Do `source setup.sh` before trying to run this notebook!

Import utils, and set environemnt variables

```
try:
    IQN_BASE = os.environ['IQN_BASE']
    print('BASE directoy properly set = ', IQN_BASE)
    utils_dir = os.path.join(IQN_BASE, 'utils')
    sys.path.append(utils_dir)
    import utils
    #usually its not recommended to import everything from a module, 
but we know
    #whats in it so its fine
    from utils import *
    print('DATA directory also properly set, in %s' % 
os.environ['DATA_DIR'])
except Exception:
    print("""\nBASE directory not properly set. Read repo README.\
    If you need a function from utils, use the decorator below, or add 
utils to sys.path\n
    You can also do os.environ['IQN_BASE']=<ABSOLUTE PATH FOR THE IQN 
REPO>""")
    pass
```

```
BASE directoy properly set = 
/home/ali/Desktop/Pulled_Github_Repositories/torchQN
DATA directory also properly set, in 
/home/ali/Desktop/Pulled_Github_Repositories/IQN_HEP/Davidson/data
```

A user is competent enought to do `source setup.sh` on a `setup.sh` script that comes in the repo, such as the next cell uncommented

```
# %%writefile setup.sh
# #!/bin/bash
# export IQN_BASE=/home/ali/Desktop/Pulled_Github_Repositories/torchQN
# #DAVIDSON
# #export 
DATA_DIR='/home/DAVIDSON/alalkadhim.visitor/IQN/DAVIDSON_NEW/data'
# #LOCAL
# export 
DATA_DIR='/home/ali/Desktop/Pulled_Github_Repositories/IQN_HEP/Davidso
n/data'
# echo 'DATA DIR'
# ls -l $DATA_DIR
# #ln -s $DATA_DIR $IQN_BASE, if you want
# #conda create env -n torch_env -f torch_env.yml
# #conda activate torch_env
# mkdir -p ${IQN_BASE}/images/loss_plots ${IQN_BASE}/trained_models  $
{IQN_BASE}/hyperparameters ${IQN_BASE}/predicted_data
# tree $IQN_BASE
```

External Imports

If you don't have some of these packages installed, you can also use the conda environment that has all of the packages by doing `conda env create -f IQN_env.yml && conda activate IQN_env`

```python
import numpy as np; import pandas as pd
import scipy as sp; import scipy.stats as st
import torch; import torch.nn as nn; print(f"using torch version
{torch.__version__}")
#use numba's just-in-time compiler to speed things up
from numba import njit
from sklearn.preprocessing import StandardScaler; from
sklearn.model_selection import train_test_split
import matplotlib as mp; import matplotlib.pyplot as plt;
#reset matplotlib stle/parameters
import matplotlib as mpl
#reset matplotlib parameters to their defaults
mpl.rcParams.update(mpl.rcParamsDefault)
plt.style.use('seaborn-deep')
mp.rcParams['agg.path.chunksize'] = 10000
font_legend = 15; font_axes=15
# %matplotlib inline
import copy; import sys; import os
from IPython.display import Image, display
from importlib import import_module

try:
    import optuna
    print(f"using (optional) optuna version {optuna.__version__}")
except Exception:
    print('optuna is only used for hyperparameter tuning, not
critical!')
    pass
import argparse
import time
# import sympy as sy
import ipywidgets as wid;
```

```
using torch version 1.9.0
using optuna version 2.8.0
```

```python
# update fonts
FONTSIZE = 14
font = {'family' : 'serif',
        'weight' : 'normal',
        'size'   : FONTSIZE}
mp.rc('font', **font)

# set usetex = False if LaTex is not
```

```
# available on your system or if the
# rendering is too slow
mp.rc('text', usetex=True)

# set a seed to ensure reproducibility
seed = 128
rnd  = np.random.RandomState(seed)
#sometimes jupyter doesnt initialize MathJax automatically for latex, so do this:
wid.HTMLMath('$\LaTeX$')
```

{"version_major":2,"version_minor":0,"model_id":"09e9ab7e8a51448894608 40f2f7c68a7"}

Set arguments and configurations

```
################################### ARGUMENTS
###################################
parser=argparse.ArgumentParser(description='train for different targets')
parser.add_argument('--N', type=str, help='''size of the dataset you want to use.
                    Options are 10M and 100K and 10M_2, the default is 10M_2''', required=False,default='10M_2')
#N_epochs X N_train_examples = N_iterations X batch_size
# N_iterations = (N_epochs * train_data.shape[0])/batch_size
#N_iterations = (N_epochs * train_data.shape[0])/64 = 125000 for 1 epoch
parser.add_argument('--n_iterations', type=int, help='''The number of iterations for training,
                    the default is''', required=False,default=50)
#default=5000000 )
parser.add_argument('--n_layers', type=int, help='''The number of layers in your NN,
                    the default is 5''', required=False,default=6)
parser.add_argument('--n_hidden', type=int, help='''The number of hidden layers in your NN,
                    the default is 5''', required=False,default=6)
parser.add_argument('--starting_learning_rate', type=float, help='''Starting learning rate,
                    the defulat is 10^-3''', required=False,default=1.e-2)
parser.add_argument('--show_loss_plots', type=bool, help='''Boolean to show the loss plots,
                    default is False''', required=False,default=False)
parser.add_argument('--save_model', type=bool, help='''Boolean to save the trained model dictionary''',
                    required=False,default=False)
parser.add_argument('--save_loss_plots', type=bool, help='''Boolean to save the loss plots''',
                    required=False,default=False)
```

```
################################### CONFIGURATIONS
###################################
DATA_DIR=os.environ['DATA_DIR']
JUPYTER=True

if JUPYTER:
    args = parser.parse_args(args=[])
    N = '10M_2'
    n_iterations = int(1e4)
    n_layers, n_hidden = int(1), int(10)
    starting_learning_rate = float(1.e-2)
    show_loss_plots = False
    save_model=False
    save_loss_plots = False
else:
    args = parser.parse_args()
    N = args.N
    n_iterations = args.n_iterations
    n_layers = args.n_layers
    n_hidden = args.n_hidden
    starting_learning_rate=args.starting_learning_rate
    show_loss_plots=args.show_loss_plots
    save_model=args.save_model
    save_loss_plots=args.save_loss_plots

dropout=0.2

def get_model_params():
    return n_iterations, n_layers, n_hidden, starting_learning_rate,
dropout
```

Import the numpy data, convert to dataframe and save (if you haven't saved the dataframes)

Explore the Dataframe and preprocess

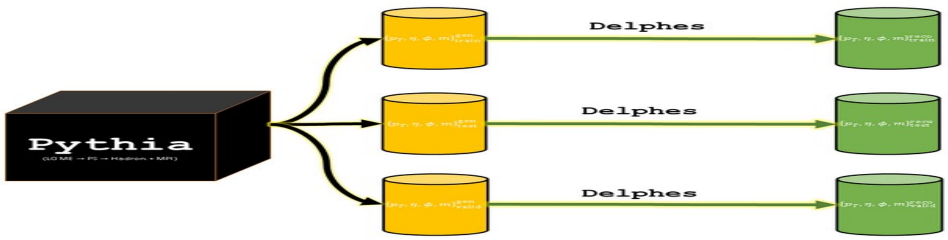
idea: do another flowchart for how IQN works autoregressively to get $p_T{}'$, etc

Plotting

```
def show_jupyter_image(image_filename, width = 1300, height = 300):
    """Show a saved image directly in jupyter. Make sure
image_filename is in your IQN_BASE !"""
    display(Image(os.path.join(IQN_BASE,image_filename), width =
width, height = height  ))
```

```python
def use_svg_display():
    """Use the svg format to display a plot in Jupyter (better
quality)"""
    from matplotlib_inline import backend_inline
    backend_inline.set_matplotlib_formats('svg')

def reset_plt_params():
    """reset matplotlib parameters - often useful"""
    use_svg_display()
    mpl.rcParams.update(mpl.rcParamsDefault)

def show_plot(legend=None):
    use_svg_display()
    plt.tight_layout();
    plt.show()
    if legend:
        plt.legend(loc='best')

def set_figsize(get_axes=False,figsize=(7, 7)):
    use_svg_display()
    plt.rcParams['figure.figsize'] = figsize
    if get_axes:
        fig, ax = plt.subplots(1,1, figsize=figsize)
        return fig, ax

def set_axes(ax, xlabel, ylabel=None, xmin=None, xmax=None, ymin=None,
ymax=None, title=None):
    """saves a lot of time in explicitly difining each axis, its title
and labels: do them all in one go"""
    use_svg_display()
    ax.set_xlabel(xlabel,fontsize=font_axes)
    if ylabel:
        ax.set_ylabel(ylabel,fontsize=font_axes)
    if xmin and xmax:
        ax.set_xlim(xmin, xmax)

    if ax.get_title()  != '':
        #if the axes (plot) does have a title (which is non-empty
string), display it
        ax.set_title(title)
    if ax.legend():
        #if an axis has a legned label, display it
        ax.legend(loc='best',fontsize=font_legend)
    if ymin and ymax:
        #sometimes we dont have ylimits since we do a lot of
histograms, but if an axis has ylimits, set them
        ax.set_ylim(ymin, ymax)
```

```python
    try:
        fig.show()
    except Exception:
        pass
    plt.tight_layout()
    plt.show()

use_svg_display()
show_jupyter_image('data_diagram_IQN.png')
```



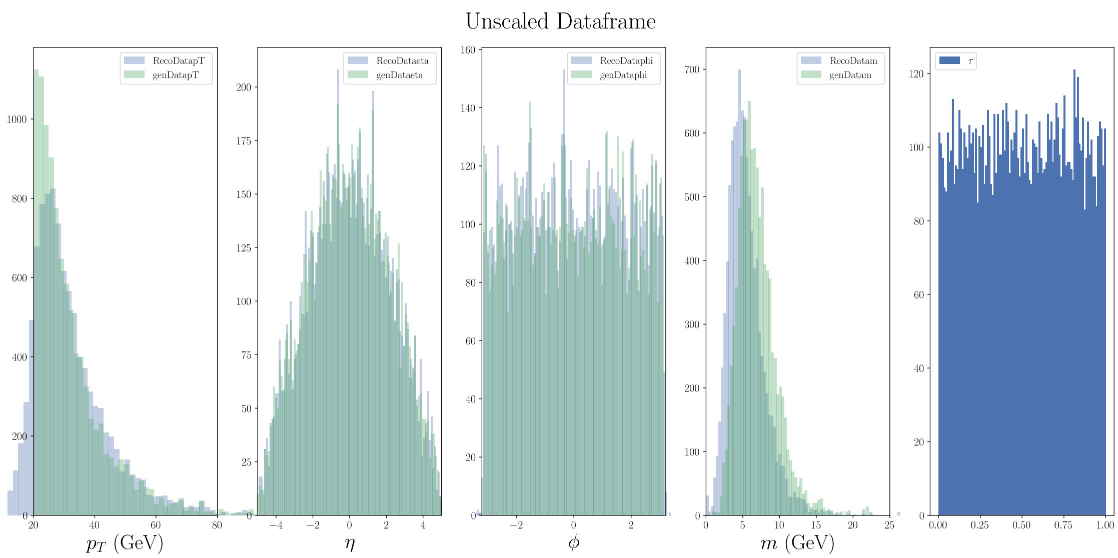
For Davidson team, please read try to all the code/comments before asking me questions!

```python
#################################### SET DATA CONFIGURATIONS
####################################
X       = ['genDatapT', 'genDataeta', 'genDataphi', 'genDatam', 'tau']

FIELDS  = {'RecoDatam' : {'inputs': X,
                           'xlabel':  r'$m$ (GeV)',
                           'xmin': 0,
                           'xmax': 25},

           'RecoDatapT': {'inputs': ['RecoDatam']+X,
                           'xlabel':  r'$p_T$ (GeV)' ,
                           'xmin'   : 20,
                           'xmax'   :  80},

           'RecoDataeta': {'inputs': ['RecoDatam','RecoDatapT'] + X,
                           'xlabel': r'$\eta$',
                           'xmin'   : -5,
                           'xmax'   :  5},

           'RecoDataphi'  : {'inputs': ['RecoDatam', 'RecodatapT',
'RecoDataeta']+X,
                           'xlabel': r'$\phi$' ,
                           'xmin'   : -3.2,
                           'xmax'   :3.2}
          }

######################################################################
#########################
y_label_dict ={'RecoDatapT':'$p(p_T)$'+' [ GeV'+'$^{-1} $'+']',
                    'RecoDataeta':'$p(\eta)$', 'RecoDataphi':'$p(\phi)
```

```
$',
                    'RecoDatam':'$p(m)$'+' [ GeV'+'$^{-1} $'+']'}

loss_y_label_dict ={'RecoDatapT':'$p_T^{reco}$',
                    'RecoDataeta':'$\eta^{reco}$', 'RecoDataphi':'$\
phi^{reco}$',
                    'RecoDatam':'$m^{reco}$'}

all_variable_cols=['genDatapT', 'genDataeta', 'genDataphi',
'genDatam','RecoDatapT', 'RecoDataeta', 'RecoDataphi', 'RecoDatam']
all_cols=['genDatapT', 'genDataeta', 'genDataphi',
'genDatam','RecoDatapT', 'RecoDataeta', 'RecoDataphi', 'RecoDatam',
'tau']
################################### Load unscaled dataframes
###################################
SUBSAMPLE=int(1e4)#subsample use for development - in production use
whole dataset
train_data=pd.read_csv(os.path.join(DATA_DIR,'train_data_10M_2.csv'),
                      usecols=all_cols,
                      nrows=SUBSAMPLE
                      )

test_data=pd.read_csv(os.path.join(DATA_DIR,'test_data_10M_2.csv'),
                      usecols=all_cols,
                     nrows=SUBSAMPLE
                     )

def explore_data(df, title, scaled=False):
    fig, ax = plt.subplots(1,5, figsize=(15,10) )
    # df = df[['genDatapT', 'genDataeta', 'genDataphi',
'genDatam','RecoDatapT', 'RecoDataeta', 'RecoDataphi', 'RecoDatam']]
    levels = ['RecoData', 'genData']
    kinematics=['pT','eta','phi','m']
    columns = [level+k for level in levels for k in kinematics]
    print(columns)
    columns = columns + ['tau']
    print(columns)
    df = df[columns]

    for k_i, k in enumerate(kinematics):
        Reco_var = levels[0]+k
        gen_var = levels[1]+k
        print('Reco_var: ', Reco_var, ', \t gen_var: ', gen_var)
        ax[k_i].hist(df[Reco_var], bins=100, label=Reco_var,
alpha=0.35)
        ax[k_i].hist(df[gen_var], bins=100, label=gen_var, alpha=0.35)
        xmin, xmax = FIELDS[Reco_var]['xmin'], FIELDS[Reco_var]
['xmax']
        xlabel=FIELDS[Reco_var]['xlabel']
        ax[k_i].set_xlim( (xmin, xmax) )
```

```
        # set_axes(ax[k_i], xlabel=xlabel, ylabel='', xmin=xmin,
xmax=xmax)
        ax[k_i].set_xlabel(xlabel,fontsize=26)



        if scaled:
            ax[k_i].set_xlim(df[gen_var].min(),df[gen_var].max() )

        ax[k_i].legend(loc='best', fontsize=13)
    ax[4].hist(df['tau'],bins=100, label=r'$\tau$')
    ax[4].legend(loc='best', fontsize=13)
    fig.suptitle(title, fontsize=30)
    show_plot()

explore_data(df=train_data, title='Unscaled Dataframe')
```

```
['RecoDatapT', 'RecoDataeta', 'RecoDataphi', 'RecoDatam', 'genDatapT',
'genDataeta', 'genDataphi', 'genDatam']
Reco_var:  RecoDatapT ,     gen_var:  genDatapT
Reco_var:  RecoDataeta ,    gen_var:  genDataeta
Reco_var:  RecoDataphi ,    gen_var:  genDataphi
Reco_var:  RecoDatam ,      gen_var:  genDatam
```




```
print(train_data.shape)
train_data.describe()#unscaled
```

```
(10000, 9)

          genDatapT    genDataeta    genDataphi      genDatam
RecoDatapT  \
count  10000.000000  10000.000000  10000.000000  10000.000000
10000.000000
mean      32.748727     -0.007169      0.004215      6.980037
```

```
32.982230
std         14.374873       2.209883       1.809176       2.751696
15.626337
min         20.004600      -5.053690      -3.140890       0.136333
11.532200
25%         23.693450      -1.636940      -1.556042       5.119607
23.495425
50%         28.400000      -0.012826      -0.023519       6.547370
29.017050
75%         36.486850       1.633903       1.552912       8.363860
37.877825
max        183.448000       5.039390       3.140640      35.081300
185.426000

        RecoDataeta    RecoDataphi      RecoDatam           tau
count  10000.000000   10000.000000   10000.000000  10000.000000
mean      -0.007198       0.004905       5.531751      0.501375
std        2.202264       1.809657       2.639882      0.288104
min       -4.936930      -3.351365      -0.000022      0.000014
25%       -1.637945      -1.555673       3.780315      0.252924
50%       -0.018205      -0.023471       5.087130      0.501390
75%        1.629590       1.557280       6.772220      0.751112
max        4.998390       3.381455      33.813600      0.999968
```

standarize:

$$X' = \frac{X - X_{min}}{X_{max} - X_{min}} \rightarrow X = X'(X_{max} - X_{min}) + X_{min}$$

```python
def standarize(values):
    expected_min, expected_max = values.min(), values.max()
    scale_factor = expected_max - expected_min
    offset = expected_min
    standarized_values = (values - offset)/scale_factor
    return standarized_values
```

standarize_2:

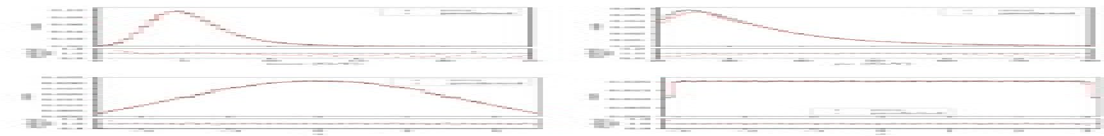
$$X' = \frac{X - E[X]}{\sigma_X} \rightarrow X = X' \sigma_X + E[X]$$

```python
def standarize_2(values):
    return values - (np.mean(values)/np.std(values))
```

Results prior to Braden-scaling

Recall that the best IQNx4 autoregressive results that I attained prior to trying the Braden scaling was the following (which was implemented in the Davidson cluster here: `/home/DAVIDSON/alalkadhim.visitor/IQN/DAVIDSON_NEW/OCT_7/*.py` and copied to my repo here):

```
show_jupyter_image('OCT_7/AUTOREGRESSIVE_RESULTS_OCT7.png',width =
800, height = 100)
```

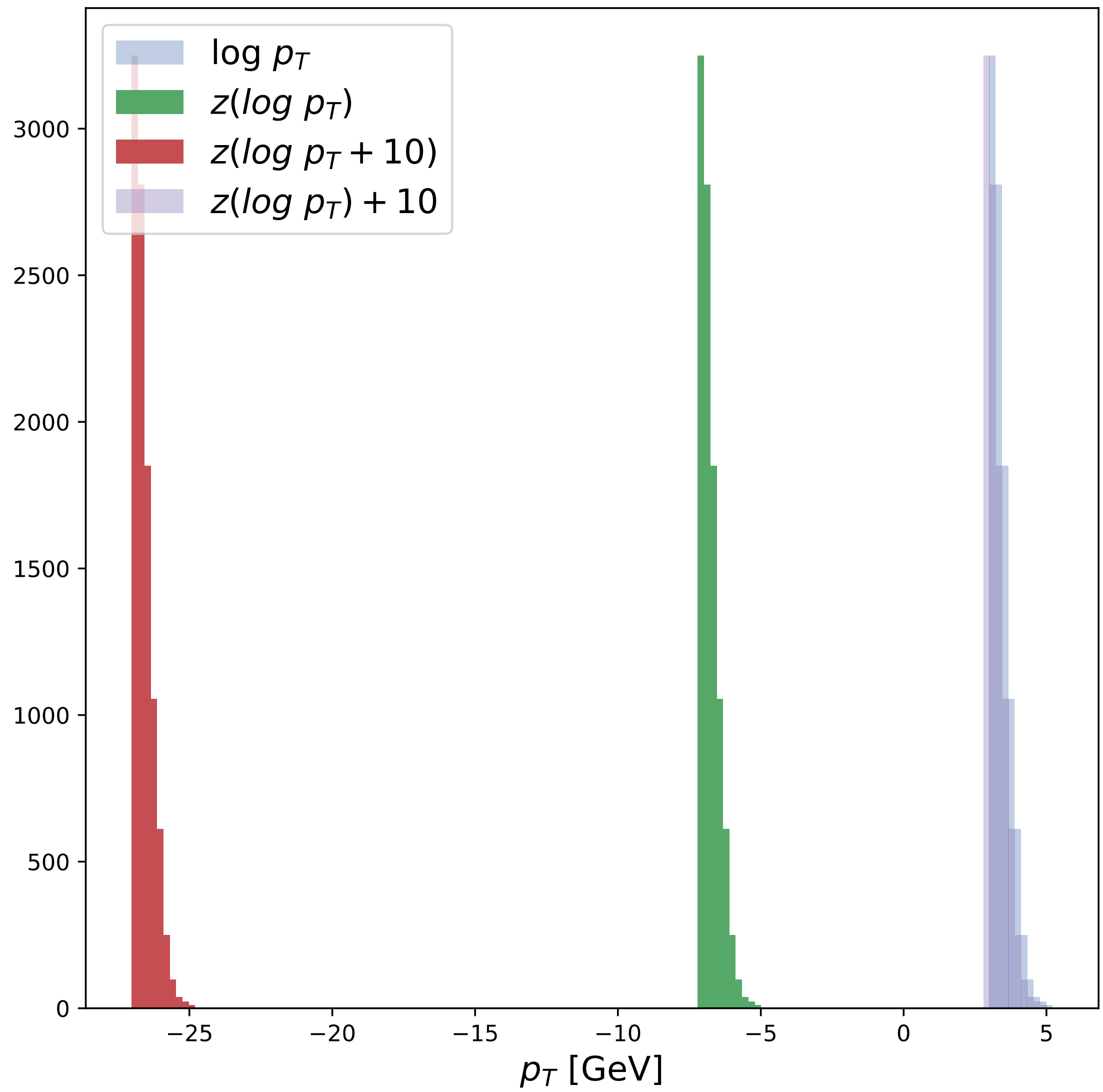


Scale the data accoding to the "Braden Kronheim scaling" :

$$T\left(p_T\right)=z\left(\log p_T\right),T\left(\eta\right)=z\left(\eta\right),T\left(\phi\right)=z\left(\phi\right),T\left(m\right)=z\left(\log\left(m+2\right)\right),T\left(\tau\right)=6\tau-3$$

```
fig, ax= set_figsize(get_axes=True)
ax.hist(np.log(train_data.iloc[:,0]), label='log $p_T$',alpha=0.35);
ax.hist(standarize_2(np.log(train_data.iloc[:,0])), label='$z(log\
p_T$)');
ax.hist(standarize_2(np.log(train_data.iloc[:,0]) +10), label='$z(log\
p_T + 10$)');
ratio_of_cons_inside_log=standarize_2(np.log(train_data.iloc[:,0])
+10)/standarize_2(np.log(train_data.iloc[:,0]) +10)

ax.hist(standarize_2(np.log(train_data.iloc[:,0]))+10, label='$z(log\
p_T)+10$',alpha=0.35)
set_axes(ax=ax, xlabel=r'$p_T$ [GeV]')
```

```
/home/ali/anaconda3/lib/python3.7/site-packages/
ipykernel_launcher.py:50: UserWarning: Matplotlib is currently using
module://matplotlib_inline.backend_inline, which is a non-GUI backend,
so cannot show the figure.
```



standarize_IQN:

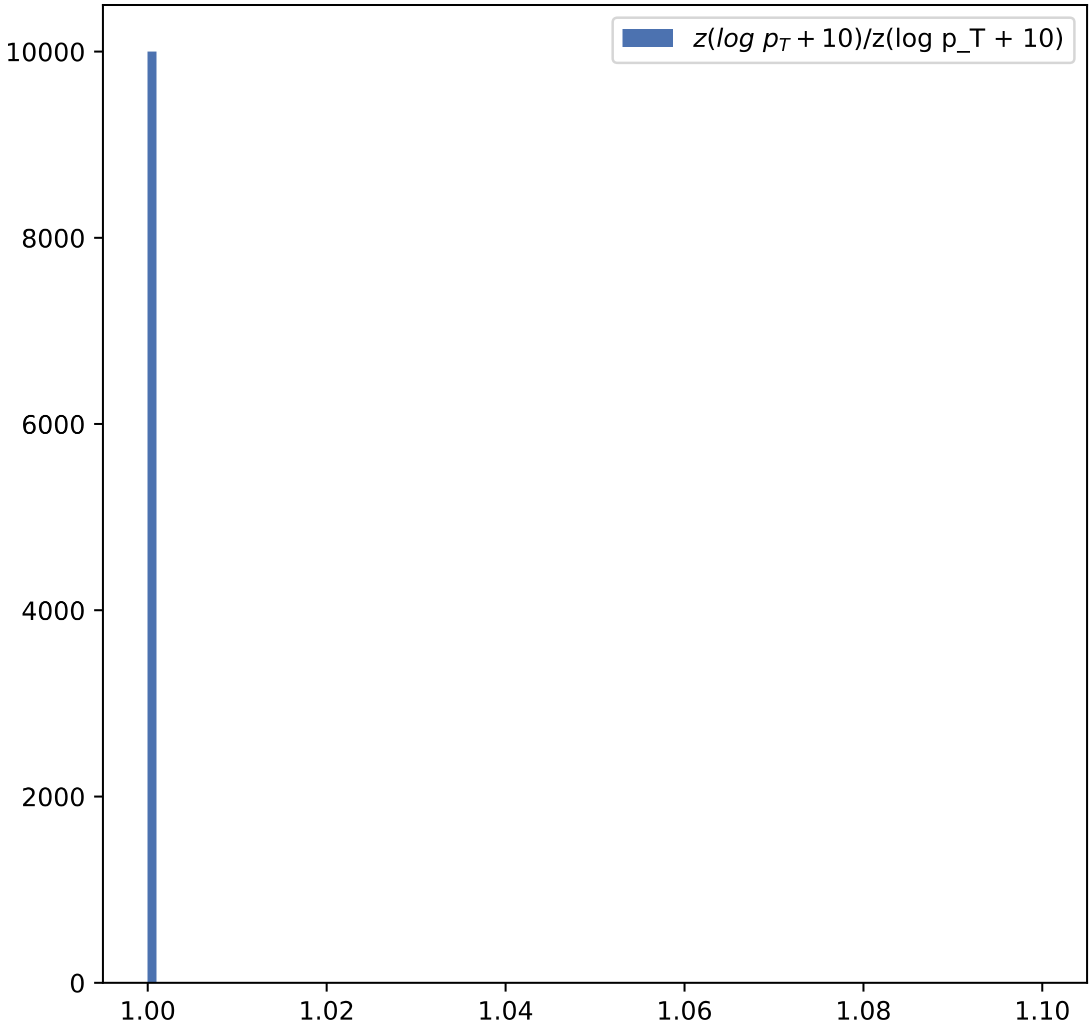
$$X' = \frac{X - X_{min}}{X_{max} - X_{min}} \rightarrow X = X'\left(X_{max} - X_{min}\right) + X_{min}$$

Standarize_IQN_2:

$$p_T^{\text{scaled}} = \frac{\log p_T - E\left[\log p_T\right]}{\sigma_{\log\left(p_T\right)}} + 10 \rightarrow p_T^{\text{unscaled}} = \exp\left(\left(p_T^{\text{scaled}} - 10\right)\sigma_{\log\left(p_T\right)} + E\left[\log\left(p_T\right)\right]\right)$$

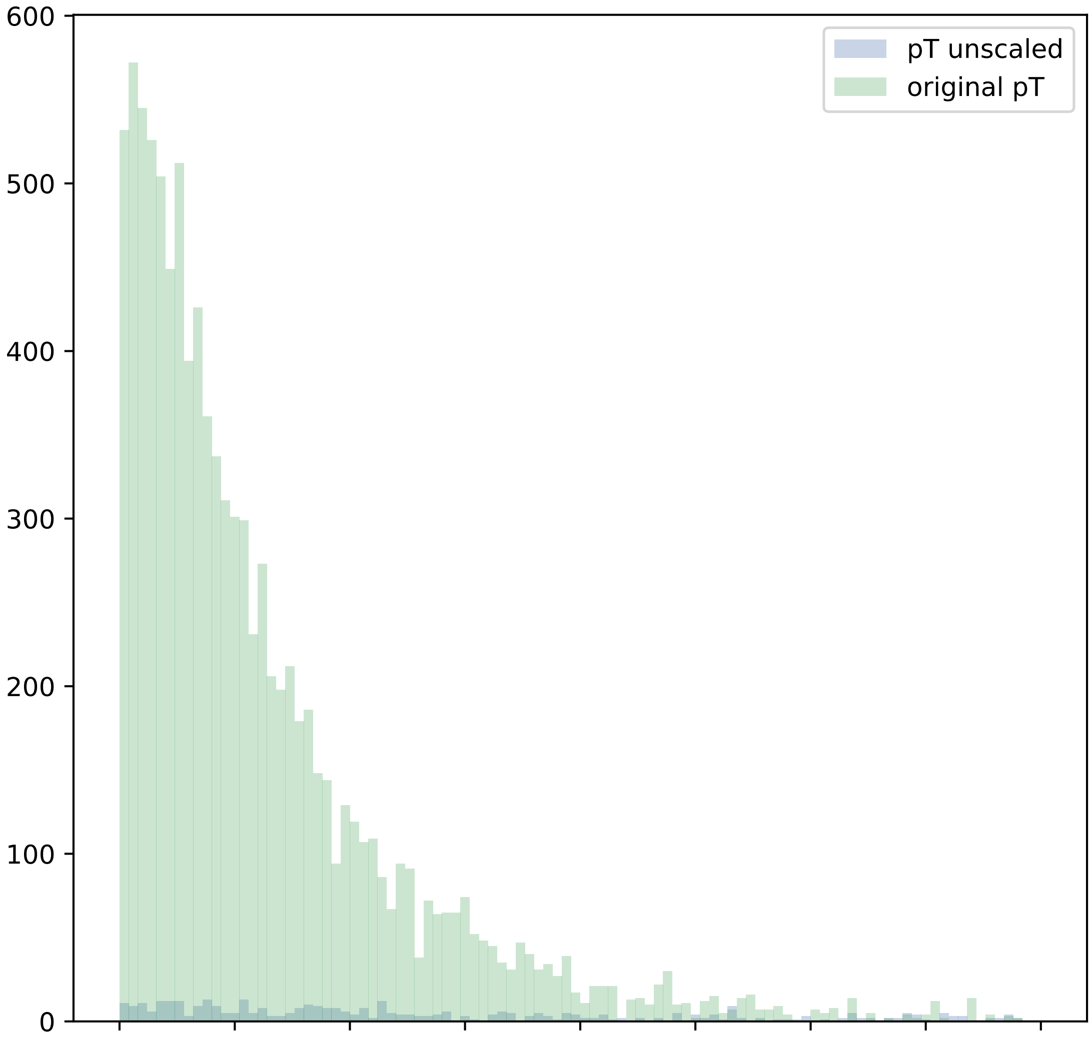
```python
def standarize_IQN(orig_values, label, const=None):
    if label=='pT':
        const=10
        log_pT=np.log(orig_values)
        pT_scaled = ((log_pT - np.mean(log_pT))/np.std(log_pT) ) + 10
        standarized_values =pT_scaled
    return standarized_values
```

```
plt.hist(ratio_of_cons_inside_log, label=r'$z(log\ p_T + 10$)/z(log
p_T + 10$)$',bins=100,range=(1,1.1) );plt.legend();plt.show()
```




```
def de_standarize_IQN(standarized_values, label, const=None):
    if label=='pT':
        const=10
        orig__unscaled_pT=train_data.iloc[:,0]
        log_orig__unscaled_pT = np.log(orig__unscaled_pT)
        pT_unscaled = np.exp( ((standarized_values-const) *
np.std(orig__unscaled_pT)) + np.mean(log_orig__unscaled_pT) )
    return pT_unscaled

# plt.hist(train_data.iloc[:,0]);plt.show()

pT_scaled = standarize_IQN(orig_values=train_data.iloc[:,0],
label='pT')
pT_unscaled = de_standarize_IQN(standarized_values=pT_scaled,
label='pT')
# plt.hist(pT_scaled,label='pT scaled');
```

```
plt.hist(pT_unscaled, label='pT unscaled',bins=100 ,
range=(20,100),alpha=0.3);
plt.hist(train_data.iloc[:,0],label='original pT',
bins=100,range=(20,100),alpha=0.3)

plt.legend();plt.show()
```

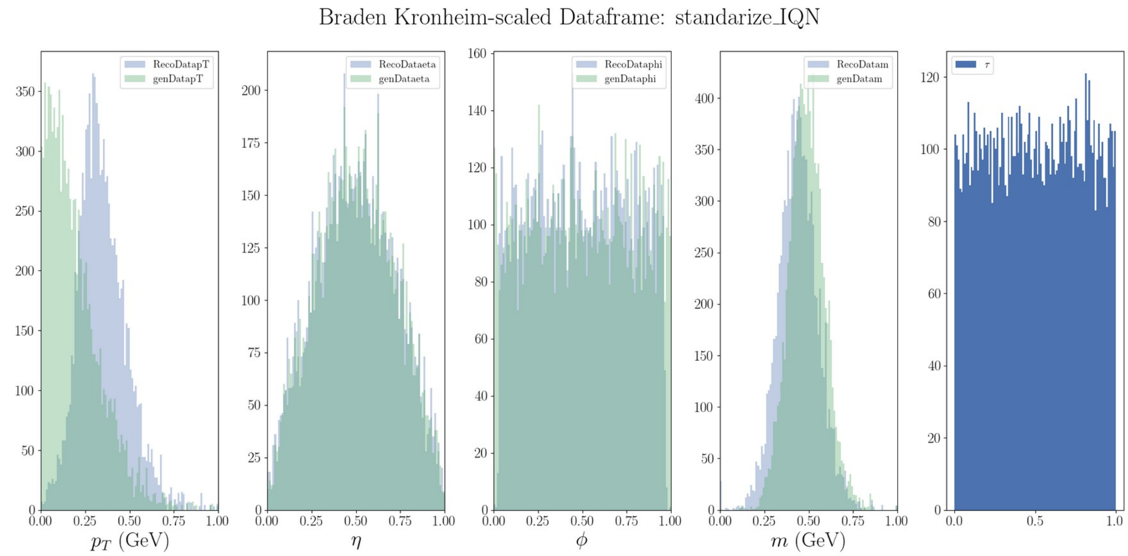



```
def scale_df(df, title, scale_func, save=False):
    #scale
    SUBSAMPLE=int(1e4)
    df = df[all_cols]#[:SUBSAMPLE]
    # print(df.head())
    scaled_df = pd.DataFrame()
    #select the columns by index:
    # 0:genDatapT, 1:genDataeta, 2:genDataphi, 3:genDatam,
    # 4:RecoDatapT, 5:RecoDataeta, 6:RecoDataphi, 7: Recodatam
    scaled_df['genDatapT'] = scale_func(np.log(df.iloc[:,0]) )
```

```
    scaled_df['RecoDatapT'] = scale_func(np.log(df.iloc[:,4]) )

    scaled_df['genDataeta'] = scale_func(df.iloc[:,1])
    scaled_df['RecoDataeta'] = scale_func(df.iloc[:,5])


    scaled_df['genDataphi'] = scale_func(df.iloc[:,2])
    scaled_df['RecoDataphi'] = scale_func(df.iloc[:,6])

    scaled_df['genDatam'] = scale_func(np.log(df.iloc[:,3] + 2) )
    scaled_df['RecoDatam'] = scale_func(np.log(df.iloc[:,7] + 2) )
    #why scale tau?
    # scaled_df['tau'] = 6 * df.iloc[:,8] - 3
    scaled_df['tau'] = df.iloc[:,8]

    print(scaled_df.describe())

    if save:
        scaled_df.to_csv(os.path.join(DATA_DIR, title) )
    return scaled_df

scaled_train_data = scale_df(train_data,
title='scaled_train_data_10M_2.csv',
                             scale_func=standarize,
                             save=False)
print('\n\n')
scaled_test_data = scale_df(test_data,
title='scaled_test_data_10M_2.csv',
                            scale_func=standarize,
                            save=False)

explore_data(df=scaled_train_data, title='Braden Kronheim-scaled
Dataframe: standarize_IQN', scaled=True)
```

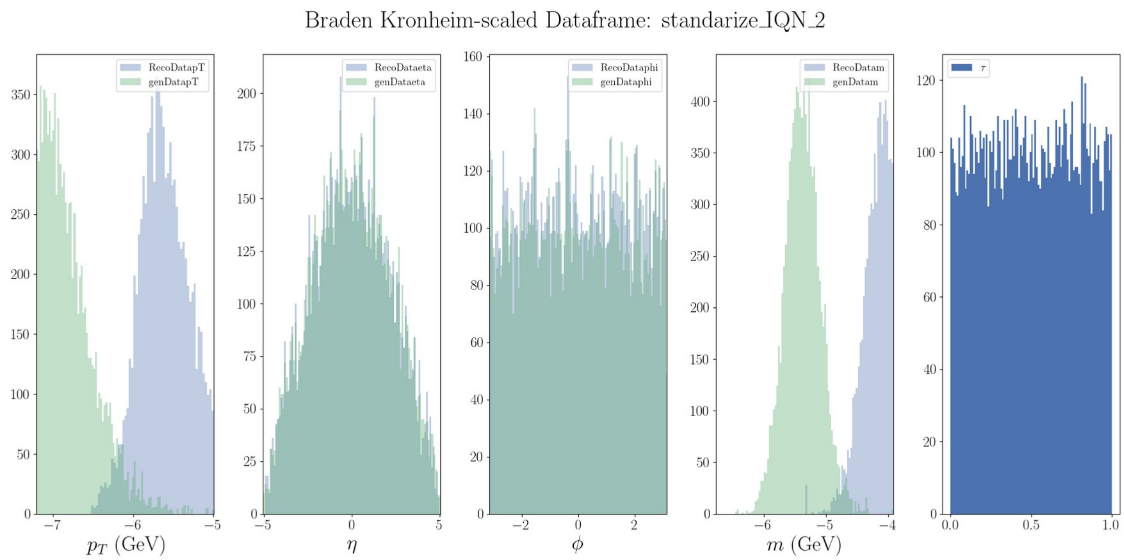
```
          genDatapT    RecoDatapT    genDataeta   RecoDataeta
genDataphi  \
count  10000.000000  10000.000000  10000.000000  10000.000000
10000.000000
mean       0.193019      0.349439      0.499998      0.496183
0.500691
std        0.151402      0.137091      0.218950      0.221660
0.288015
min        0.000000      0.000000      0.000000      0.000000
0.000000
25%        0.076371      0.256223      0.338524      0.332046
0.252303
50%        0.158137      0.332218      0.499438      0.495075
0.496276
75%        0.271209      0.428161      0.662592      0.660927
0.747239
```

```
max        1.000000     1.000000     1.000000     1.000000
1.000000

        RecoDataphi      genDatam     RecoDatam          tau
count  10000.000000  10000.000000  10000.000000  10000.000000
mean       0.498494      0.488433      0.440818      0.501375
std        0.268781      0.100227      0.113154      0.288104
min        0.000000      0.000000      0.000000      0.000014
25%        0.266707      0.421777      0.367851      0.252924
50%        0.494279      0.485817      0.438496      0.501390
75%        0.729062      0.553336      0.512428      0.751112
max        1.000000      1.000000      1.000000      0.999968



          genDatapT    RecoDatapT    genDataeta   RecoDataeta
genDataphi  \
count  10000.000000  10000.000000  10000.000000  10000.000000
10000.000000
mean       0.143909      0.275600      0.507399      0.505858
0.504341
std        0.112547      0.110219      0.217335      0.222251
0.289598
min        0.000000      0.000000      0.000000      0.000000
0.000000
25%        0.059885      0.203154      0.344565      0.339593
0.254367
50%        0.119371      0.263623      0.511950      0.510924
0.506544
75%        0.201243      0.337655      0.667306      0.669468
0.757987
max        1.000000      1.000000      1.000000      1.000000
1.000000

        RecoDataphi      genDatam     RecoDatam          tau
count  10000.000000  10000.000000  10000.000000  10000.000000
mean       0.502875      0.330795      0.354760      0.507559
std        0.277433      0.089873      0.091590      0.290743
min        0.000000      0.000000      0.000000      0.000013
25%        0.263911      0.272740      0.295975      0.259261
50%        0.504849      0.329915      0.354809      0.511120
75%        0.745752      0.387605      0.412537      0.762087
max        1.000000      1.000000      1.000000      0.999989
['RecoDatapT', 'RecoDataeta', 'RecoDataphi', 'RecoDatam', 'genDatapT',
'genDataeta', 'genDataphi', 'genDatam']
Reco_var:  RecoDatapT ,     gen_var:  genDatapT
Reco_var:  RecoDataeta ,    gen_var:  genDataeta
Reco_var:  RecoDataphi ,    gen_var:  genDataphi
Reco_var:  RecoDatam ,      gen_var:  genDatam
```




```
scaled_train_data = scale_df(train_data,
title='scaled_train_data_10M_2.csv',
                             scale_func=standarize_2,
                             save=False)
print('\n\n')
scaled_test_data = scale_df(test_data,
title='scaled_test_data_10M_2.csv',
                            scale_func=standarize_2,
                            save=False)

explore_data(df=scaled_train_data, title='Braden Kronheim-scaled
Dataframe: standarize_IQN_2', scaled=True)

          genDatapT    RecoDatapT    genDataeta    RecoDataeta
genDataphi  \
count  10000.000000  10000.000000  10000.000000  10000.000000
10000.000000
mean      -6.781494     -5.555223     -0.003925     -0.003929
0.001885
std        0.335502      0.380772      2.209883      2.202264
1.809176
min       -7.209217     -6.525794     -5.050446     -4.933662     -
3.143220
25%       -7.039981     -5.814132     -1.633696     -1.634677     -
1.558373
50%       -6.858790     -5.603054     -0.009582     -0.014936     -
0.025849
75%       -6.608227     -5.336572      1.637147      1.632858
1.550582
max       -4.993248     -3.748282      5.042634      5.001658
3.138310

        RecoDataphi      genDatam     RecoDatam           tau
```

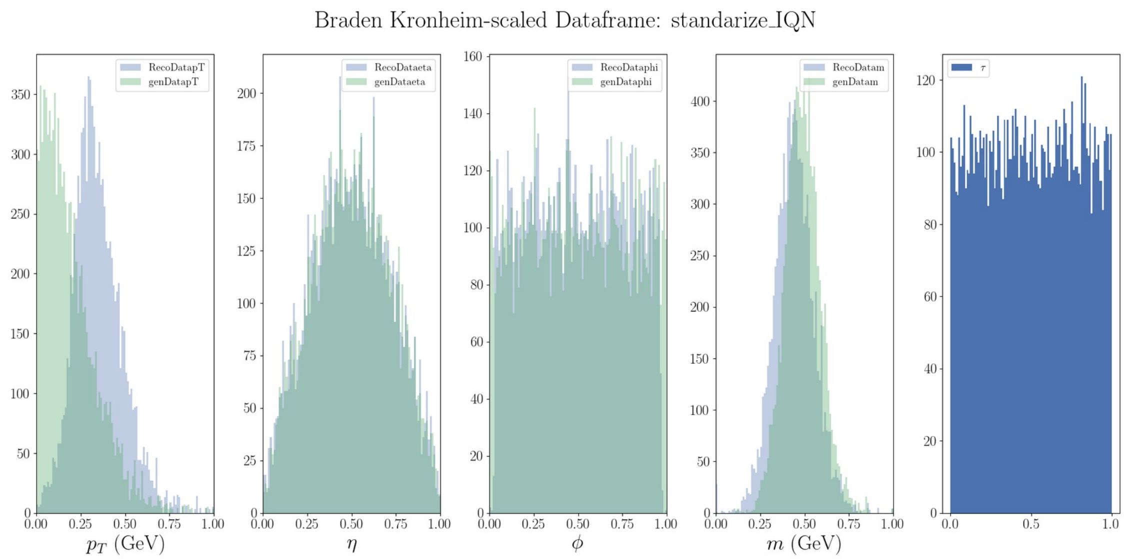
```
count  10000.000000  10000.000000  10000.000000  10000.000000
mean       0.002195     -5.374291     -4.054152      0.501375
std        1.809657      0.286049      0.326472      0.288104
min       -3.354076     -6.768290     -5.325995      0.000014
25%       -1.558383     -5.564528     -4.264673      0.252924
50%       -0.026182     -5.381757     -4.060851      0.501390
75%        1.554569     -5.189056     -3.847541      0.751112
max        3.378745     -3.914268     -2.440804      0.999968



          genDatapT    RecoDatapT    genDataeta   RecoDataeta
genDataphi  \
count  10000.000000  10000.000000  10000.000000  10000.000000
10000.000000
mean      -6.629865     -5.331596      0.018054      0.017897
0.012041
std        0.341107      0.390866      2.211242      2.206106
1.819197
min       -7.066024     -6.308946     -5.144407     -5.003340     -
3.156130
25%       -6.884524     -5.588510     -1.638677     -1.632480     -
1.558245
50%       -6.704234     -5.374067      0.064356      0.068187
0.025877
75%       -6.456097     -5.111531      1.645003      1.641920
1.605392
max       -4.035226     -2.762678      5.029953      4.922840
3.125670

        RecoDataphi      genDatam     RecoDatam           tau
count  10000.000000  10000.000000  10000.000000  10000.000000
mean       0.012016     -5.314733     -4.012887      0.507559
std        1.818557      0.288388      0.329008      0.290743
min       -3.284307     -6.376207     -5.287256      0.000013
25%       -1.554381     -5.501024     -4.224053      0.259261
50%        0.024950     -5.317557     -4.012707      0.511120
75%        1.604059     -5.132437     -3.805338      0.762087
max        3.270644     -3.167348     -1.695051      0.999989
['RecoDatapT', 'RecoDataeta', 'RecoDataphi', 'RecoDatam', 'genDatapT',
'genDataeta', 'genDataphi', 'genDatam']
Reco_var:  RecoDatapT ,      gen_var:  genDatapT
Reco_var:  RecoDataeta ,     gen_var:  genDataeta
Reco_var:  RecoDataphi ,     gen_var:  genDataphi
Reco_var:  RecoDatam ,       gen_var:  genDatam
```



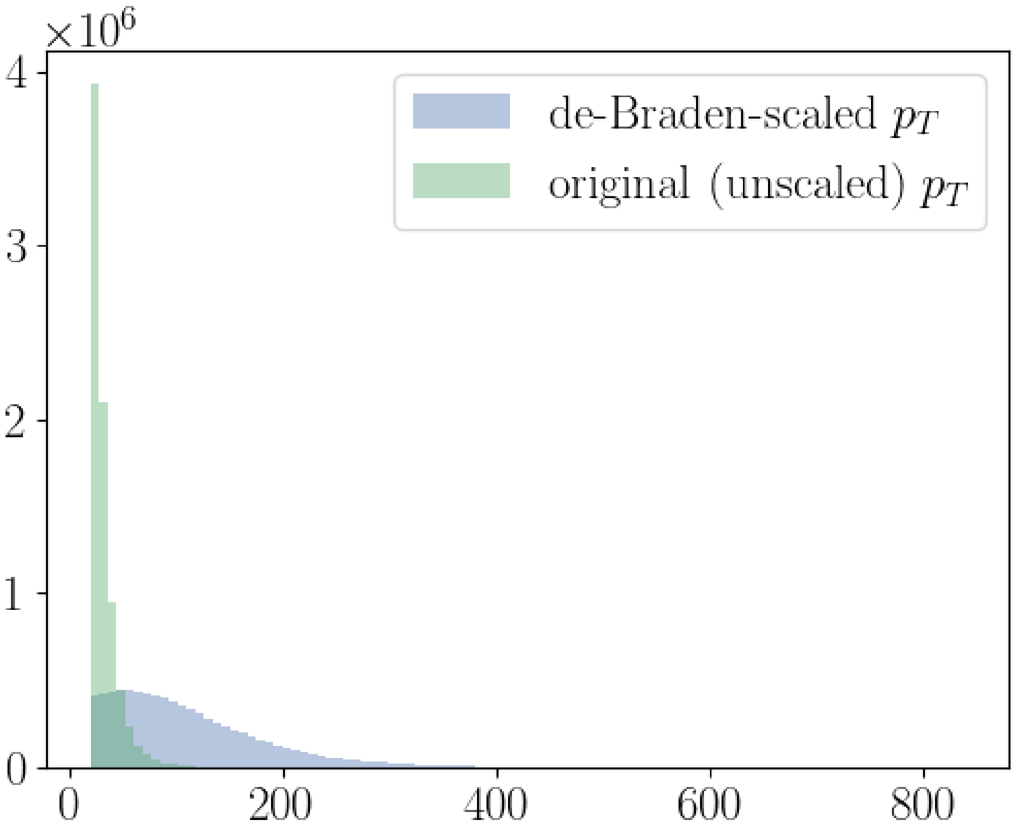
standarize is better than standarize_2

```
scaled_train_data = scale_df(train_data,
title='scaled_train_data_10M_2.csv',
                             scale_func=standarize,
                             save=True)
print('\n\n')
scaled_test_data = scale_df(test_data,
title='scaled_test_data_10M_2.csv',
                            scale_func=standarize,
                            save=True)

explore_data(df=scaled_train_data, title='Braden Kronheim-scaled
Dataframe: standarize_IQN', scaled=True)

          genDatapT    RecoDatapT    genDataeta    RecoDataeta
genDataphi  \
count  10000.000000  10000.000000  10000.000000  10000.000000
10000.000000
mean       0.193019      0.349439      0.499998      0.496183
0.500691
std        0.151402      0.137091      0.218950      0.221660
0.288015
min        0.000000      0.000000      0.000000      0.000000
0.000000
25%        0.076371      0.256223      0.338524      0.332046
0.252303
50%        0.158137      0.332218      0.499438      0.495075
0.496276
75%        0.271209      0.428161      0.662592      0.660927
0.747239
max        1.000000      1.000000      1.000000      1.000000
1.000000
```

```
        RecoDataphi      genDatam     RecoDatam           tau
count  10000.000000  10000.000000  10000.000000  10000.000000
mean       0.498494      0.488433      0.440818      0.501375
std        0.268781      0.100227      0.113154      0.288104
min        0.000000      0.000000      0.000000      0.000014
25%        0.266707      0.421777      0.367851      0.252924
50%        0.494279      0.485817      0.438496      0.501390
75%        0.729062      0.553336      0.512428      0.751112
max        1.000000      1.000000      1.000000      0.999968



          genDatapT    RecoDatapT    genDataeta   RecoDataeta
genDataphi  \
count  10000.000000  10000.000000  10000.000000  10000.000000
10000.000000
mean       0.143909      0.275600      0.507399      0.505858
0.504341
std        0.112547      0.110219      0.217335      0.222251
0.289598
min        0.000000      0.000000      0.000000      0.000000
0.000000
25%        0.059885      0.203154      0.344565      0.339593
0.254367
50%        0.119371      0.263623      0.511950      0.510924
0.506544
75%        0.201243      0.337655      0.667306      0.669468
0.757987
max        1.000000      1.000000      1.000000      1.000000
1.000000

        RecoDataphi      genDatam     RecoDatam           tau
count  10000.000000  10000.000000  10000.000000  10000.000000
mean       0.502875      0.330795      0.354760      0.507559
std        0.277433      0.089873      0.091590      0.290743
min        0.000000      0.000000      0.000000      0.000013
25%        0.263911      0.272740      0.295975      0.259261
50%        0.504849      0.329915      0.354809      0.511120
75%        0.745752      0.387605      0.412537      0.762087
max        1.000000      1.000000      1.000000      0.999989
['RecoDatapT', 'RecoDataeta', 'RecoDataphi', 'RecoDatam', 'genDatapT',
'genDataeta', 'genDataphi', 'genDatam']
Reco_var:  RecoDatapT ,     gen_var:  genDatapT
Reco_var:  RecoDataeta ,    gen_var:  genDataeta
Reco_var:  RecoDataphi ,    gen_var:  genDataphi
Reco_var:  RecoDatam ,      gen_var:  genDatam
```




```
def denormalize_IQN(original_values, scaled_values):
    expected_min, expected_max = original_values.min(),
original_values.max()
    scale_factor = expected_max - expected_min
    offset = expected_min
    return scaled_values  * scale_factor + offset

de_scaled_m = denormalize_IQN(original_values=train_data.iloc[:,0],
scaled_values=scaled_train_data.iloc[:,0])
plt.hist(de_scaled_m,bins=100, label='de-Braden-scaled
$p_T$',alpha=0.4)
plt.hist(train_data.iloc[:,0],bins=100,label='original (unscaled)
$p_T$',alpha=0.4)
plt.legend();plt.show()
```



ML

Note that this ideas is very powerful and has the potential to replace the use of Delphes/GEANT for most people. According to the previous paper this method already works for a single IQN.

It's important to remember "the master formula" of all of machine learning:

$$\int \frac{\partial L}{\partial f} p(y \vee x) d y = 0$$

or, equivalently,

$$\frac{\delta R}{\delta f} = 0,$$

where L is the loss function, f is the model (in this case IQN) (implicitly parameterized by potentially a gazillion parameters), y is the target(s) that we want to estimate, x is the (set of) training features, R is the risk functional.

So, for IQNs,

$$L_{\text{IQN}}(f,y)=\begin{cases}\tau\left(y-f(x,\tau;\theta)\right) & y\geq f(x,\tau;\theta)\\ (1-\tau)\left(f(x,\tau;\theta)-y\right) & y<f(x,\tau;\theta)\end{cases},$$

Means that what was done previously is that the risk functional, which is generally a functional of many models f, was a only a functional of a single model: $R[f_1,\ldots,f_n]=f[f_1]$. Here we have 4 models

$$R_{\text{IQN}\,x\,4}=R_{\text{IQN}}[f_m,f_{p_T},f_\eta,f_\phi],$$

and since we're choosing the evaluation order:

$$\begin{array}{ll} p(y\vee x) & \text{¿}\,p(m'\vee x)\\ \text{¿} & \times\, p(\eta'\vee x,m',p_T')\\ \text{¿} & \text{¿}\end{array}$$

$$\begin{array}{ll} R_{\text{IQN}\,x\,4} & \text{¿}\int L_{\text{IQN}}\left(f_m(x_m,\tau),y_m\right)p(x_m,y_m)\,d\,x_m\,d\,y_m\\ \text{¿} & \times\int L_{\text{IQN}}\left(f_\phi(x_\phi,\tau),y_\phi\right)p(x_\phi,y_\phi)\,d\,x_\phi\,d\,y_\phi\end{array},$$

where, again, each model f_i is also dependent on a set of parameters θ_i (dropped for simplicity)

Our risk functional is minimized for

$$\frac{\delta R_{\text{IQN}\,x\,4}}{\delta f_m}=0$$

(which is basically what's done in the training process to get $f_m^{\text{¿}}$ whose weights/parameters minimize the loss). Suppose we factorize the risk as

$$R_{\text{IQN}\,x\,4}=R_{\text{IQN}}^{m}\,R_{\text{IQN}}^{p_T}\,R_{\text{IQN}}^{\eta}\,R_{\text{IQN}}^{\phi},$$

then, by Eq (4),

$$R_{\text{IQN}}^{m}\equiv\int L_{\text{IQN}}\left(f_m(x_m,\tau),y_m\right)p(x_m,y_m,\tau)\,d\,x_m\,d\,y_m\,d\,\tau,$$

and by Eq (5)

$$\int d\,x_m\,d\,y_m\,d\,\tau\,p(x_m,y_m,\tau)\frac{\delta L_{\text{IQN}}\left(f_m(x_m,\tau),y_m\right)}{\delta f_m}=0$$

and by Eq (2)

$$\int d\,x_m\,d\,y_m\,d\,\tau\,p(x_m,y_m,\tau)\frac{\delta L_{\text{IQN}}\left(f_m(x_m,\tau),y_m\right)}{\delta f_m}=0$$

...

Expand Eq (2) in Eq (7) and integrate wrt y to see that $f(x,\tau)$ is the quantile function for $p(y \vee x)$, i.e. (I believe) that IQNx4 should work basically exactly.

$$R_{\mathrm{IQN}\,x\,4} = ¿$$

Train Mass

for mass, $y_m = m_{\mathrm{reco}}$ and $x_m = \{p_T^{\mathrm{gen}}, \eta^{\mathrm{gen}}, \phi^{\mathrm{gen}}, m^{\mathrm{gen}}, \tau\}$.

```
SUBSAMPLE=int(1e4)
target = 'RecoDatam'
source  = FIELDS[target]
features= source['inputs']
########

print('USING NEW DATASET\n')
#UNSCALED
#
train_data_m=pd.read_csv(os.path.join(DATA_DIR,'train_data_10M_2.csv')
,
#                        usecols=features,
#                        nrows=SUBSAMPLE)

# print('TRAINING FEATURES\n', train_data.head())

# test_data_m=
pd.read_csv(os.path.join(DATA_DIR,'test_data_10M_2.csv'),
#                        usecols=features,
#                        nrows=SUBSAMPLE)
# print('\nTESTING FEATURES\n', test_data.head())
# valid_data=
pd.read_csv(os.path.join(DATA_DIR,'valid_data_10M_2.csv'),
#                        usecols=features,
#                        nrows=SUBSAMPLE)


# SCALED
train_data_m=pd.read_csv(os.path.join(DATA_DIR,'train_data_10M_2.csv')
,
                       usecols=all_cols,
                       nrows=SUBSAMPLE)

print('TRAINING FEATURES\n', train_data.head())

test_data_m= pd.read_csv(os.path.join(DATA_DIR,'test_data_10M_2.csv'),
                       usecols=all_cols,
                       nrows=SUBSAMPLE)
print('\nTESTING FEATURES\n', test_data.head())
```

```
print('\ntrain set shape:',  train_data.shape)
print('\ntest set shape:  ', test_data.shape)
# print('validation set shape:', valid_data.shape)
```

```
USING NEW DATASET

TRAINING FEATURES
    genDatapT  genDataeta  genDataphi  genDatam  RecoDatapT
RecoDataeta  \
0    29.4452    0.828187    2.902130   2.85348     31.9132
0.817082
1    24.3193   -1.163510    0.636469   5.83685     27.3513    -
1.151020
2    24.3193   -1.163510    0.636469   5.83685     27.3513    -
1.151020
3    24.3193   -1.163510    0.636469   5.83685     27.3513    -
1.151020
4    20.1703    1.844410   -0.186685   5.69090     24.2158
1.837910

   RecoDataphi  RecoDatam       tau
0     2.919510    2.59587  0.361310
1     0.652153    5.35538  0.126899
2     0.652153    5.35538  0.962307
3     0.652153    5.35538  0.457282
4    -0.160621    4.59370  0.840862

TESTING FEATURES
    genDatapT  genDataeta  genDataphi  genDatam  RecoDatapT
RecoDataeta  \
0    43.6113    0.824891    -1.26949   5.93310     44.3274
0.824645
1    43.6113    0.824891    -1.26949   5.93310     44.3274
0.824645
2    26.0153    3.529970     1.55495   7.41270     27.4750
3.590390
3    28.4944   -1.159650     1.82602   7.84157     33.8797    -
1.139940
4    21.9840    2.747660     2.03085   5.18315     23.3141
2.775790

   RecoDataphi  RecoDatam       tau
0     -1.26117    5.80270  0.250046
1     -1.26117    5.80270  0.847493
2      1.52062    4.81403  0.851995
3      1.76254    7.06425  0.052378
4      2.10209    4.08061  0.542549

train set shape: (8000000, 9)
```

```
test set shape:   (1000000, 9)
```

Batches, validation, losses, and plotting of losses functions

```python
def get_batch(x, t, batch_size):
    # the numpy function choice(length, number)
    # selects at random "batch_size" integers from
    # the range [0, length-1] corresponding to the
    # row indices.
    rows    = np.random.choice(len(x), batch_size)
    batch_x = x[rows]
    batch_t = t[rows]
    # batch_x.T[-1] = np.random.uniform(0, 1, batch_size)
    return (batch_x, batch_t)

# Note: there are several average loss functions available
# in pytorch, but it's useful to know how to create your own.
def average_quadratic_loss(f, t, x):
    # f and t must be of the same shape
    return  torch.mean((f - t)**2)

def average_cross_entropy_loss(f, t, x):
    # f and t must be of the same shape
    loss = torch.where(t > 0.5, torch.log(f), torch.log(1 - f))
    return -torch.mean(loss)

def average_quantile_loss(f, t, x):
    # f and t must be of the same shape
    tau = x.T[-1] # last column is tau.
    #Eq (2)
    return torch.mean(torch.where(t >= f,
                                  tau * (t - f),
                                  (1 - tau)*(f - t)))

# function to validate model during training.
def validate(model, avloss, inputs, targets):
    # make sure we set evaluation mode so that any training specific
    # operations are disabled.
    model.eval() # evaluation mode

    with torch.no_grad(): # no need to compute gradients wrt. x and t
        x = torch.from_numpy(inputs).float()
        t = torch.from_numpy(targets).float()
        # remember to reshape!
        o = model(x).reshape(t.shape)
    return avloss(o, t, x)


def mkdir(dir_):
    """make a directory without overwriting what's in it if it
```

```
exists"""
    # assert isinstance(dir_, str)
    try:
        os.system('mkdir -p %s' % str(dir_) )
    except Exception:
        pass


def plot_average_loss(traces, ftsize=18,save_loss_plots=False,
show_loss_plots=True):

    xx, yy_t, yy_v, yy_v_avg = traces

    # create an empty figure
    fig = plt.figure(figsize=(6, 4.5))
    fig.tight_layout()

    # add a subplot to it
    nrows, ncols, index = 1,1,1
    ax  = fig.add_subplot(nrows,ncols,index)

    ax.set_title("Average loss")

    ax.plot(xx, yy_t, 'b', lw=2, label='Training')
    ax.plot(xx, yy_v, 'r', lw=2, label='Validation')
    #ax.plot(xx, yy_v_avg, 'g', lw=2, label='Running average')

    ax.set_xlabel('Iterations', fontsize=ftsize)
    ax.set_ylabel('average loss', fontsize=ftsize)
    ax.set_xscale('log')
    ax.set_yscale('log')
    ax.grid(True, which="both", linestyle='-')
    ax.legend(loc='upper right')
    if save_loss_plots:
        filename='IQNx4_%s_Loss.dict' % target
        mkdir('images/loss_plots')
        PATH = os.path.join(IQN_BASE, 'images', 'loss_plots',
filename)

plt.savefig('images/loss_curves/IQN_'+N+T+'_Consecutive_2.png')
        print('\nloss curve saved in
images/loss_curves/IQN_'+N+target+'_Consecutive.png')
    if show_loss_plots:
        plt.show()
```

Get training and testing features and targets

```
target = 'RecoDatam'
source  = FIELDS[target]
features= source['inputs']
################################################
```

```
def split_t_x(df, target, input_features):
    # change from pandas dataframe format to a numpy
    # array of the specified types
    t = np.array(df[target])
    x = np.array(df[input_features])
    return t, x

print(f'spliting data for {target}')
train_t, train_x = split_t_x(df= train_data_m, target = target,
input_features=features)
print('train_t shape = ',train_t.shape , 'train_x shape = ',
train_x.shape)
print('\n Training features:\n')
print(train_x)
valid_t, valid_x = split_t_x(df= test_data_m, target = target,
input_features=features)
print('valid_t shape = ',valid_t.shape , 'valid_x shape = ',
valid_x.shape)

print('no need to train_test_split since we already have the split
dataframes')
```

```
spliting data for RecoDatam
train_t shape =  (10000,) train_x shape =  (10000, 5)

 Training features:

[[29.4452      0.828187    2.90213     2.85348     0.36130954]
 [24.3193     -1.16351     0.636469    5.83685     0.12689925]
 [24.3193     -1.16351     0.636469    5.83685     0.96230681]
 ...
 [36.0059      3.537       3.1117      7.61186     0.30763637]
 [36.0059      3.537       3.1117      7.61186     0.83365051]
 [31.3881      2.70158     0.267685    9.22485     0.89913462]]
valid_t shape =  (10000,) valid_x shape =  (10000, 5)
no need to train_test_split since we already have the split dataframes
```

Training and running-of-training functions

```
def train(model, optimizer, avloss, getbatch,
          train_x, train_t,
          valid_x, valid_t,
          batch_size,
          n_iterations, traces,
          step=10, window=10):

    # to keep track of average losses
    xx, yy_t, yy_v, yy_v_avg = traces

    n = len(valid_x)
```

```python
print('Iteration vs average loss')
print("%10s\t%10s\t%10s" % \
      ('iteration', 'train-set', 'valid-set'))

for ii in range(n_iterations):

    # set mode to training so that training specific
    # operations such as dropout are enabled.
    model.train()

    # get a random sample (a batch) of data (as numpy arrays)
    batch_x, batch_t = getbatch(train_x, train_t, batch_size)

    # convert the numpy arrays batch_x and batch_t to tensor
    # types. The PyTorch tensor type is the magic that permits
    # automatic differentiation with respect to parameters.
    # However, since we do not need to take the derivatives
    # with respect to x and t, we disable this feature
    with torch.no_grad(): # no need to compute gradients
        # wrt. x and t
        x = torch.from_numpy(batch_x).float()
        t = torch.from_numpy(batch_t).float()

    # compute the output of the model for the batch of data x
    # Note: outputs is
    #   of shape (-1, 1), but the tensor targets, t, is
    #   of shape (-1,)
    # In order for the tensor operations with outputs and t
    # to work correctly, it is necessary that they have the
    # same shape. We can do this with the reshape method.
    outputs = model(x).reshape(t.shape)

    # compute a noisy approximation to the average loss
    empirical_risk = avloss(outputs, t, x)

    # use automatic differentiation to compute a
    # noisy approximation of the local gradient
    optimizer.zero_grad()       # clear previous gradients
    empirical_risk.backward()   # compute gradients

    # finally, advance one step in the direction of steepest
    # descent, using the noisy local gradient.
    optimizer.step()            # move one step

    if ii % step == 0:

        acc_t = validate(model, avloss, train_x[:n], train_t[:n])
        acc_v = validate(model, avloss, valid_x[:n], valid_t[:n])
        yy_t.append(acc_t)
        yy_v.append(acc_v)
```

```
        # compute running average for validation data
        len_yy_v = len(yy_v)
        if   len_yy_v < window:
            yy_v_avg.append( yy_v[-1] )
        elif len_yy_v == window:
            yy_v_avg.append( sum(yy_v) / window )
        else:
            acc_v_avg  = yy_v_avg[-1] * window
            acc_v_avg += yy_v[-1] - yy_v[-window-1]
            yy_v_avg.append(acc_v_avg / window)

        if len(xx) < 1:
            xx.append(0)
            print("%10d\t%10.6f\t%10.6f" % \
                  (xx[-1], yy_t[-1], yy_v[-1]))
        else:
            xx.append(xx[-1] + step)

            print("\r%10d\t%10.6f\t%10.6f\t%10.6f" % \
                      (xx[-1], yy_t[-1], yy_v[-1], yy_v_avg[-1]),
                  end='')

    print()
    return (xx, yy_t, yy_v, yy_v_avg)


def run(model, target,
        train_x, train_t,
        valid_x, valid_t, traces,
        n_batch=256,
        n_iterations=n_iterations,
        traces_step=500,
        traces_window=500,
        save_model=False):

    learning_rate= starting_learning_rate
    optimizer = torch.optim.Adam(model.parameters(), lr=learning_rate)

    #starting at 10^-3
    traces = train(model, optimizer,
                      average_quantile_loss,
                      get_batch,
                      train_x, train_t,
                      valid_x, valid_t,
                      n_batch,
                  n_iterations,
                  traces,
                  step=traces_step,
                  window=traces_window)
```

```
    # learning_rate=learning_rate/10
    # optimizer = torch.optim.Adam(model.parameters(),
lr=learning_rate)
    # #10^-4
    # traces = train(model, optimizer,
    #                   average_quantile_loss,
    #                   get_batch,
    #                   train_x, train_t,
    #                   valid_x, valid_t,
    #                   n_batch,
    #               n_iterations,
    #               traces,
    #               step=traces_step,
    #               window=traces_window)


    # learning_rate=learning_rate/100
    # optimizer = torch.optim.Adam(model.parameters(),
lr=learning_rate)
    # #10^-6
    # traces = train(model, optimizer,
    #                   average_quantile_loss,
    #                   get_batch,
    #                   train_x, train_t,
    #                   valid_x, valid_t,
    #                   n_batch,
    #               n_iterations,
    #               traces,
    #               step=traces_step,
    #               window=traces_window)

    plot_average_loss(traces)

    if save_model:
        filename='Trained_IQNx4_%s_%sK_iter.dict' % (target,
str(int(n_iterations/1000)) )
        PATH = os.path.join(IQN_BASE, 'trained_models', filename)
        torch.save(model.state_dict(), PATH)
        print('\ntrained model dictionary saved in %s' % PATH)
    #utils.ModelHandler(model, scalers)
    return  model
```

Define basic NN model

```
class RegularizedRegressionModel(nn.Module):
    #inherit from the super class
    def __init__(self, nfeatures, ntargets, nlayers, hidden_size,
dropout):
        super().__init__()
        layers = []
```

```
        for _ in range(nlayers):
            if len(layers) ==0:
                #inital layer has to have size of input features as
its input layer
                #its output layer can have any size but it must match
the size of the input layer of the next linear layer
                #here we choose its output layer as the hidden size
(fully connected)
                layers.append(nn.Linear(nfeatures, hidden_size))
                #batch normalization
                layers.append(nn.BatchNorm1d(hidden_size))
                #Dropout seems to worsen model performance
                layers.append(nn.Dropout(dropout))
                #ReLU activation
                layers.append(nn.ReLU())
            else:
                #if this is not the first layer (we dont have layers)
                layers.append(nn.Linear(hidden_size, hidden_size))
                layers.append(nn.BatchNorm1d(hidden_size))
                #Dropout seems to worsen model performance
                # layers.append(nn.Dropout(dropout))
                layers.append(nn.ReLU())
                #output layer:
        layers.append(nn.Linear(hidden_size, ntargets))

        # only for classification add sigmoid
        # layers.append(nn.Sigmoid())
            #we have defined sequential model using the layers in
oulist
        self.model = nn.Sequential(*layers)


    def forward(self, x):
        return self.model(x)

n_iterations, n_layers, n_hidden, starting_learning_rate, dropout =
get_model_params()

NFEATURES=train_x.shape[1]
model=RegularizedRegressionModel(nfeatures=NFEATURES, ntargets=1,
                                 nlayers=n_layers, hidden_size=n_hidden,
dropout=dropout)

print(model)
```

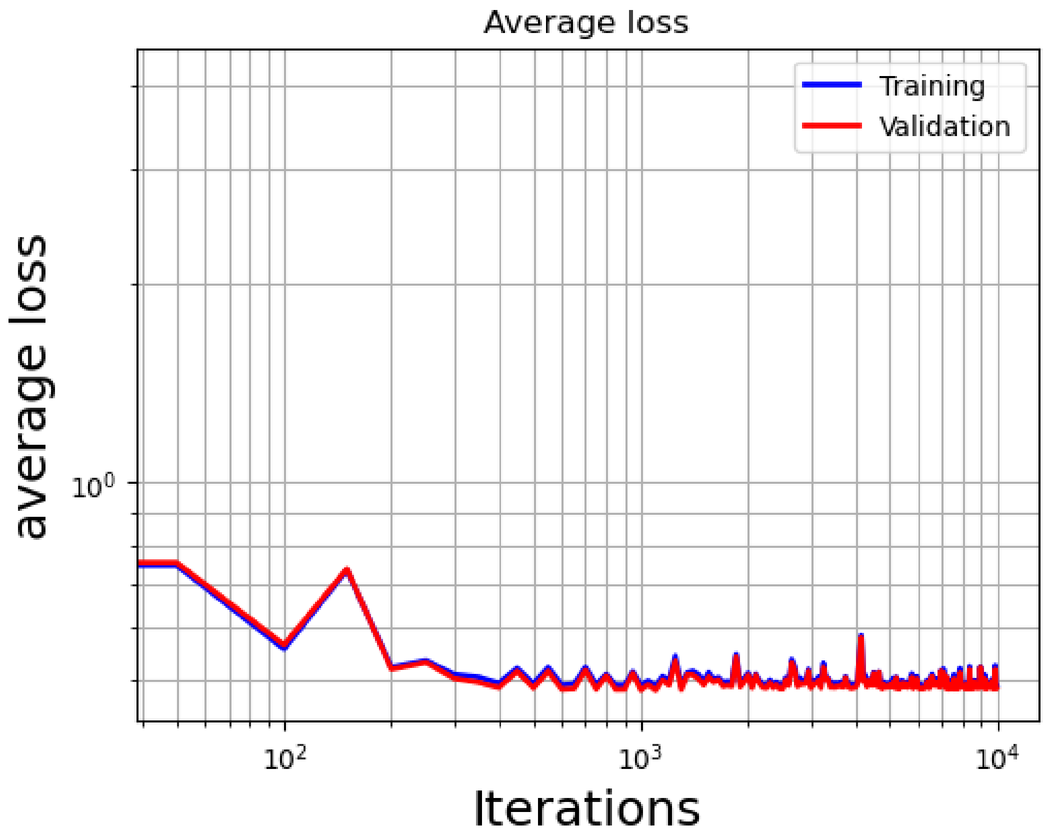
```
RegularizedRegressionModel(
  (model): Sequential(
    (0): Linear(in_features=5, out_features=10, bias=True)
    (1): BatchNorm1d(10, eps=1e-05, momentum=0.1, affine=True,
track_running_stats=True)
```

```
    (2): Dropout(p=0.2, inplace=False)
    (3): ReLU()
    (4): Linear(in_features=10, out_features=1, bias=True)
  )
)
```

Run training

```
print(f'Training for {n_iterations} iterations')
start=time.time()
print('estimating %s\n' % target)
IQN_trace=([], [], [], [])
traces_step = 50
IQN = run(model=model, target=target,train_x=train_x, train_t=train_t,

        valid_x=valid_x, valid_t=valid_t, traces=IQN_trace,
n_batch=256,
        n_iterations=n_iterations, traces_step=50, traces_window=50,
        save_model=False)

end=time.time()
difference=end-start
print('evaluating m took ',difference, 'seconds')
```

```
Training for 10000 iterations
estimating RecoDatam

Iteration vs average loss
 iteration  train-set  valid-set
         0   4.042081   4.107997
      9950   0.490166   0.486542   0.493084
```



Evalute model and save evaluated data
```
if target== 'RecoDatapT':
    label= '$p_T$ [GeV]'
    x_min, x_max = 20, 60
elif target== 'RecoDataeta':
    label = '$\eta$'
    x_min, x_max = -5.4, 5.4
elif target =='RecoDataphi':
    label='$\phi$'
    x_min, x_max = -3.4, 3.4
elif target == 'RecoDatam':
    label = ' $m$ [GeV]'
    x_min, x_max = 0, 18



def evaluate_model(dnn, target, src,
                   fgsize=(6, 6),
                   ftsize=20,save_image=False, save_pred=False,
                   show_plot=True):

eval_data=pd.read_csv(os.path.join(DATA_DIR,'test_data_10M_2.csv'))
    ev_features=X
    #['genDatapT', 'genDataeta', 'genDataphi', 'genDatam','tau']
```

```
    eval_data=eval_data[ev_features]

    print('EVALUATION DATA OLD INDEX\n', eval_data.head())




    dnn.eval()
    y = dnn(eval_data)
    eval_data['RecoDatam']=y
    new_cols= ['RecoDatam'] + X
    eval_data=eval_data.reindex(columns=new_cols)
    print('EVALUATION DATA NEW INDEX\n', eval_data.head())

    eval_data.to_csv('AUTOREGRESSIVE_m_Prime.csv')


    if save_pred:
        pred_df = pd.DataFrame({T+'_predicted':y})

pred_df.to_csv('predicted_data/dataset2/'+T+'_predicted_MLP_iter_50000
00.csv')

    if save_image or show_plot:
        gfile ='fig_model_%s.png' % target
        xbins = 100
        xmin  = src['xmin']
        xmax  = src['xmax']
        xlabel= src['xlabel']
        xstep = (xmax - xmin)/xbins

        fig, ax = plt.subplots(nrows=1, ncols=1, figsize=fgsize)

        ax.set_xlim(xmin, xmax)
        ax.set_xlabel(xlabel, fontsize=ftsize)
        ax.set_xlabel('reco jet '+label, fontsize=ftsize)
        ax.set_ylabel(y_label_dict[target], fontsize=ftsize)

        ax.hist(train_data['RecoDatam'],
                bins=xbins,
                range=(xmin, xmax),
                alpha=0.3,
                color='blue',
                density=True,
                label='simulation')
        ax.hist(y,
                bins=xbins,
                range=(xmin, xmax),
```

```
                alpha=0.3,
                color='red',
                density=True,
                label='$y^\prime$')
        ax.grid()
        ax.legend()


        if save_image:
            plt.savefig('images/'+T+'IQN_Consecutive_'+N+'.png')
            print('images/'+T+'IQN_Consecutive_'+N+'.png')
        if show_plot:
            plt.tight_layout()
            plt.show()
##########
################################################CNN







def main():
    start=time.time()
    print('estimating mass\n')
    model =
utils.RegularizedRegressionModel(nfeatures=train_x.shape[1],
ntargets=1,nlayers=n_layers, hidden_size=n_hidden)
    traces = ([], [], [], [])
    dnn = run(model, scalers, target, train_x, train_t, valid_x,
valid_t, traces)
    evaluate_model( dnn, target, source)



if __name__ == "__main__":
    main()
```

Plot predicted vs real reco (in our paper's format)

Train p_T using saved variables above

Evaluate p_T and save predicted distribution

Plot reco p_T and predicted reco p_T marginal densities

```
# show_jupyter_image('screenshot.png')
```

commented new ideas below