# Model Tuning

June 2, 2022

```
[1]: import numpy as np
  import h5py
  import torch
  from torch.utils.data import Dataset, DataLoader
  import torch.nn as nn
  from collections.abc import Iterable
  import time
  import math

batchSize = 32 #Batch size of training set
```

```
[2]: def trainNetwork(model, loss_function, optimizer, numEpochs, dataloader,__
     →numOutputs):
         #Set model to training mode
         model.train()
         for epoch in range(numEpochs):
             # Print epoch
             print(f'Starting epoch {epoch+1}')
             # Set current loss value
             current_loss = 0.0
             #Reset model parameters
             # Iterate over the DataLoader for training data
             for i, data in enumerate(dataloader, 0):
                 # Get and prepare input
                 preProcessedInputs = data[:, 0:4] #This line doesn't really do⊔
     → anything, delete later?
                 targets = data[:, 4:(4+numOutputs)]
                 #Process intensity by putting it on a log scale
```

```
intens = data[:, 0:1]
        intens = np.log(intens)
        inputs = torch.cat((intens, data[:,1:4]), axis = 1)
        #Process targets by putting them on a log scale
        targets = np.log(targets)
        #print(type(inputs))
        #Comment the next two lines out if not using GPU
        inputs = inputs.to('cuda')
        targets = targets.to('cuda')
        #Normalize inputs
        inputs, targets = inputs.float(), targets.float()
        targets = targets.reshape((targets.shape[0], numOutputs))
        # Zero the gradients
        optimizer.zero_grad()
        # Perform forward pass
        inputs = inputs
        outputs = model(inputs)
        #The following two lines are for debugging only
#
          if i \% 10 == 0:
             print("Targets:", targets[0:2])
             print("Outputs:", outputs[0:2])
#
              print()
             print()
        # Compute loss
        loss = loss_function(outputs, targets)
        # Perform backwards propagation
        loss.backward()
        # Perform optimization
        optimizer.step()
        # Print statistics
        current_loss += loss.item()
        if i % 10 == 0:
           print('Loss after mini-batch %5d: %.3f' %
                 (i + 1, current_loss / 500))
            current_loss = 0.0
```

```
# Process is complete.
         print('Training process has finished.\n')
[3]: def calc_MSE_Error(target, output, index):
         targetNP = np.exp(target[:, index].cpu().detach().numpy())
         outputNP = np.exp(output[:, index].cpu().detach().numpy())
           print(targetNP)
           print(outputNP)
         result = np.square(np.subtract(targetNP, outputNP)).mean()
          print("Index: ", index)
     #
          print(target)
          print(output)
         print("Result:", result)
         return result
[4]: def calc_Avg_Percent_Error(target, output, index):
         targetNP = np.exp(target[:, index].cpu().detach().numpy())
         outputNP = np.exp(output[:, index].cpu().detach().numpy())
         difference = targetNP - outputNP
         difference = np.abs(difference)
         error = np.divide(difference, outputNP) * 100
         result = error.mean()
         return result
[5]: def getModelError(model, epochList, loss_function, trainDataset, testDataset):
         mseErrorList = []
         avgErrorList = []
         mseTrainList = []
         avgTrainList = []
         timeList = □
         #print("Epochs to test:", epochList)
         for numEpochs in epochList:
             #Reset model parameters
```

```
for layer in model.children():
           if hasattr(layer, 'reset_parameters'):
               layer.reset_parameters()
       print("Training with", numEpochs, "epochs.")
       #Define optimizer
       optimizer = torch.optim.Adam(model.parameters(), lr=1e-2)
       #Create dataloader for training set
       dataloader = DataLoader(trainDataset, batch size=batchSize,
→shuffle=True)
       #Start clock
       startTime = time.time()
       #First train the network
       trainNetwork(model, loss_function, optimizer, numEpochs, dataloader, __
→numOutputs = 3)
       #End clock
       endTime = time.time()
       timeSpent = endTime - startTime #In seconds
       #Next test the network
       model.eval()
       #Create dataloader for testing set
       testDataloader = DataLoader(testDataset, batch_size=math.floor(0.
→1*numPoints), shuffle=True)
       iterDataLoader = iter(testDataloader)
       testData = next(iterDataLoader)
       #Process the intens value so it is in a log scale
       intens = testData[:, 0:1]
       logIntens = np.log(intens)
       #Create the final tensor of inputs we will feed into the model
       inputs = torch.cat((logIntens, testData[:,1:4]), axis = 1)
       #Create the tensor of our actual values
       target = testData[:, 4:7]
       target = np.log(target)
       #Push our tensors to the GPU
       inputs = inputs.to('cuda')
       target = target.to('cuda')
```

```
inputs, target = inputs.float(), target.float()
       target = target.reshape((target.shape[0], 3))
       #Get the model predictions and apply a log-scale to our actual values
       #(Model predictions already have a log-scale applied to them)
       output = model(inputs)
       target = np.log(testData[:, 4:7])
         print(output)
         print(target)
        print(' \ n')
       #Initialize error lists
       #Index mappings:
       \#O = Max KE
       #1 = Total Energy
       #2 = Average Energy
       error = [0., 0., 0.]
      percentError = [0., 0., 0.]
      print("Calculate error for test")
       for index in range(3):
           error[index] = calc_MSE_Error(target, output, index)
           percentError[index] = calc_Avg_Percent_Error(target, output, index)
       #Append error values into our list
       mseErrorList.append(error)
       avgErrorList.append(percentError)
       timeList.append(timeSpent)
       #Also retrieve the testing error
       dataloader = DataLoader(trainDataset, batch_size=math.floor(0.1 *_
→numPoints), shuffle=True)
       iterDataLoader = iter(dataloader)
       trainData = next(iterDataLoader)
       #Process the intens value so it is in a log scale
       intens = trainData[:, 0:1]
       logIntens = np.log(intens)
       #Create the final tensor of inputs we will feed into the model
       inputs = torch.cat((logIntens, trainData[:,1:4]), axis = 1)
```

```
#Create the tensor of our actual values
       target = trainData[:, 4:7]
       target = np.log(target)
       #Push our tensors to the GPU
       inputs = inputs.to('cuda')
       target = target.to('cuda')
       inputs, target = inputs.float(), target.float()
       target = target.reshape((target.shape[0], 3))
       #Get the model predictions and apply a log-scale to our actual values
       #(Model predictions already have a log-scale applied to them)
       trainOutput = model(inputs)
       trainTarget = np.log(trainData[:, 4:7])
         print(output)
        print(target)
      print("Calculate error for train")
      trainError = [0., 0., 0.]
       trainPercentError = [0., 0., 0.]
      for index in range(3):
           trainError[index] = calc_MSE_Error(trainTarget, trainOutput, index)
           trainPercentError[index] = calc_Avg_Percent_Error(trainTarget,_
→trainOutput, index)
       #Append error values
      mseTrainList.append(trainError)
       avgTrainList.append(trainPercentError)
  return mseErrorList, avgErrorList, mseTrainList, avgTrainList, timeList
```

### 1 Define our neural networks

```
super().__init__()
  self.norm0 = nn.BatchNorm1d(4)
  self.linear1 = nn.Linear(in_features=4, out_features=64)
  self.norm1 = nn.BatchNorm1d(64)
  self.act1 = nn.LeakyReLU()
  self.dropout = nn.Dropout()
  self.linear2 = nn.Linear(in_features=64, out_features=16)
  self.norm2 = nn.BatchNorm1d(16)
  #self.dropout = nn.Dropout()
  self.act2 = nn.LeakyReLU()
  self.linear3 = nn.Linear(in_features=16, out_features=8)
  self.act3 = nn.LeakyReLU()
  #self.dropout = nn.Dropout()
  self.output = nn.Linear(in_features=8, out_features = 3)
def forward(self, x):
   Forward pass
  x = self.norm0(x)
  x = self.linear1(x)
 x = self.norm1(x)
 x = self.act1(x)
 \#x = self.dropout(x)
  x = self.linear2(x)
 x = self.norm2(x)
  \#x = self.dropout(x)
 x = self.act2(x)
 x = self.linear3(x)
  x = self.act3(x)
  \#x = self.dropout(x)
  x = self.output(x)
  return x
```

```
[7]: #Neural network with 1 hidden layer

class MultiRegressor1Layer(nn.Module):
    '''
    Multilayer Perceptron for regression.
    '''
    def __init__(self):
        super().__init__()
        self.norm0 = nn.BatchNorm1d(4)
```

```
self.linear1 = nn.Linear(in_features=4, out_features=64)
  self.norm1 = nn.BatchNorm1d(64)
  self.act1 = nn.LeakyReLU()
  self.dropout = nn.Dropout()
  self.linear2 = nn.Linear(in_features=64, out_features=16)
  self.norm2 = nn.BatchNorm1d(16)
  #self.dropout = nn.Dropout()
  self.act2 = nn.LeakyReLU()
  self.output = nn.Linear(in_features=16, out_features = 3)
def forward(self, x):
  111
   Forward pass
  111
  x = self.normO(x)
  x = self.linear1(x)
 x = self.norm1(x)
  x = self.act1(x)
 \#x = self.dropout(x)
 x = self.linear2(x)
  x = self.norm2(x)
  \#x = self.dropout(x)
  x = self.act2(x)
  x = self.output(x)
  return x
```

### 2 Read in the data

```
[30]: #Read columns

intens = h5File['Intensity_(W_cm2)']
duration = h5File['Pulse_Duration_(fs)']
```

```
thickness = h5File['Target_Thickness (um)']
      spotSize = h5File['Spot_Size_(FWHM um)']
      maxEnergy = h5File['Max_Proton_Energy_(MeV)']
      totalEnergy = h5File['Total_Proton_Energy_(MeV)']
      avgEnergy = h5File['Avg_Proton_Energy_(MeV)']
      #Convert columns into numpy arrays
      npIntens = np.fromiter(intens, float)
      npDuration = np.fromiter(duration, float)
      npThickness = np.fromiter(thickness, float)
      npSpot = np.fromiter(spotSize, float)
      npMaxEnergy = np.fromiter(maxEnergy, float)
      npTotalEnergy = np.fromiter(totalEnergy, float)
      npAvgEnergy = np.fromiter(avgEnergy, float)
      #Join all of those arrays into one big numpy array
      \#npFile = np.dstack((npIntens, npDuration, npThickness, npSpot, npMaxEnergy, \sqcup
       →npTotalEnergy, npAvqEnergy))
      npFile = npFile.reshape(numPoints, 7)
      #npTrain = npFile[:math.floor(.9*numPoints), 0:7]
      #npTest = npFile[math.floor(.9*numPoints):, 0:7]
      npTrain = npFile[:, 0:7]
      #print(npFile.shape)
[31]: filename_test = 'Data_Fuchs_v_2.2_Wright_Pat_Narrow_Range_lambda_um_0.
       \rightarrow 8 \text{ points '} + \text{str}(100000) + ' \text{ seed } 1.h5'
      h5FileTest = h5py.File(filename_test, 'r+')
      #Read columns
      intens = h5FileTest['Intensity_(W_cm2)']
      duration = h5FileTest['Pulse_Duration_(fs)']
      thickness = h5FileTest['Target_Thickness (um)']
      spotSize = h5FileTest['Spot_Size_(FWHM um)']
      maxEnergy = h5FileTest['Max_Proton_Energy_(MeV)']
      totalEnergy = h5FileTest['Total Proton Energy (MeV)']
      avgEnergy = h5FileTest['Avg_Proton_Energy_(MeV)']
      #Convert columns into numpy arrays
```

```
npIntens = np.fromiter(intens, float)
npDuration = np.fromiter(duration, float)
npThickness = np.fromiter(thickness, float)
npSpot = np.fromiter(spotSize, float)
npMaxEnergy = np.fromiter(maxEnergy, float)
npTotalEnergy = np.fromiter(totalEnergy, float)
npAvgEnergy = np.fromiter(avgEnergy, float)
#Join all of those arrays into one big numpy array
npFile = np.dstack((npIntens, npDuration, npThickness, npSpot, npMaxEnergy,
 →npTotalEnergy, npAvgEnergy))
npFile = npFile.reshape(100000, 7)
#npTrain = npFile[:math.floor(.9*numPoints), 0:7]
#npTest = npFile[math.floor(.9*numPoints):, 0:7]
npTest = npFile[:, 0:7]
print(npFile.shape)
(100000, 7)
```

# 3 Prepare our dataset

```
[32]: training_dataset = h5File.create_dataset(name=None, data=npTrain)
test_dataset = h5File.create_dataset(name=None, data=npTest)
```

```
[33]: #Choose our loss function

loss_function = nn.MSELoss()
```

```
[34]: #List which epochs we should test

#epochList = [1]
#epochList = [1, 2, 3]
epochList = [1, 5, 10, 15, 20, 25, 30, 35, 40, 45, 50, 55, 60, 65, 70, 75, 80, 40, 45, 90, 100, 150, 200, 250]
#epochList = [1, 5, 10, 15, 20, 25, 50, 75, 100, 150, 200]
#epochList = [1, 5, 10, 15, 20, 50]
#epochList = [1, 5, 10, 15, 20, 25]
```

```
[]: #Initialize neural network and dataloader
model1Layer = MultiRegressor1Layer().to('cuda')
```

```
[36]: def splitErrorList(errorList):
    maxEnergyError = []
    totalEnergyError = []

    for element in errorList:
        maxEnergyError.append(element[0])
        totalEnergyError.append(element[1])
        avgEnergyError.append(element[2])

    return maxEnergyError, totalEnergyError, avgEnergyError
```

# 4 Now plot errors and running time

```
[38]: %matplotlib inline
import matplotlib.pyplot as plt

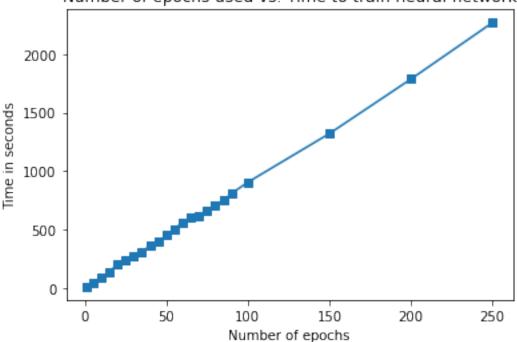
#Time spent plot
fig = plt.figure()
ax1 = fig.add_subplot(1,1,1)

plt.plot(epochList, timeList, marker='s')
```

```
plt.title("Number of epochs used vs. Time to train neural network")
plt.xlabel("Number of epochs")
plt.ylabel("Time in seconds")

#plt.legend(loc='upper left');
plt.show()
```

# Number of epochs used vs. Time to train neural network



```
[39]: for epochElement, timeElement in zip(epochList, timeList):
    minuteValue = timeElement / 60

    print("Number of epochs:", epochElement)
    print("Time spent:", minuteValue, "minutes", '\n')
```

Number of epochs: 1

Time spent: 0.14703834056854248 minutes

Number of epochs: 5

Time spent: 0.7457958658536276 minutes

Number of epochs: 10

Time spent: 1.4910252849260965 minutes

Time spent: 2.292820946375529 minutes

Number of epochs: 20

Time spent: 3.344715170065562 minutes

Number of epochs: 25

Time spent: 3.9810705820719403 minutes

Number of epochs: 30

Time spent: 4.580164515972138 minutes

Number of epochs: 35

Time spent: 5.102071925004323 minutes

Number of epochs: 40

Time spent: 6.038470617930094 minutes

Number of epochs: 45

Time spent: 6.526627858479817 minutes

Number of epochs: 50

Time spent: 7.543764340877533 minutes

Number of epochs: 55

Time spent: 8.418479128678639 minutes

Number of epochs: 60

Time spent: 9.331233354409536 minutes

Number of epochs: 65

Time spent: 10.031408512592316 minutes

Number of epochs: 70

Time spent: 10.151241747538249 minutes

Number of epochs: 75

Time spent: 11.008545513947805 minutes

Number of epochs: 80

Time spent: 11.8485617518425 minutes

Number of epochs: 85

Time spent: 12.469416495164236 minutes

Number of epochs: 90

Time spent: 13.462661596139272 minutes

Time spent: 15.062532075246175 minutes

Number of epochs: 150

Time spent: 22.001067531108855 minutes

Number of epochs: 200

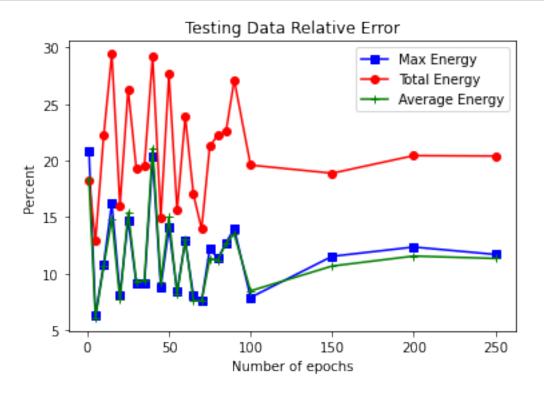
Time spent: 29.7786949634552 minutes

Number of epochs: 250

Time spent: 37.83274068832397 minutes

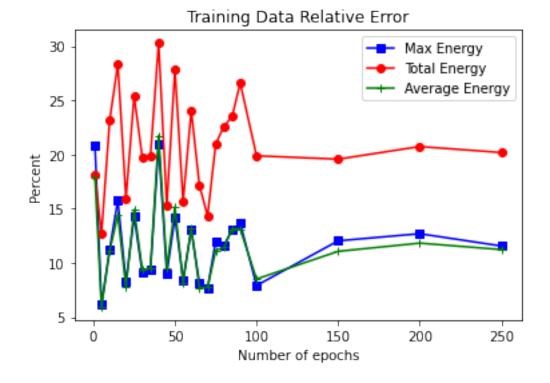
```
[51]: #Percent Error plot
    fig = plt.figure()
    ax1 = fig.add_subplot(1,1,1)

plt.plot(epochList, maxEnergyPercent, c='b', marker="s", label='Max Energy')
    plt.plot(epochList, totalEnergyPercent, c='r', marker="o", label='Total Energy')
    plt.plot(epochList, avgEnergyPercent, c='g', marker='+', label='Average Energy')
    plt.title("Testing Data Relative Error")
    plt.xlabel("Number of epochs")
    plt.ylabel("Percent")
    plt.legend(loc='upper right')
    plt.show()
```



```
[52]: #Percent Error plot for training data
fig = plt.figure()
ax1 = fig.add_subplot(1,1,1)

plt.plot(epochList, trainMaxPercent, c='b', marker="s", label='Max Energy')
plt.plot(epochList, trainTotalPercent, c='r', marker="o", label='Total Energy')
plt.plot(epochList, trainAvgPercent, c='g', marker='+', label='Average Energy')
plt.title("Training Data Relative Error")
plt.xlabel("Number of epochs")
plt.ylabel("Percent")
plt.legend(loc='upper right')
plt.show()
```



```
[53]: #Compare errors of train and test using just the max energy % error

fig = plt.figure()
#ax1 = fig.add_subplot(1,1,1)

plt.plot(epochList, trainMaxPercent, c='b', marker="s", label='Training Data')
plt.plot(epochList, maxEnergyPercent, c='r', marker="s", label='Testing Data')
```

```
plt.title("Testing vs. Training Data Error")
plt.xlabel("Number of epochs")
plt.ylabel("Max Energy Percent Error")
plt.legend(loc='upper right')
plt.show()
```

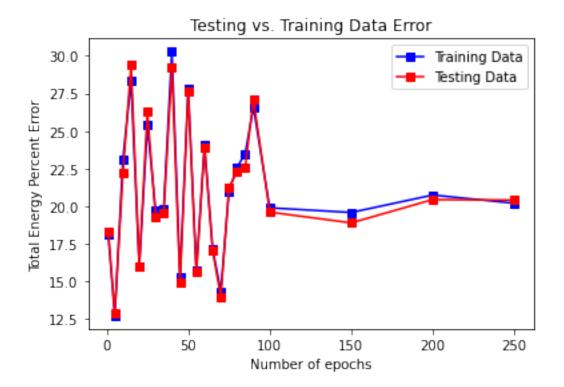


```
[54]: #Compare errors of train and test using just the total energy % error

fig = plt.figure()
    #ax1 = fig.add_subplot(1,1,1)

plt.plot(epochList, trainTotalPercent, c='b', marker="s", label='Training Data')
plt.plot(epochList, totalEnergyPercent, c='r', marker="s", label='Testing Data')

plt.title("Testing vs. Training Data Error")
plt.xlabel("Number of epochs")
plt.ylabel("Total Energy Percent Error")
plt.legend(loc='upper right')
plt.show()
```



```
[55]: #Compare errors of train and test using just the avg energy % error

fig = plt.figure()
    #ax1 = fig.add_subplot(1,1,1)

plt.plot(epochList, trainAvgPercent, c='b', marker="s", label='Training Data')
plt.plot(epochList, avgEnergyPercent, c='r', marker="s", label='Testing Data')

plt.title("Testing vs. Training Data Error")
plt.xlabel("Number of epochs")
plt.ylabel("Total Energy Percent Error")
plt.legend(loc='upper right')
plt.show()
```



Max energy percent error: 20.87278003795522 Total energy percent error: 18.278400748824065 Average energy percent error: 18.300609469347663

Number of epochs: 5

Max energy percent error: 6.292433321827366 Total energy percent error: 12.894555185327413 Average energy percent error: 6.099359933356997

Number of epochs: 10

Max energy percent error: 10.824749565167979 Total energy percent error: 22.20004334964132 Average energy percent error: 10.645141615041783

Number of epochs: 15

Max energy percent error: 16.23049546093938

Total energy percent error: 29.41500321625747 Average energy percent error: 14.87635943268122

Number of epochs: 20

Max energy percent error: 8.109079144438734 Total energy percent error: 16.021951408149125 Average energy percent error: 7.682810163347712

Number of epochs: 25

Max energy percent error: 14.75316779293649 Total energy percent error: 26.293908007551746 Average energy percent error: 15.416446130359935

Number of epochs: 30

Max energy percent error: 9.130424157808424 Total energy percent error: 19.295348564525987 Average energy percent error: 9.275129060466746

Number of epochs: 35

Max energy percent error: 9.141269329040213 Total energy percent error: 19.579482206878268 Average energy percent error: 9.397601465528368

Number of epochs: 40

Max energy percent error: 20.307473421023865 Total energy percent error: 29.198628130719502 Average energy percent error: 21.102139122343043

Number of epochs: 45

Max energy percent error: 8.8341279915337 Total energy percent error: 14.919483201244534 Average energy percent error: 9.289932889614821

Number of epochs: 50

Max energy percent error: 14.074466067224789

Total energy percent error: 27.63038883666942

Average energy percent error: 14.996706746114512

Number of epochs: 55

Max energy percent error: 8.416797538776743 Total energy percent error: 15.586736914469085 Average energy percent error: 8.160750172149728

Number of epochs: 60

Max energy percent error: 12.914375112271223 Total energy percent error: 23.88993033294988 Average energy percent error: 13.027638933574712

Max energy percent error: 8.057336357181724 Total energy percent error: 17.01902153882975 Average energy percent error: 7.6058993829144566

Number of epochs: 70

Max energy percent error: 7.565505299744417 Total energy percent error: 13.952628163527562 Average energy percent error: 7.586146700376765

Number of epochs: 75

Max energy percent error: 12.193658759300002 Total energy percent error: 21.248828568475126 Average energy percent error: 11.330218968109268

Number of epochs: 80

Max energy percent error: 11.346021844652919 Total energy percent error: 22.27386942219833 Average energy percent error: 11.212229891098604

Number of epochs: 85

Max energy percent error: 12.743847457485478 Total energy percent error: 22.59085550378961 Average energy percent error: 12.71617667457452

Number of epochs: 90

Max energy percent error: 13.988382036383832 Total energy percent error: 27.12014269309939 Average energy percent error: 13.495641069467952

Number of epochs: 100

Max energy percent error: 7.897922616144397 Total energy percent error: 19.59624919618485 Average energy percent error: 8.48123049936957

Number of epochs: 150

Max energy percent error: 11.536754725405073 Total energy percent error: 18.87969310548973 Average energy percent error: 10.676295011760246

Number of epochs: 200

Max energy percent error: 12.356540707101708

Total energy percent error: 20.43384763316827

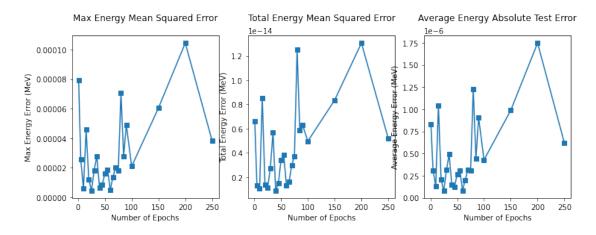
Average energy percent error: 11.558902502372193

Number of epochs: 250

Max energy percent error: 11.703276505441663 Total energy percent error: 20.399311833860175

```
[56]: fig = plt.figure(figsize = (12, 4))
      plt.subplot(1, 3, 1)
      plt.plot(epochList, maxEnergyMSE, marker = 's')
      plt.title("Max Energy Mean Squared Error", pad = 20)
      plt.xlabel('Number of Epochs')
      plt.ylabel('Max Energy Error (MeV)')
      plt.subplot(1, 3, 2)
      plt.plot(epochList, totalEnergyMSE, marker = 's')
      plt.title("Total Energy Mean Squared Error", pad = 20)
      plt.xlabel('Number of Epochs')
      plt.ylabel('Total Energy Error (MeV)')
      plt.subplot(1, 3, 3)
      plt.plot(epochList, avgEnergyMSE, marker = 's')
      plt.title("Average Energy Absolute Test Error", pad = 20)
      plt.xlabel('Number of Epochs')
      plt.ylabel('Average Energy Error (MeV)')
```

[56]: Text(0, 0.5, 'Average Energy Error (MeV)')



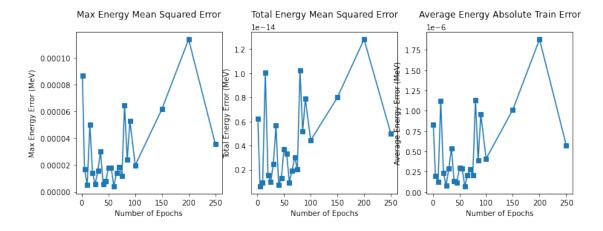
```
[57]: fig = plt.figure(figsize = (12, 4))

plt.subplot(1, 3, 1)
 plt.plot(epochList, trainMaxMSE, marker='s')
 plt.title("Max Energy Mean Squared Error", pad = 20)
 plt.xlabel('Number of Epochs')
 plt.ylabel('Max Energy Error (MeV)')
```

```
plt.subplot(1, 3, 2)
plt.plot(epochList, trainTotalMSE, marker='s')
plt.title("Total Energy Mean Squared Error", pad = 20)
plt.xlabel('Number of Epochs')
plt.ylabel('Total Energy Error (MeV)')

plt.subplot(1, 3, 3)
plt.plot(epochList, trainAvgMSE, marker='s')
plt.title("Average Energy Absolute Train Error", pad = 20)
plt.xlabel('Number of Epochs')
plt.ylabel('Average Energy Error (MeV)')
```

#### [57]: Text(0, 0.5, 'Average Energy Error (MeV)')



```
[62]: def listSubtract(list1, list2):
    result = []

    for x, y in zip(list1, list2):
        difference = x - y
        difference = abs(difference)
        result.append(difference)
```

```
[69]: #Compare train and test MSE errors on the max energy

fig = plt.figure()
  #ax1 = fig.add_subplot(1,1,1)

maxMSEDiff = listSubtract(trainMaxMSE, maxEnergyMSE)
```

```
plt.plot(epochList, maxMSEDiff, c='b', marker="s")

plt.title("Max Energy Error MSE Difference Between Training and Testing", pad =

→20)

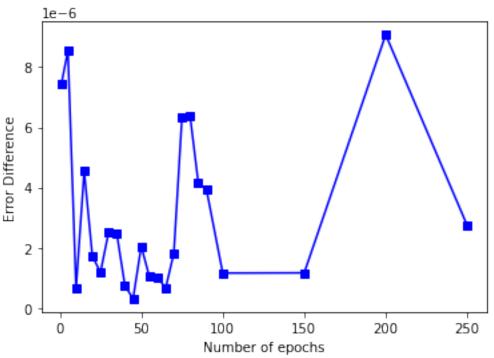
plt.xlabel("Number of epochs")

plt.ylabel("Error Difference")

#plt.legend(loc='upper left')

plt.show()
```

## Max Energy Error MSE Difference Between Training and Testing



```
[67]: #Compare train and test percent errors on the max energy

fig = plt.figure()
#ax1 = fig.add_subplot(1,1,1)

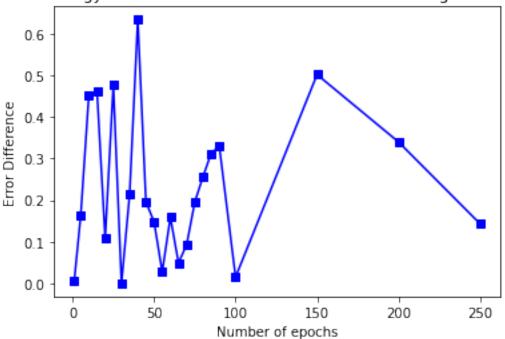
maxPercentDiff = listSubtract(trainMaxPercent, maxEnergyPercent)

plt.plot(epochList, maxPercentDiff, c='b', marker="s")

plt.title("Max Energy Relative Error Difference Between Training and Testing")
plt.xlabel("Number of epochs")
plt.ylabel("Error Difference")
```

```
#plt.legend(loc='upper left')
plt.show()
```

## Max Energy Relative Error Difference Between Training and Testing



```
[48]: for epoch, maxError, totalError, avgError in zip(epochList, maxEnergyMSE, u

→totalEnergyMSE, avgEnergyMSE):

print("Number of epochs:", epoch)

print("Max energy MSE:", maxError)

print("Total energy MSE:", totalError)

print("Average energy MSE:", avgError, '\n')
```

Number of epochs: 1

Max energy MSE: 7.90678981275435e-05 Total energy MSE: 6.628874470347595e-15 Average energy MSE: 8.270581280748943e-07

Number of epochs: 5

Max energy MSE: 2.56097509304956e-05 Total energy MSE: 1.3159836973675904e-15 Average energy MSE: 3.052881171627591e-07

Number of epochs: 10

Max energy MSE: 5.843151638475434e-06 Total energy MSE: 1.0487468404820815e-15 Average energy MSE: 1.3450930758344612e-07

Max energy MSE: 4.573764136075536e-05 Total energy MSE: 8.539439887026031e-15 Average energy MSE: 1.043652028339493e-06

Number of epochs: 20

Max energy MSE: 1.2225174624579374e-05 Total energy MSE: 1.4019149672236502e-15 Average energy MSE: 2.0449766341159457e-07

Number of epochs: 25

Max energy MSE: 4.617832026437266e-06 Total energy MSE: 1.1386756715137832e-15 Average energy MSE: 8.176574557675277e-08

Number of epochs: 30

Max energy MSE: 1.8398282073741432e-05 Total energy MSE: 2.738247805600269e-15 Average energy MSE: 3.1320008596527395e-07

Number of epochs: 35

Max energy MSE: 2.7830366415829203e-05 Total energy MSE: 5.691832001998356e-15 Average energy MSE: 4.916228436796306e-07

Number of epochs: 40

Max energy MSE: 6.417194722972398e-06 Total energy MSE: 8.916700181568558e-16 Average energy MSE: 1.455500193902616e-07

Number of epochs: 45

Max energy MSE: 8.540746332391318e-06 Total energy MSE: 1.47539524937632e-15 Average energy MSE: 1.2596657171892955e-07

Number of epochs: 50

Max energy MSE: 1.6168281817421286e-05 Total energy MSE: 3.403557766137718e-15 Average energy MSE: 2.642834794067944e-07

Number of epochs: 55

Max energy MSE: 1.8911618411471807e-05 Total energy MSE: 3.842817341325633e-15 Average energy MSE: 3.124143072395634e-07

Number of epochs: 60

Max energy MSE: 5.27086171034873e-06

Total energy MSE: 1.3366690771814578e-15 Average energy MSE: 8.476458235106203e-08

Number of epochs: 65

Max energy MSE: 1.3720378880948688e-05 Total energy MSE: 1.6251378711588333e-15 Average energy MSE: 2.0060483950655062e-07

Number of epochs: 70

Max energy MSE: 2.025310256572672e-05 Total energy MSE: 3.009400704078984e-15 Average energy MSE: 3.2010991889383347e-07

Number of epochs: 75

Max energy MSE: 1.8158031675834693e-05 Total energy MSE: 3.744467968609542e-15 Average energy MSE: 3.081494290984527e-07

Number of epochs: 80

Max energy MSE: 7.07717333755127e-05 Total energy MSE: 1.2551130044070479e-14 Average energy MSE: 1.223065524918084e-06

Number of epochs: 85

Max energy MSE: 2.804888512250297e-05 Total energy MSE: 5.851463281155415e-15 Average energy MSE: 4.4407015455334704e-07

Number of epochs: 90

Max energy MSE: 4.901962701589263e-05 Total energy MSE: 6.330414435933989e-15 Average energy MSE: 9.035084792530954e-07

Number of epochs: 100

Max energy MSE: 2.107425527150117e-05 Total energy MSE: 4.9675397124597325e-15 Average energy MSE: 4.2803590030569e-07

Number of epochs: 150

Max energy MSE: 6.050833718744156e-05 Total energy MSE: 8.351028222649266e-15 Average energy MSE: 9.87727346500104e-07

Number of epochs: 200

Max energy MSE: 0.00010443767923438354 Total energy MSE: 1.3065264444251528e-14 Average energy MSE: 1.7464690807542189e-06

Max energy MSE: 3.848314989036754e-05 Total energy MSE: 5.206516255650622e-15 Average energy MSE: 6.201112748931364e-07

[25]: