.array(joined_dataFrame_original.x <= 0.46) * numpy.array(joined_dataFra
         x_mask5 = numpy.array(joined_dataFrame_original.x <= 0.58) * numpy.array(joined_dataFra
         x_mask6 = numpy.array(joined_dataFrame_original.x <= 0.70) * numpy.array(joined_dataFra
         x_mask7 = numpy.array(joined_dataFrame_original.x <= 0.85) * numpy.array(joined_dataFra
         x_mask8 = numpy.array(joined_dataFrame_original.x <= 1.00) * numpy.array(joined_dataFra

         x_anti_mask1 = numpy.array(joined_dataFrame_original.x >= 0.10) * numpy.array(joined_da
         x_anti_mask2 = numpy.array(joined_dataFrame_original.x >= 0.22) * numpy.array(joined_da
         x_anti_mask3 = numpy.array(joined_dataFrame_original.x >= 0.34) * numpy.array(joined_da
         x_anti_mask4 = numpy.array(joined_dataFrame_original.x >= 0.46) * numpy.array(joined_da
         x_anti_mask5 = numpy.array(joined_dataFrame_original.x >= 0.58) * numpy.array(joined_da
         x_anti_mask6 = numpy.array(joined_dataFrame_original.x >= 0.70) * numpy.array(joined_da
         x_anti_mask7 = numpy.array(joined_dataFrame_original.x >= 0.85) * numpy.array(joined_da
         x_anti_mask8 = numpy.array(joined_dataFrame_original.x >= 1.00) * numpy.array(joined_da
```

Ti_Te

```
In [48]: Ti_Te_mask1 = joined_dataFrame_original.Ti_Te == 0.25
         Ti_Te_mask2 = joined_dataFrame_original.Ti_Te == 0.5
         Ti_Te_mask3 = joined_dataFrame_original.Ti_Te == 0.75
         Ti_Te_mask4 = joined_dataFrame_original.Ti_Te == 1
         Ti_Te_mask5 = numpy.array(joined_dataFrame_original.Ti_Te <= 1.34) * numpy.array(joined
         Ti_Te_mask6 = numpy.array(joined_dataFrame_original.Ti_Te <= 1.67) * numpy.array(joined
         Ti_Te_mask7 = joined_dataFrame_original.Ti_Te == 2.50
```

6 Plots

```
In [49]: '''
         {'An': 3,
         'Ati': 5.75,
         'Ti_Te': 1.33,
         'q': 3,
         'smag': 0.7,
         'x': 0.45}
         '''

         newDF = joined_dataFrame[An_mask10 & Ati_mask7 & qx_mask5 & smag_mask4 & x_mask4 & Ti_T
         newDF_Mk2 = joined_dataFrame_original[An_mask10 & Ati_mask7 & qx_mask5 & smag_mask4 & x
         print(newDF)
         print(type(newDF))

         print(newDF_Mk2)
         print(type(newDF_Mk2))
```

```
           efeETG_GB       Ati       Ate        An        qx      smag  \
30963559  -0.813345  0.105471 -1.407881  0.546038 -0.320359  0.203593
31366759  -0.556873  0.105471 -1.159999  0.546038 -0.320359  0.203593
32576359   1.644625  0.105471 -0.416355  0.546038 -0.320359  0.203593

                 x    Ti_Te
30963559 -0.118598 -0.06698
31366759 -0.118598 -0.06698
32576359 -0.118598 -0.06698
<class 'pandas.core.frame.DataFrame'>
          efeETG_GB   Ati   Ate   An   qx  smag     x  Ti_Te
30963559   7.413384  5.75  4.25  3.0  3.0   0.7  0.45   1.33
31366759  13.286460  5.75  5.00  3.0  3.0   0.7  0.45   1.33
32576359  63.699650  5.75  7.25  3.0  3.0   0.7  0.45   1.33
<class 'pandas.core.frame.DataFrame'>
```

```
In [50]: efeETG_DF = newDF['efeETG_GB']
         efeETG_DF_np_array = efeETG_DF.values
         print(efeETG_DF_np_array)

         Ate_DF = newDF['Ate']
         Ate_DF_np_array = Ate_DF.values
         print(Ate_DF_np_array)
```

```
[-0.81334497 -0.5568731   1.64462486]
[-1.40788083 -1.15999925 -0.41635451]
```

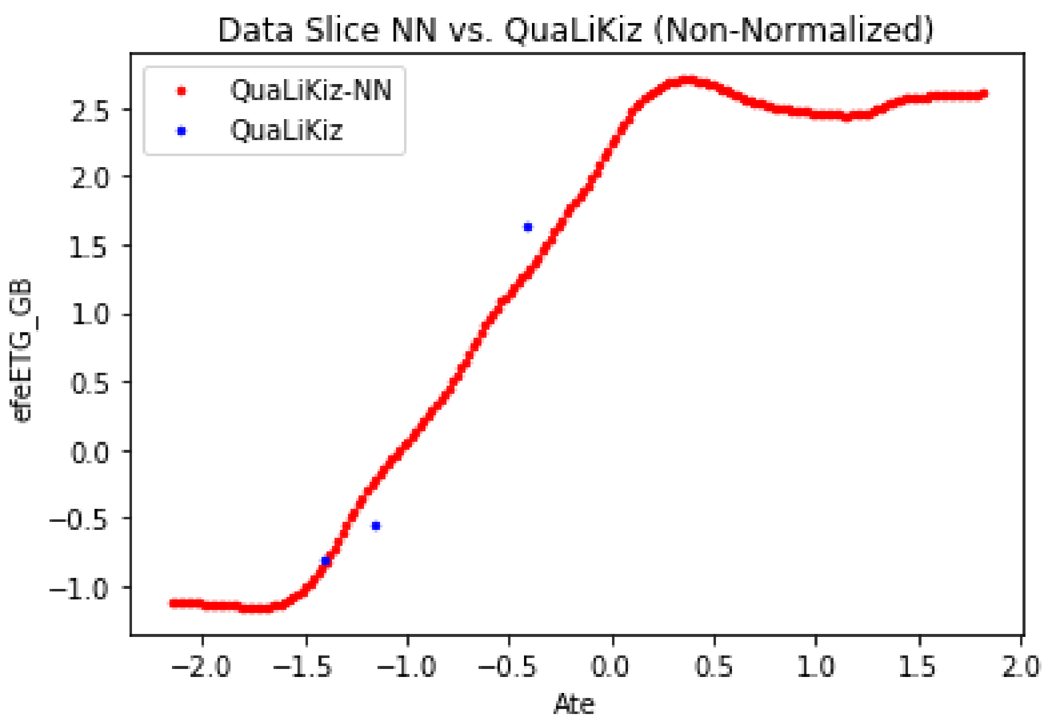
```
In [51]: efeETG_DF_Mk2 = newDF_Mk2['efeETG_GB']
         efeETG_DF_Mk2_np_array = efeETG_DF_Mk2.values
```

```
print(efeETG_DF_Mk2_np_array)

Ate_DF_Mk2 = newDF_Mk2['Ate']
Ate_DF_Mk2_np_array = Ate_DF_Mk2.values
print(Ate_DF_Mk2_np_array)
```

```
[ 7.413384 13.28646  63.69965 ]
[4.25 5.   7.25]
```

```
In [52]: efeETG_DF = newDF['efeETG_GB']
         Ate_DF = newDF['Ate']
         plt.plot(table_normalized[:,1], predictions, 'r.', ms = 5, label = 'QuaLiKiz-NN')
         plt.plot(Ate_DF_np_array, efeETG_DF_np_array, 'b.', ms = 5, label = 'QuaLiKiz')
         plt.title('Data Slice NN vs. QuaLiKiz (Non-Normalized)')
         plt.xlabel('Ate')
         plt.ylabel('efeETG_GB')
         plt.legend()
         plt.show()
```




```
In [53]: predictions_deNormalized = (predictions * joined_dataFrame_original['efeETG_GB'].std())
         print(predictions_deNormalized.shape)
```

```
(200,)
```

In [54]:
```
plt.plot(table[:,1], predictions_deNormalized, 'r.', ms = 5, label = 'QuaLiKiz-NN')
plt.plot(Ate_DF_Mk2_np_array, efeETG_DF_Mk2_np_array, 'b.', ms = 5, label = 'QuaLiKiz')
plt.title('Data Slice NN vs. QuaLiKiz (De-Normalized)')
plt.xlabel('Ate')
plt.ylabel('efeETG_GB')
plt.legend()
# plt.savefig('./2018-07-17_TableTestingNotebook_Mk2/NN_Predictions.png', dpi = 100)
plt.show()
```