

ml4sci-task3-2-1

March 14, 2023

1 ML4SCI Task 3.2

Converting array of (8,) into (8,125,125) and making the dataset and dataloader

the array (8,) contains each element as array of 125 elements which inturn is an array of 125 elements

2 End-to-End Deep Learning Regression for Measurements with the CMS Experiment

```
[1]: # importing basic modules"
import pandas as pd
import numpy as np
```

Lets import the data.....

We find that the data is tooooo huge and normal `pd.read_parquet("")` causes cpu overload and hence doesnt get read

SO WHAT IS MY APPROACH??

I ran a for loop from 0 to total rows with step size of `chunk_size` variable Then reading the `ith` element and converting it into pandas Lastly appending them all to form the dataframe TO SET THE NUMBER OF EXAMPLES TO EXTRACT

If u set the value of chunk size as `n` , then u will get `total rows//n` number of examples

```
[20]: import pyarrow.parquet as pq
# Set the size of each chunk in rows
chunk_size = 50

# Create a Parquet file reader object
parquet_file = pq.ParquetFile('/kaggle/input/ml4sci-regression-dataset/
↳top_gun_opendata_3.parquet')

# Determine the total number of rows in the file
total_rows = parquet_file.metadata.num_rows

# Loop over the file in chunks
```

```

dfs = []
for i in range(0, total_rows, chunk_size):
    # Read a chunk of rows from the file
    chunk = parquet_file.read_row_group(i)
    df = chunk.to_pandas()
    # print(i)
    dfs.append(df)

# Concatenate all the DataFrames into a single DataFrame
final_df3 = pd.concat(dfs, ignore_index=True)

```

```
[21]: parquet_file.metadata    #Shows us what is there inside the parquet file
```

```

[21]: <pyarrow._parquet.FileMetaData object at 0x7f5d735ca350>
      created_by: parquet-cpp version 1.5.1-SNAPSHOT
      num_columns: 5
      num_rows: 150448
      num_row_groups: 150448
      format_version: 1.0
      serialized_size: 72299402

```

```
[22]: parquet_file.read_row_group(0).to_pandas()    # to convert into pandas
```

```

[22]:
      X_jet      m   iphi  \
0  [[0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0...  232.846863  66.0

      pt   ieta
0  865.297302  26.0

```

```
[23]: final_df3['X_jet'][0].shape
```

```
[23]: (8,)
```

Above we see that the each element under the X_jets is just an array of 8 elements... but that 8 elements is it self an array of 125 elements where that 125 elements is an array of 125 elements

I created a function that stacks this and creates a 8,125,125 matrix

```
[24]: final_df3.head()
```

```

[24]:
      X_jet      m   iphi  \
0  [[0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0...  232.846863  66.0
1  [[0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0...  413.781799  53.0
2  [[0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0...  288.204926  63.0
3  [[0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0...  269.854034  44.0
4  [[0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0...  118.995079  46.0

      pt   ieta

```

```
0  865.297302  26.0
1  962.853760  38.0
2  926.835327  39.0
3  656.809326  37.0
4  411.588104  38.0
```

```
[25]: total_rows
```

```
[25]: 150448
```

```
[26]: final_df3['X_jet'][0].shape
```

```
[26]: (8,)
```

3 created function to convert

```
[27]: def to_3d(arr):
      vishak=[]
      for i in range (0,4):
          vis=np.stack(np.stack(arr)[i],axis=-1)
          vishak.append(vis)
      vishak=np.array(vishak)
      return vishak
```

```
[28]: rr=final_df3['X_jet'].shape[0]
```

```
[29]: for i in range (0,rr):
      final_df3['X_jet'][i]=to_3d(final_df3['X_jet'][i])
```

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See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy

```
[30]: final_df3['X_jet'][0].shape
```

```
[30]: (4, 125, 125)
```

So we see that our dataframe final_df now has a column called X_jets which contains 8,125,125 sized matrix

```
[31]: import matplotlib.pyplot as plt
```

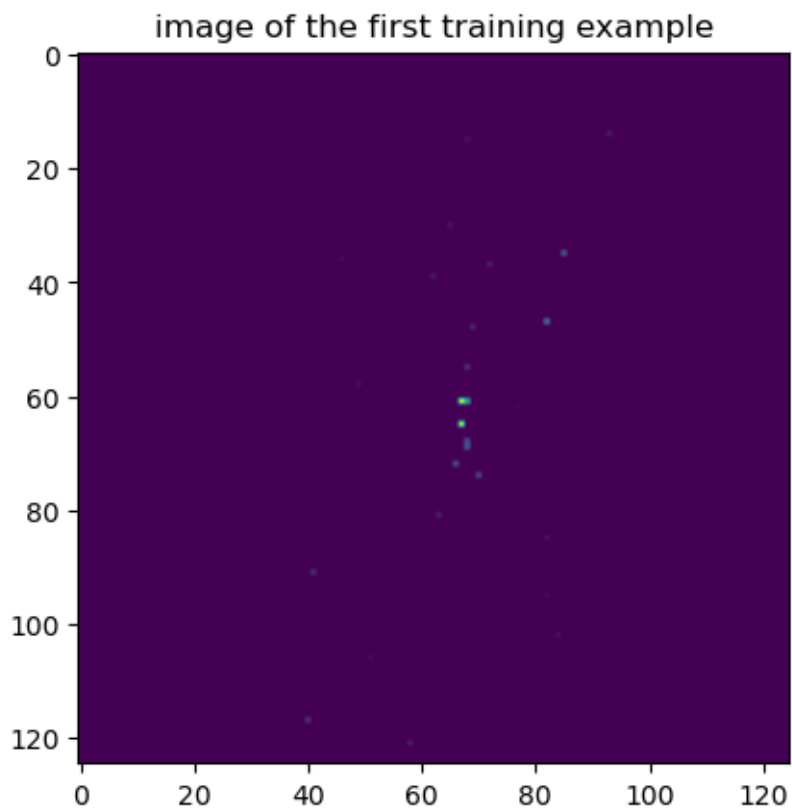
Lets plot and see how the image looks like

4 visualizing the data

```
[32]: plt.imshow(final_df3['X_jet'][0][0,:,:])

plt.title("image of the first training example");
label=final_df3['m'][0]
print(f"Mass is ={label}")
```

Mass is =232.84686279296875



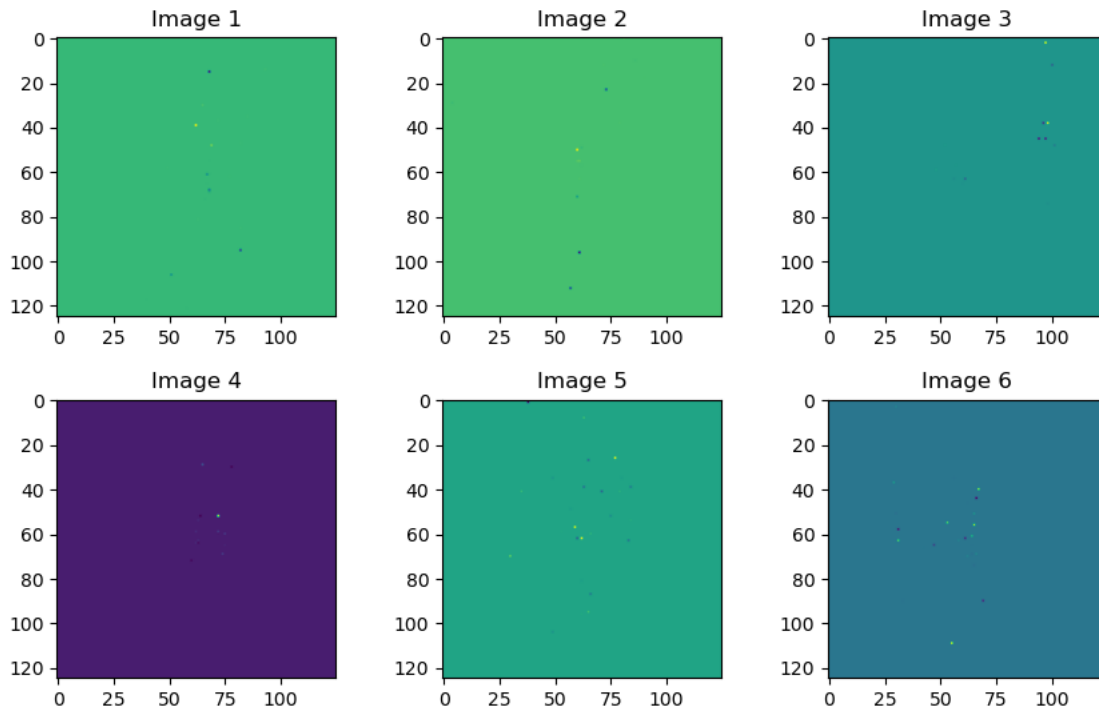
```
[33]: fig, axes = plt.subplots(nrows=2, ncols=3, figsize=(10, 6))

# Loop over the axes and image ids, and plot each image on a separate subplot
for i, ax in enumerate(axes.flatten()):
    image = final_df3['X_jet'][i][2,:,:]
    ax.imshow(image)
    ax.set_title(f'Image {i+1}')

# Adjust spacing between subplots
```

```
plt.subplots_adjust(left=0.1, right=0.9, bottom=0.1, top=0.9, wspace=0.3, hspace=0.3)
```

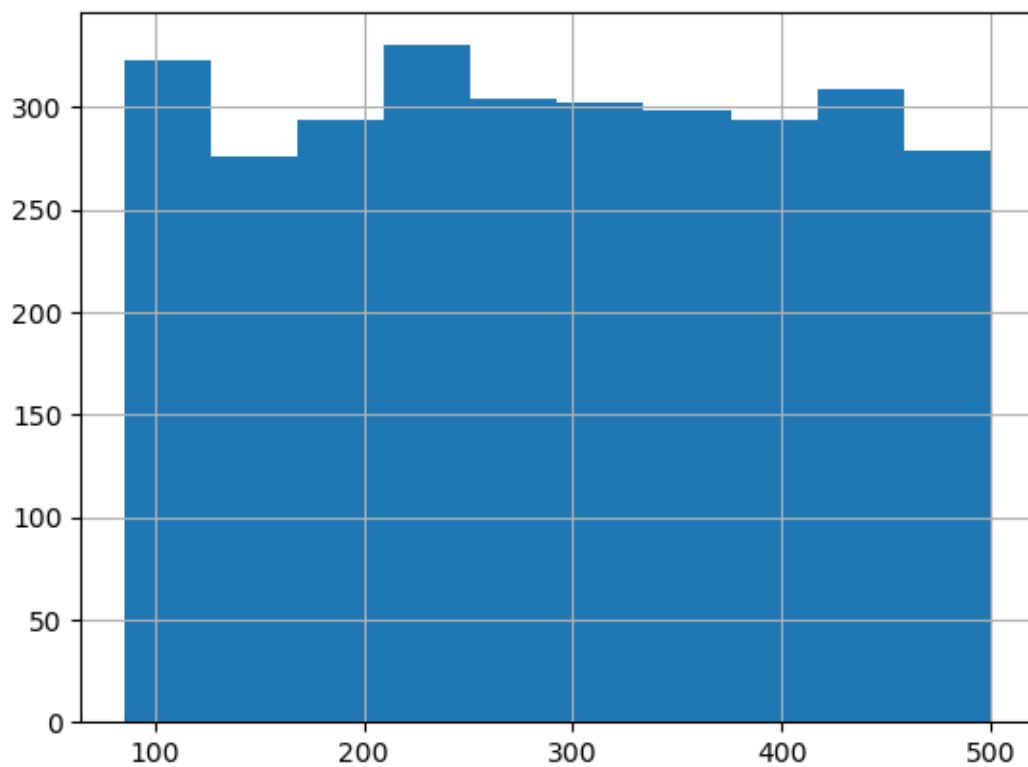
```
# Show the plot  
plt.show()
```



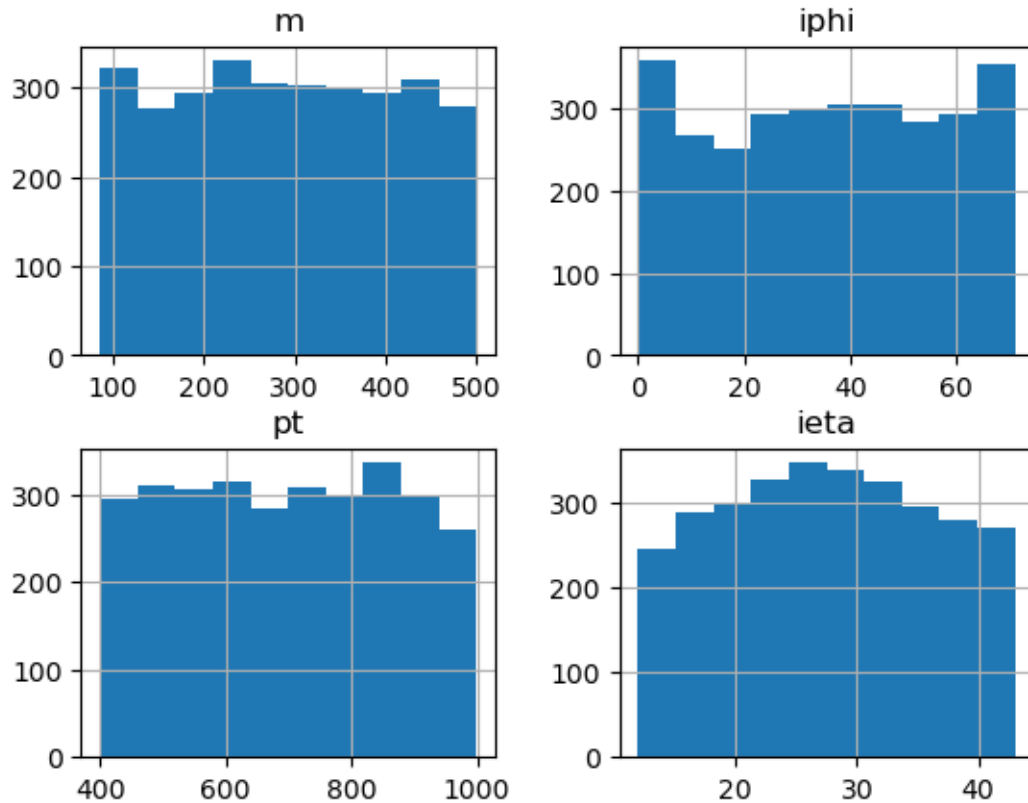
the plot of the mass lets plot the histogram

```
[34]: final_df3['m'].hist()
```

```
[34]: <AxesSubplot:>
```



```
[35]: final_df3.hist();
```



Lets scale the data using standard scaler

THIS function below scales the values

```
[36]: from sklearn.preprocessing import StandardScaler

def scale_matrix(matrix):
    """
    Scale the pixel values of a 3D numpy array using the StandardScaler.

    Parameters:
    matrix (numpy.ndarray): A 3D numpy array of shape (n_samples, height, width).

    Returns:
    numpy.ndarray: A 3D numpy array of the same shape as input, with scaled pixel values.
    """
    # Reshape the matrix to a 2D array
    reshaped_matrix = matrix.reshape(matrix.shape[0], -1)
```

```

# Initialize the StandardScaler object
scaler = StandardScaler()

# Scale the pixel values of the matrix
scaled_matrix = scaler.fit_transform(reshaped_matrix)

# Reshape the scaled matrix back to its original shape
scaled_matrix = scaled_matrix.reshape(matrix.shape)

return scaled_matrix

```

```

[37]: for i in range (0,rr):
      final_df3['X_jet'][i]=scale_matrix(final_df3['X_jet'][i]);

```

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See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy

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5 Dataset and DataLoader

Splitting the data into train and test set in ratio 80/100

```
[38]: from sklearn.model_selection import train_test_split
```

```
[39]: import torch
import torch.nn as nn
from torch.utils.data import Dataset, DataLoader, random_split
```

```
[40]: final_df3.head()
```

```
[40]:
```

		X_jet	m	iphi	\
0	[[[0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0...	232.846863	66.0		
1	[[[0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0...	413.781799	53.0		
2	[[[0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0...	288.204926	63.0		
3	[[[0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0...	269.854034	44.0		
4	[[[0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0...	118.995079	46.0		

	pt	ieta
0	865.297302	26.0
1	962.853760	38.0
2	926.835327	39.0
3	656.809326	37.0
4	411.588104	38.0

DataSet Description: 125x125 image matrices with name of variables: ieta and iphi, with 4 channels called X_jet (Track pT, DZ and D0, ECAL). Please use at least ECAL and Track pT channels and 'am' as the target feature. Please train your model on 80% of the data and evaluate on the remaining 20%. Please make sure not to overfit on the test dataset - it will be checked with an independent sample.

electromagnetic calorimeter (ECAL)

momentum pT > 20 GeV

```
[41]: Dataset
```

```
[41]: torch.utils.data.dataset.Dataset
```

```
[42]: class regdataset(Dataset):

    def __init__(self,data):
        self.df= data
        self.X= data['X_jet']
        self.y=data['m']

    def __len__(self):
        return len(self.df)

    def __getitem__(self,idx):
        return torch.tensor(self.X[idx],dtype=torch.float32), torch.tensor(self.
↪ y[idx],dtype=torch.float32)
```

create the instance of the above class

```
[43]: train_data=regdataset(final_df3)
```

```
[44]: next(iter(train_data))[0].shape
```

```
[44]: torch.Size([4, 125, 125])
```

Splitting the data into train and test set in ratio 80/100

```
[45]: train_size = int(0.8 * len(train_data))  # use 80% of data for training
test_size = len(train_data) - train_size  # use remaining 20% for testing
train_dataset, test_dataset = random_split(train_data, [train_size, test_size])
↪ # split dataset into train and test
```

6 DataLoader

```
[46]: train_loader= DataLoader(train_dataset, batch_size=32,shuffle=True)
test_loader = DataLoader(test_dataset,batch_size=32,shuffle=True)
```

```
[47]: next(iter(train_loader))[0].shape
```

```
[47]: torch.Size([32, 4, 125, 125])
```

7 Architecture

```
[52]: import torch.nn.functional as F

class RegressionModel(nn.Module):
    def __init__(self):
        super(RegressionModel, self).__init__()
```



```

self.conv1 = nn.Conv2d(4, 16, 3, padding=1)
self.conv2 = nn.Conv2d(16, 32, 3, padding=1)
self.conv3 = nn.Conv2d(32, 64, 3, padding=1)
self.fc1 = nn.Linear(64 * 31 * 31, 256)
self.fc2 = nn.Linear(256, 1)

```

```

def forward(self, x):
    x = F.relu(self.conv1(x))
    x = F.max_pool2d(F.relu(self.conv2(x)), 2)
    x = F.max_pool2d(F.relu(self.conv3(x)), 2)
    x = x.view(-1, 64 * 31 * 31)
    x = F.relu(self.fc1(x))
    x = self.fc2(x)
    return x.squeeze()

```

```
[53]: model= RegressionModel()
```

```
[56]: model(next(iter(train_loader))[0])
```

```
[56]: tensor([0.0097, 0.0127, 0.0119, 0.0056, 0.0104, 0.0051, 0.0070, 0.0089, 0.0122,
            0.0087, 0.0083, 0.0062, 0.0055, 0.0133, 0.0101, 0.0114, 0.0092, 0.0046,
            0.0086, 0.0115, 0.0110, 0.0155, 0.0217, 0.0145, 0.0119, 0.0135, 0.0069,
            0.0128, 0.0191, 0.0130, 0.0147, 0.0123], grad_fn=<SqueezeBackward0>)
```

```
[57]: final_df3['X_jet'][0].shape
```

```
[57]: (4, 125, 125)
```

8 Training Loop

```

[82]: import torch.optim as optim
import matplotlib.pyplot as plt
import numpy as np

# Instantiate the model and move it to the GPU (if available)
device = torch.device("cuda" if torch.cuda.is_available() else "cpu")
model = RegressionModel().to(device)

# Define the loss function and optimizer
criterion = nn.MSELoss()
optimizer = optim.Adam(model.parameters(), lr=0.001)

```

```

[109]: model_state_dict = torch.load('/kaggle/working/checkpoint_epoch20.pth')['model']

# Load the saved state_dict
model.load_state_dict(model_state_dict)

```

[109]: <All keys matched successfully>

```
[90]: # Training loop
num_epochs = 5
train_losses = []
for epoch in range(num_epochs):
    flag=0
    running_loss = 0.0
    for i, data in enumerate(train_loader, 0):
        inputs, labels = data
        inputs, labels = inputs.to(device), labels.to(device) # move to GPU if
        ↪available
        optimizer.zero_grad()
        outputs = model(inputs)
        loss = criterion(outputs, labels)
        loss.backward()
        optimizer.step()
        running_loss += loss.item()

    # Print statistics every 100 mini-batches
    if (flag==0):
        print('[Epoch %d, Batch %d] Loss: %.3f' %
              (epoch + 1, i + 1, running_loss / len(train_loader)))
        train_losses.append(running_loss / len(train_loader))
        running_loss = 0.0
        flag=1

    # Save model checkpoint after each epoch
    # checkpoint = {
    #     'model': model.state_dict(),
    #     'optimizer': optimizer.state_dict(),
    #     'epoch': epoch + 1,
    #     'train_losses': train_losses
    # }
    # torch.save(checkpoint, f'checkpoint_epoch{epoch+1}.pth')

# Plot learning curve
plt.plot(train_losses, label='Training Loss')
plt.xlabel('Epoch')
plt.ylabel('Loss')
plt.legend()
plt.show()
```

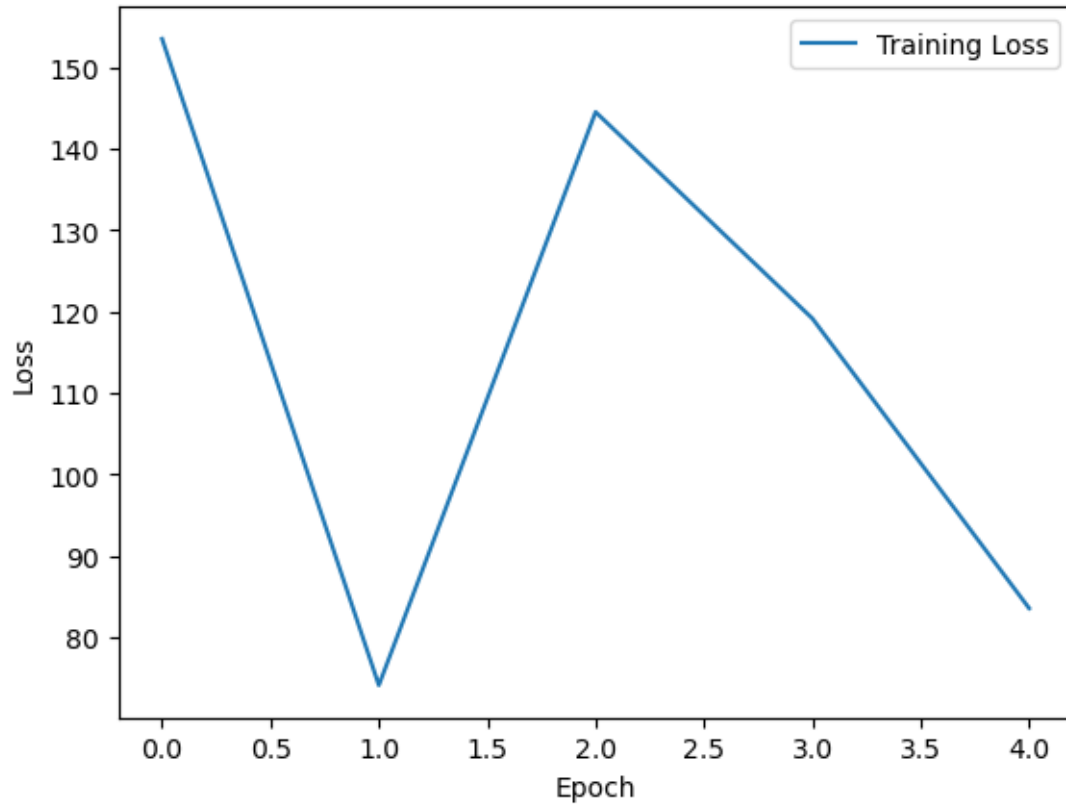
[Epoch 1, Batch 1] Loss: 153.510

[Epoch 2, Batch 1] Loss: 74.120

[Epoch 3, Batch 1] Loss: 144.523

[Epoch 4, Batch 1] Loss: 119.168

[Epoch 5, Batch 1] Loss: 83.565



```
[91]: # Save model checkpoint after each epoch
checkpoint = {
    'model': model.state_dict(),
    'optimizer': optimizer.state_dict(),
    'epoch': epoch + 1,
    'train_losses': train_losses
}
torch.save(checkpoint, f'checkpoint_epoch{epoch+1}.pth')
```

```
[92]: epoch
```

```
[92]: 4
```

```
[93]: model(next(iter(train_loader))[0].to(device))
```

```
[93]: tensor([471.8888, 279.9029, 277.7546, 274.4968, 251.9696, 162.9466, 306.3516,
        301.8897, 388.4455, 274.2234, 274.9473, 300.4969, 264.4630, 318.0904,
        275.2048, 470.1100, 206.7000, 319.9237, 269.8929, 420.4942, 472.6387,
        257.5468, 261.6323, 352.6745, 162.2177, 168.9116, 268.5382, 259.6030,
```

```
257.7735, 302.7849, 172.7616, 155.4103], device='cuda:0',
grad_fn=<SqueezeBackward0>)
```

```
[94]: next(iter(train_loader))[1]
```

```
[94]: tensor([403.6158, 490.6981, 402.5923, 367.9812, 415.8146, 219.4500, 222.5574,
          251.6791, 276.5468, 381.8850, 221.5687, 208.9986, 153.3036, 282.8660,
          258.0343, 176.8999, 138.2467, 388.2806, 401.5501, 429.7057, 369.3040,
          466.6577, 477.6188, 316.0166, 385.8481, 187.2014, 288.4980, 120.7616,
          401.0101, 444.4043, 279.8681, 499.8500])
```

9 Final loss on train data

```
[95]: device = torch.device("cuda" if torch.cuda.is_available() else "cpu")
      model.to(device)

      # Set the model to evaluation mode for testing
      model.eval()

      # Lists to store actual and predicted values
      y_true = []
      y_pred = []

      # Disable gradient calculation during testing
      with torch.no_grad():
          for batch_idx, (data, target) in enumerate(train_loader):
              # Move data to device
              data, target = data.to(device), target.to(device)

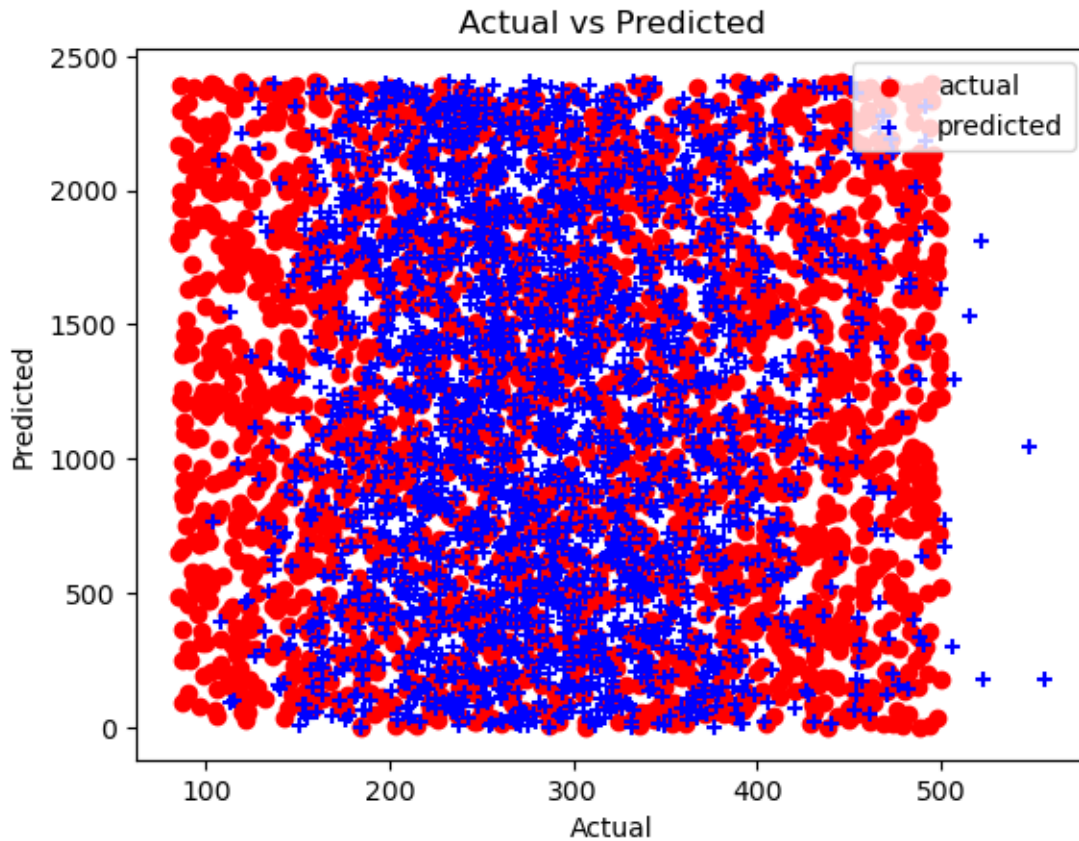
              # Forward pass to get predicted output
              output = model(data)

              # Append actual and predicted values to the lists
              y_true.extend(target.cpu().numpy().tolist())
              y_pred.extend(output.cpu().numpy().tolist())

      # Plot the actual vs predicted values with actual values in blue and predicted
      ↪ values in red
      plt.scatter(y_true, range(len(train_dataset)), color='red', label='actual')
      plt.scatter(y_pred, range(len(train_dataset)), ↪
      ↪ color='blue', marker='+', label="predicted")
      # plt.scatter(x, y, marker='+')
      # plt.plot([min(y_true+y_pred), max(y_true+y_pred)], [min(y_true+y_pred), ↪
      ↪ max(y_true+y_pred)], color='blue')
      plt.xlabel('Actual')
      plt.ylabel('Predicted')
```

```
plt.legend()

plt.title('Actual vs Predicted')
plt.show()
```



lets see the MSE of the train data

```
[96]: criterion(torch.tensor(y_pred),torch.tensor(y_true))
```

```
[96]: tensor(6858.3896)
```

```
[97]: device = torch.device("cuda" if torch.cuda.is_available() else "cpu")
      model.to(device)

      # Set the model to evaluation mode for testing
      model.eval()

      # Lists to store actual and predicted values
      y_true = []
      y_pred = []
```

```

# Disable gradient calculation during testing
with torch.no_grad():
    for batch_idx, (data, target) in enumerate(test_loader):
        # Move data to device
        data, target = data.to(device), target.to(device)

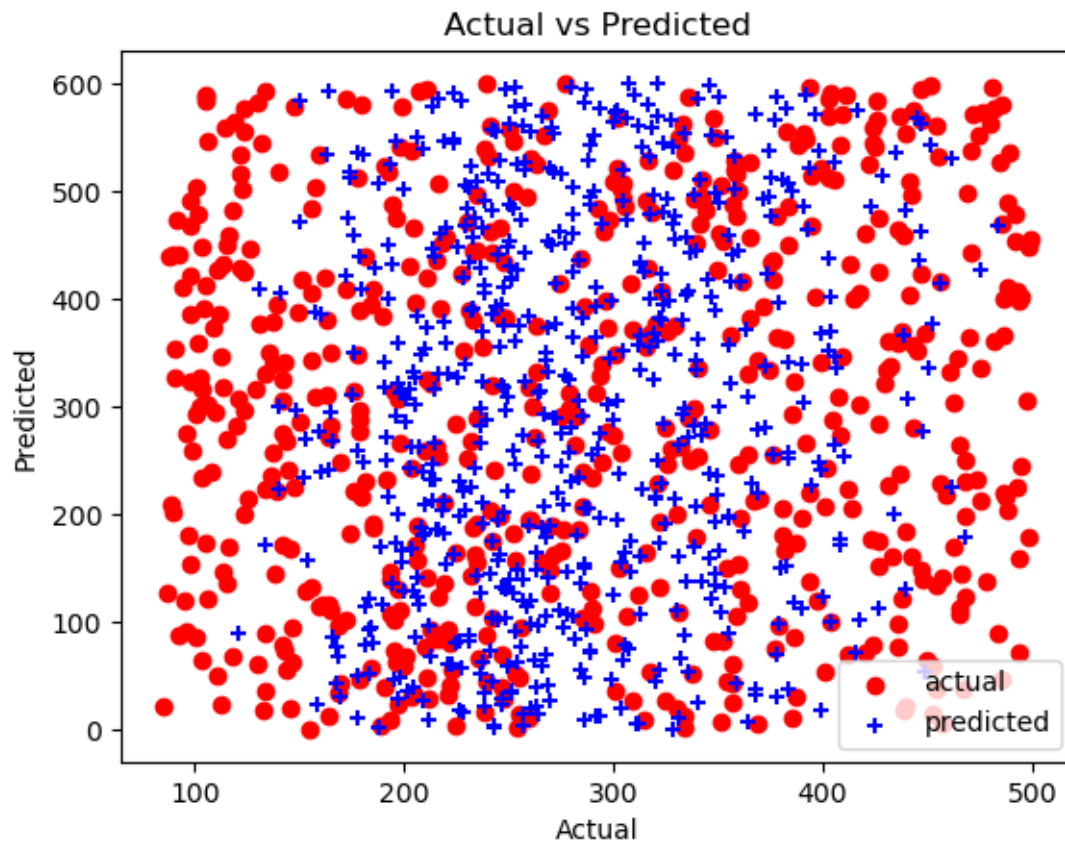
        # Forward pass to get predicted output
        output = model(data)

        # Append actual and predicted values to the lists
        y_true.extend(target.cpu().numpy().tolist())
        y_pred.extend(output.cpu().numpy().tolist())

# Plot the actual vs predicted values with actual values in blue and predicted
    ↪ values in red
plt.scatter(y_true, range(len(test_dataset)), color='red', label='actual')
plt.scatter(y_pred, range(len(test_dataset)), ↪
    ↪ color='blue', marker='+', label="predicted")
# plt.scatter(x, y, marker='+')
# plt.plot([min(y_true+y_pred), max(y_true+y_pred)], [min(y_true+y_pred), ↪
    ↪ max(y_true+y_pred)], color='blue')
plt.xlabel('Actual')
plt.ylabel('Predicted')
plt.legend()

plt.title('Actual vs Predicted')
plt.show()

```



Above we see that the actual values are marked by the red dots and the predicted values are marked by blue +

we are able to see closeness in overlapping

```
[98]: #lets see the MSE of the test data
```

```
[99]: criterion(torch.tensor(y_pred),torch.tensor(y_true))
```

```
[99]: tensor(11195.8789)
```

```
[ ]:
```

```
[ ]:
```

```
[ ]:
```