Wright_Pat_Optimal_Points

June 1, 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 backward pass
        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):
    result = np.square(np.subtract(np.exp(target[:, index].cpu().detach().
 ↪numpy()), np.exp(output[:, index].cpu().detach().numpy())).mean())

    return result
```

[4]:
```
def calc_Avg_Percent_Error(target, output, index):
    difference = np.exp(target[:, index].cpu().detach().numpy()) - np.
 ↪exp(output[:, index].cpu().detach().numpy())
    difference = np.abs(difference)
    error = np.divide(difference, np.exp(output[:, index].cpu().detach().
 ↪numpy())) * 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*points), 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:
    #0 = 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 *␣
↪points), 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

[6]:
```
class MultiRegressor3Layers(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.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]:
```
class MultiRegressor2Layers(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.dropout = nn.Dropout()
    self.output = nn.Linear(in_features=16, 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
```

[8]:
```
def splitErrorList(errorList):
    maxEnergyError = []
    totalEnergyError = []
    avgEnergyError = []

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

    return maxEnergyError, totalEnergyError, avgEnergyError
```

2 Read in the data

[ ]:
```
numPoints = [100, 500, 1000, 2000, 3000, 4000, 5000, 10000, 20000, 30000,␣
 ↪40000, 50000, 100000]

timeList = []
maxEnMSE = []
totalEnMSE = []
avgEnMSE = []
maxEnPercent = []
totalEnPercent = []
avgEnPercent = []
trainMaxMSEList = []
trainTotalMSEList = []
trainAvgMSEList = []
trainMaxPercentList = []
trainTotalPercentList = []
trainAvgPercentList = []
```

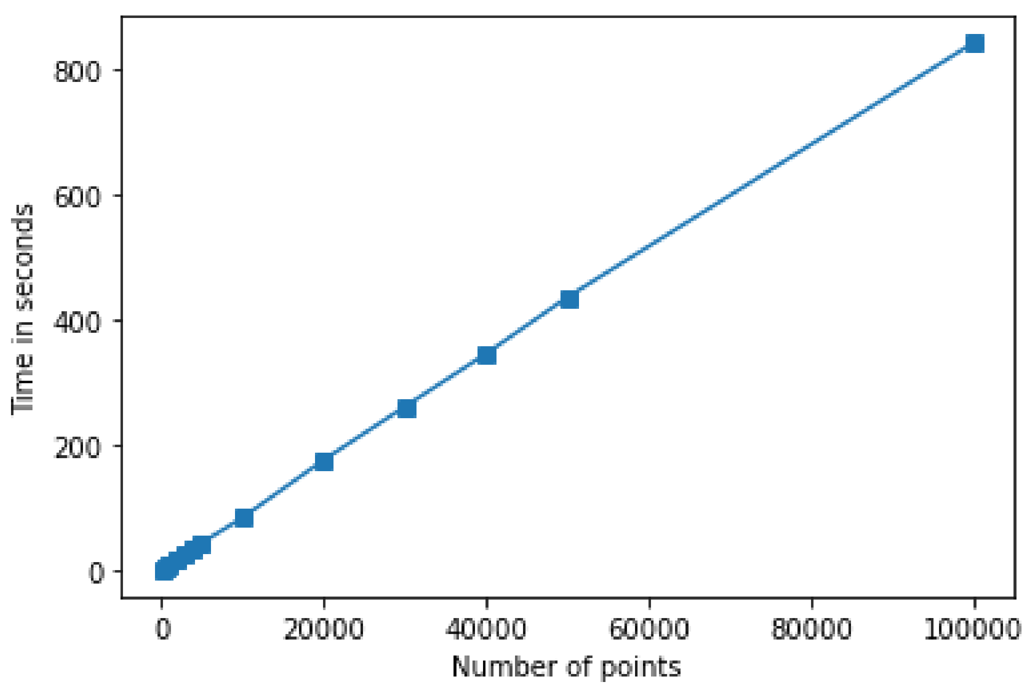
```python
for points in numPoints:

    print("Processing " + str(points) + " points.")

    filename = 'Data_Fuchs_v_2.2_Wright_Pat_Narrow_Range_lambda_um_0.8_points_'␣
↪+ str(points) + '_seed_0.h5'

    h5File = h5py.File(filename, 'r+')

    #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,␣
↪npTotalEnergy, npAvgEnergy))

    npFile = npFile.reshape(points, 7)

    npTrain = npFile[:math.floor(.9 * points), 0:7]
    npTest = npFile[math.floor(.9*points):, 0:7]

    print(npFile.shape)

    training_dataset = h5File.create_dataset(name=None, data=npTrain)
    test_dataset = h5File.create_dataset(name=None, data=npTest)

    #Choose our loss function and optimizer
```

```
    loss_function = nn.MSELoss()
    #optimizer = torch.optim.Adam(model.parameters(), lr=1e-2)

    #List which epochs we should test

    #epochList = [1, 2, 3]
    epochList = [20]
    #epochList = [1, 5, 10]

    #Initialize neural network and dataloader
    model2Layer = MultiRegressor2Layers().to('cuda')


    model2LayerMSE, model2LayerPercentError, trainMSE, trainPercent, timeSpent␣
↪= getModelError(model2Layer, epochList, loss_function, training_dataset,␣
↪test_dataset)

    #print(model2LayerMSE) #For debugging purposes

    model2LayerMSE = model2LayerMSE[0]
    model2LayerPercentError = model2LayerPercentError[0]
    trainMSE = trainMSE[0]
    trainPercent = trainPercent[0]

#     print(model2LayerPercentError)
#      print(trainMSE)
#     print(trainPercent)

    maxEnergyMSE, totalEnergyMSE, avgEnergyMSE = model2LayerMSE[0],␣
↪model2LayerMSE[1], model2LayerMSE[2]
    maxEnergyPercent, totalEnergyPercent, avgEnergyPercent =␣
↪model2LayerPercentError[0], model2LayerPercentError[1],␣
↪model2LayerPercentError[2]
    trainMaxMSE, trainTotalMSE, trainAvgMSE = trainMSE[0], trainMSE[1],␣
↪trainMSE[2]
    trainMaxPercent, trainTotalPercent, trainAvgPercent = trainPercent[0],␣
↪trainPercent[1], trainPercent[2]


    #Append values to list
    timeList.append(timeSpent)
    maxEnMSE.append(maxEnergyMSE)
    totalEnMSE.append(totalEnergyMSE)
    avgEnMSE.append(avgEnergyMSE)
    maxEnPercent.append(maxEnergyPercent)
    totalEnPercent.append(totalEnergyPercent)
    avgEnPercent.append(avgEnergyPercent)
```

```python
    trainMaxMSEList.append(trainMaxMSE)
    trainTotalMSEList.append(trainTotalMSE)
    trainAvgMSEList.append(trainAvgMSE)
    trainMaxPercentList.append(trainMaxPercent)
    trainTotalPercentList.append(trainTotalPercent)
    trainAvgPercentList.append(trainAvgPercent)
```

3 Now plot errors and time spent

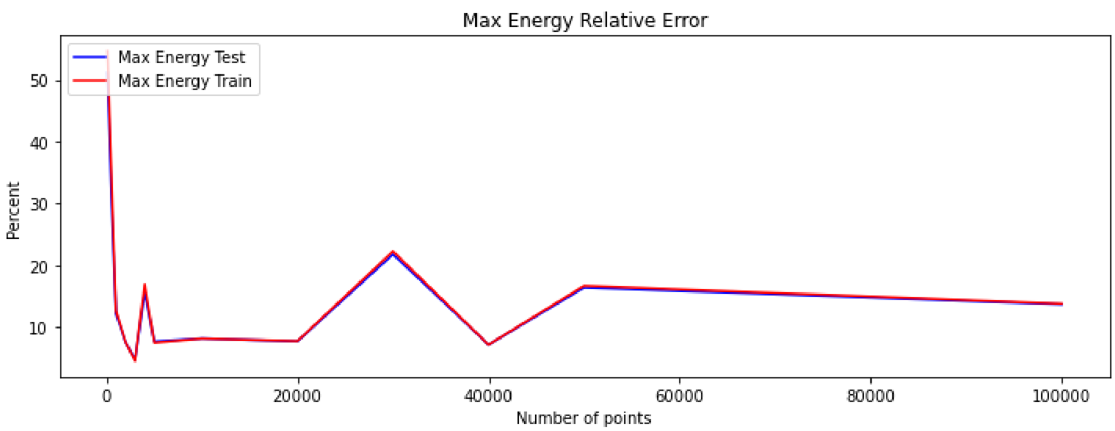
[24]:
```python
%matplotlib inline
import matplotlib.pyplot as plt

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

plt.plot(numPoints, timeList, marker='s')
plt.xlabel("Number of points")
plt.ylabel("Time in seconds")


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



[26]:
```
for point, time in zip(numPoints, timeList):

    minuteValue = time[0] / 60

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

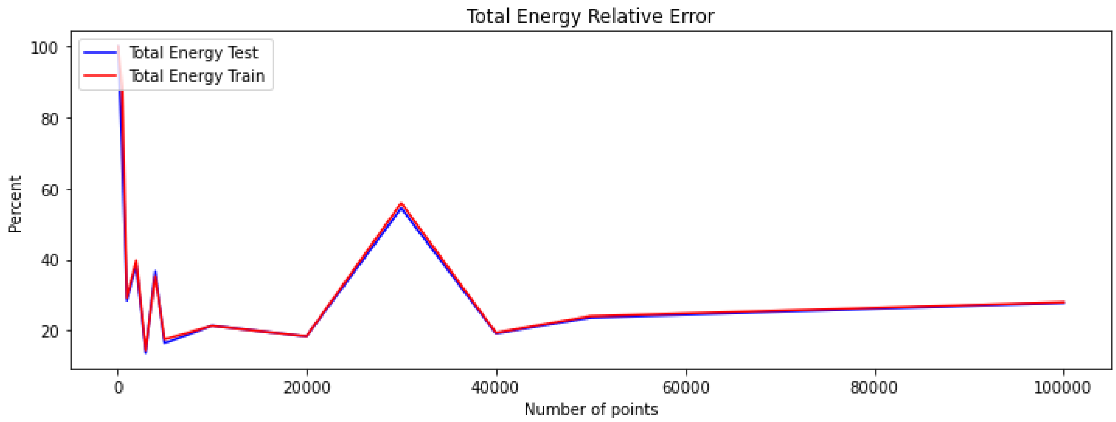
```
Number of points: 100
Time spent: 0.016349951426188152 minutes

Number of points: 500
Time spent: 0.0662332812945048 minutes

Number of points: 1000
Time spent: 0.13165001471837362 minutes

Number of points: 2000
Time spent: 0.2971670071283976 minutes

Number of points: 3000
Time spent: 0.4507332722345988 minutes

Number of points: 4000
Time spent: 0.5440333008766174 minutes

Number of points: 5000
Time spent: 0.7354166666666667 minutes

Number of points: 10000
Time spent: 1.396066709359487 minutes

Number of points: 20000
Time spent: 2.9307833274205524 minutes

Number of points: 30000
Time spent: 4.34896692832311 minutes

Number of points: 40000
Time spent: 5.7557332754135135 minutes

Number of points: 50000
Time spent: 7.2570499340693155 minutes

Number of points: 100000
Time spent: 14.018451070785522 minutes
```

[55]:
```python
#Percent Error plot
fig = plt.figure(figsize = (12, 4))
#ax1 = fig.add_subplot(1,1,1)

#ax1.scatter(numPoints, maxEnPercent, s=10, c='b', marker="s", label='Max␣
↪Energy')
#ax1.scatter(numPoints, totalEnPercent, s=10, c='r', marker="o", label='Total␣
↪Energy')
#ax1.scatter(numPoints, avgEnPercent, s=10, c='g', marker='+', label='Average␣
↪Energy')

#print(trainMaxPercent)

plt.plot(numPoints, maxEnPercent, c='b', label = 'Max Energy Test')
plt.plot(numPoints, trainMaxPercentList, c='r', label = 'Max Energy Train')

plt.legend(loc='upper left');
plt.title("Max Energy Relative Error")
plt.xlabel("Number of points")
plt.ylabel("Percent")
plt.show()
```

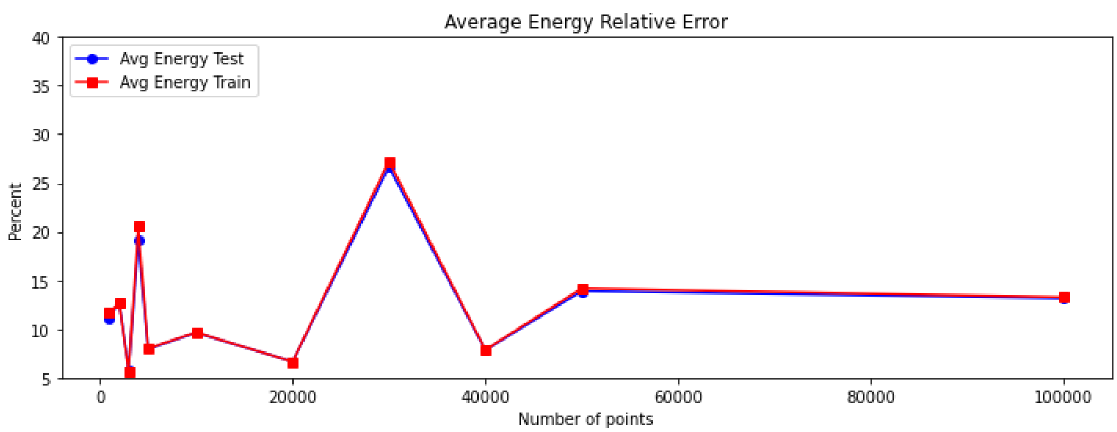


[53]:
```python
#Percent Error plot
fig = plt.figure(figsize = (12, 4))

plt.plot(numPoints, totalEnPercent, c='b', label = 'Total Energy Test')
plt.plot(numPoints, trainTotalPercentList, c='r', label = 'Total Energy Train')

plt.legend(loc='upper left');
plt.title("Total Energy Relative Error")
plt.xlabel("Number of points")
```

```
plt.ylabel("Percent")
plt.show()
```

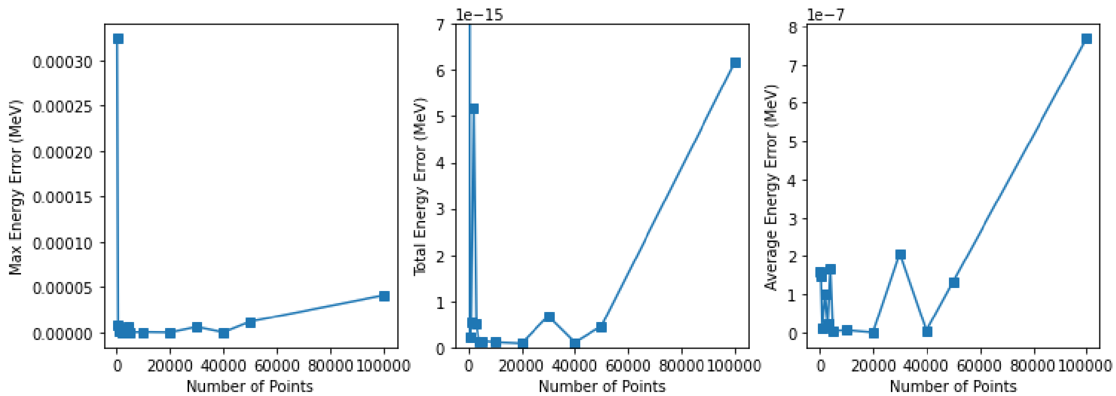


[47]:
```
#Percent Error plot
fig = plt.figure(figsize = (12, 4))

plt.plot(numPoints[2:], avgEnPercent[2:], c='b', label = 'Avg Energy Test',␣
 ↪marker='o')
plt.plot(numPoints[2:], trainAvgPercentList[2:], c='r', label = 'Avg Energy␣
 ↪Train', marker='s')

plt.legend(loc='upper left');
plt.title("Average Energy Relative Error")
plt.ylim([5, 40])
plt.xlabel("Number of points")
plt.ylabel("Percent")
plt.show()
```



[41]:
```python
#MSE Error plot

fig = plt.figure(figsize = (12, 4))

plt.subplot(1, 3, 1)
plt.plot(numPoints, maxEnMSE, marker = 's')
plt.xlabel('Number of Points')
plt.ylabel('Max Energy Error (MeV)')

plt.subplot(1, 3, 2)
plt.plot(numPoints, totalEnMSE, marker = 's')
plt.ylim([0,7e-15])
plt.xlabel('Number of Points')
plt.ylabel('Total Energy Error (MeV)')

plt.subplot(1, 3, 3)
plt.plot(numPoints, avgEnMSE, marker = 's')
plt.xlabel('Number of Points')
plt.ylabel('Average Energy Error (MeV)')
```

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



4 Raw data

[50]:
```python
#Percent error for test data

for pointAmount, maxError, totalError, avgError in zip(numPoints, maxEnPercent,␣
↪totalEnPercent, avgEnPercent):
    print("Number of points:", pointAmount)
    print("Max energy percent error:", maxError)
```

```python
    print("Total energy percent error:", totalError)
    print("Average energy percent error:", avgError, '\n')
```

```
Number of points: 100
Max energy percent error: 51.11900025833421
Total energy percent error: 99.98962941565023
Average energy percent error: 92.06623913889993

Number of points: 500
Max energy percent error: 31.7130884128016
Total energy percent error: 71.70924289187744
Average energy percent error: 30.444354461976836

Number of points: 1000
Max energy percent error: 12.225570114240474
Total energy percent error: 28.289086821938877
Average energy percent error: 11.112863087619408

Number of points: 2000
Max energy percent error: 7.634712186955392
Total energy percent error: 38.53267480321875
Average energy percent error: 12.773827834138816

Number of points: 3000
Max energy percent error: 4.7807257071036915
Total energy percent error: 13.610958572411532
Average energy percent error: 5.793757286592924

Number of points: 4000
Max energy percent error: 15.72988713494614
Total energy percent error: 36.643413602412735
Average energy percent error: 19.191929489703465

Number of points: 5000
Max energy percent error: 7.740988039596059
Total energy percent error: 16.358408671130558
Average energy percent error: 7.9470515835964735

Number of points: 10000
Max energy percent error: 8.218539451605398
Total energy percent error: 21.27512833088069
Average energy percent error: 9.621474899173721

Number of points: 20000
Max energy percent error: 7.755136474822557
Total energy percent error: 18.318747630568126
Average energy percent error: 6.643765700292708
```

```
Number of points: 30000
Max energy percent error: 21.81489696538571
Total energy percent error: 54.423029325021254
Average energy percent error: 26.664761271988755

Number of points: 40000
Max energy percent error: 7.208469240647593
Total energy percent error: 19.137370812851515
Average energy percent error: 7.832867341416962

Number of points: 50000
Max energy percent error: 16.428523476075302
Total energy percent error: 23.551487312703223
Average energy percent error: 13.889921998133033

Number of points: 100000
Max energy percent error: 13.739276659230274
Total energy percent error: 27.712716521911997
Average energy percent error: 13.167279450137736
```

[52]:

```
#Percent error for train data

for pointAmount, maxError, totalError, avgError in zip(numPoints,␣
↪trainMaxPercentList, trainTotalPercentList, trainAvgPercentList):
    print("Number of points:", pointAmount)
    print("Max energy percent error:", maxError)
    print("Total energy percent error:", totalError)
    print("Average energy percent error:", avgError, '\n')
```

```
Number of points: 100
Max energy percent error: 54.63157349309175
Total energy percent error: 99.97209152102648
Average energy percent error: 193.6955188099462

Number of points: 500
Max energy percent error: 35.79257651007673
Total energy percent error: 88.61831979070939
Average energy percent error: 33.75493788607352

Number of points: 1000
Max energy percent error: 12.657612007833643
Total energy percent error: 29.062842134856414
Average energy percent error: 11.678415683068431

Number of points: 2000
Max energy percent error: 7.659335190828313
Total energy percent error: 39.72604578477168
```

```
Average energy percent error: 12.694137070706443

Number of points: 3000
Max energy percent error: 4.565684333709083
Total energy percent error: 14.353136947386513
Average energy percent error: 5.628487545162926

Number of points: 4000
Max energy percent error: 17.01154243382638
Total energy percent error: 35.31984559481986
Average energy percent error: 20.533979384032335

Number of points: 5000
Max energy percent error: 7.537758450635185
Total energy percent error: 17.49797831580657
Average energy percent error: 8.005513997153368

Number of points: 10000
Max energy percent error: 8.202407706515636
Total energy percent error: 21.229954584960627
Average energy percent error: 9.652426864403544

Number of points: 20000
Max energy percent error: 7.805855118542531
Total energy percent error: 18.34684094363325
Average energy percent error: 6.641070587968039

Number of points: 30000
Max energy percent error: 22.312358563117847
Total energy percent error: 55.88541281402567
Average energy percent error: 27.248888839223383

Number of points: 40000
Max energy percent error: 7.21850233227473
Total energy percent error: 19.334020862576825
Average energy percent error: 7.8696615631938105

Number of points: 50000
Max energy percent error: 16.723942321011716
Total energy percent error: 23.978883205499763
Average energy percent error: 14.176065522958089

Number of points: 100000
Max energy percent error: 13.838275334965825
Total energy percent error: 27.903372192443786
Average energy percent error: 13.26646167034334
```

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[ ]:
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