# final-ml4sci-task-2

March 8, 2023

# 1 ML4SCI TASK 2

## 2 Quark-Gluon Classification

ACTUALLY THE ARRAY IS OF SIZE 3 IN WHICH EACH ELEMENT IS ITSELF AN ARRAY OF 125 ELEMENTS AND THAT 125 ELEMENTS IS AN ARRAY OF 125 ELEMENTS

THIS NOTEBOOK SHOWS THE CONVERSION OF THIS TYPE OF MATRIX INTO 3,125,125

THE KAGGLE NOTEBOOK LINK IS HERE-https://www.kaggle.com/code/vishakkbhat/ml4scitask-2

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

Lets import the data.....

We find that the data is toooo huge and normal pd.read\_parquet(") causes cpu overload and hence doesnt get read

#### SO WHAT IS MY APPRACH??

- 1) I ran a for loop from 0 to total rows with step size of chunk\_size variable
- 2) Then reading the ith elementand converting it into pandas
- 3) 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

```
# 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_df = pd.concat(dfs, ignore_index=True)
[33]: parquet_file.metadata
                            #Shows us what is there inside the parquet file
[33]: <pyarrow._parquet.FileMetaData object at 0x7f161d0b46b0>
       created_by: parquet-cpp version 1.3.1-SNAPSHOT
       num_columns: 4
       num_rows: 36272
       num_row_groups: 36272
       format_version: 1.0
       serialized_size: 14143781
[34]: parquet_file.read_row_group(0).to_pandas()
[34]:
                                                X_jets
                                                               pt
                                                                         mO \
     у
     0.0
[35]: final_df['X_jets'][0].shape
[35]: (3,)
```

Above we see that the each element under the X\_jets is just an array of 3 elements... but that 3 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 3,125,125 matrix

```
[36]: def to_3d(arr):
    vishak=[]
    for i in range (0,3):
        vis=np.stack(np.stack(arr)[i],axis=-1)
        vishak.append(vis)
```

```
vishak=np.array(vishak)
return vishak
```

#### calling the above created function

```
[37]: rr=final_df['X_jets'].shape[0]
[38]: for i in range (0,rr):
          final_df['X_jets'][i]=to_3d(final_df['X_jets'][i])
     /opt/conda/lib/python3.7/site-packages/ipykernel_launcher.py:2:
     SettingWithCopyWarning:
     A value is trying to be set on a copy of a slice from a DataFrame
     See the caveats in the documentation: https://pandas.pydata.org/pandas-
     docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
[39]: final_df['X_jets'][0],final_df['X_jets'][0].shape
[39]: (array([[[0., 0., 0., ..., 0., 0., 0.],
                [0., 0., 0., ..., 0., 0., 0.]
               [0., 0., 0., ..., 0., 0., 0.],
               [0., 0., 0., ..., 0., 0., 0.]
               [0., 0., 0., ..., 0., 0., 0.]
               [0., 0., 0., ..., 0., 0., 0.]],
              [[0., 0., 0., ..., 0., 0., 0.],
               [0., 0., 0., ..., 0., 0., 0.]
               [0., 0., 0., ..., 0., 0., 0.]
               [0., 0., 0., ..., 0., 0., 0.]
               [0., 0., 0., ..., 0., 0., 0.],
               [0., 0., 0., ..., 0., 0., 0.]
              [[0., 0., 0., ..., 0., 0., 0.],
               [0., 0., 0., ..., 0., 0., 0.]
               [0., 0., 0., ..., 0., 0., 0.]
               [0., 0., 0., ..., 0., 0., 0.],
               [0., 0., 0., ..., 0., 0., 0.]
               [0., 0., 0., ..., 0., 0., 0.]])
       (3, 125, 125))
```

So we see that our dataframe final\_df now has a column called X\_jets which contains 3,125,125 sized matrix

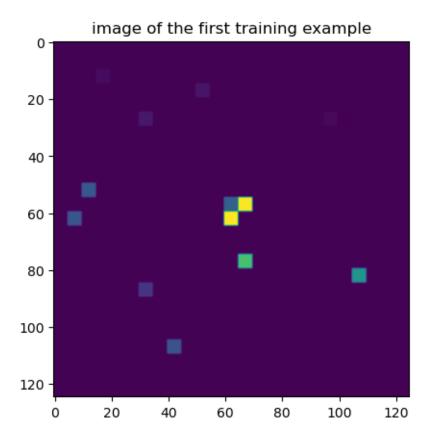
```
[40]: import matplotlib.pyplot as plt
```

#### Lets plot and see how the image looks like

```
[41]: plt.imshow(final_df['X_jets'][0][0,:,:])
    plt.imshow(final_df['X_jets'][0][1,:,:])
    plt.imshow(final_df['X_jets'][0][2,:,:])

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

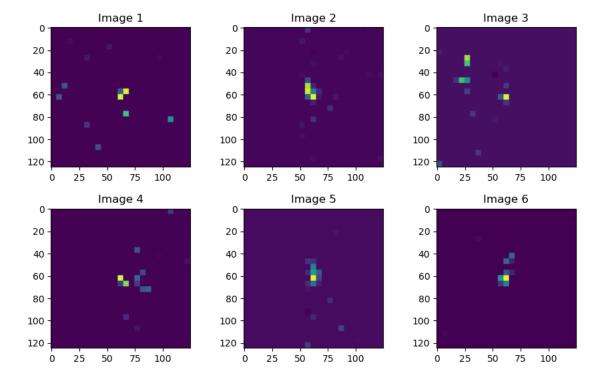
Label is =0.0



#### Plotting multiple images and seeing

```
[42]: 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_df['X_jets'][i][2,:,:]
    ax.imshow(image)
```



## 3 TASKS PERFORMED

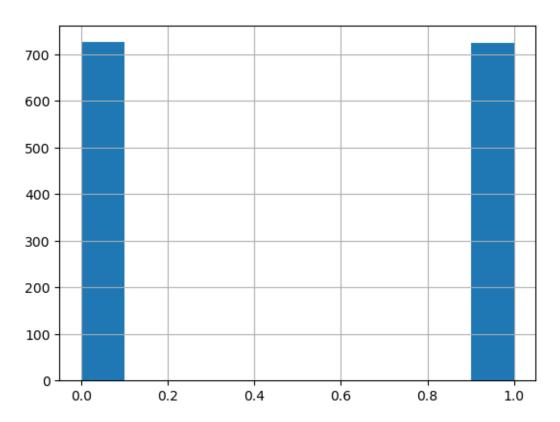
- 1. Created a dataframe now which has the matrix of 3,125,125 and pt m0 and label y
- 2. Now lets create the class dataset and dataloader and then split the data into training and testing set
- 3. Lets now create the class of architecture which contains the architecture from nn.module
- 4. Setting the optimizer and the scheduler and the criterion
- 5. Validating our model with the help of metrics like accuracy and roc auc etc

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

```
import torch.optim as optim
```

```
[44]: final_df['y'].hist()
```

[44]: <AxesSubplot:>



Almost equal examples for both the classes... NO DATA IMBALANCE

This class below converts returns us the value of X and y which is the matrix for image and the respected targer in tensor float 32

```
[45]: class QGdset(Dataset):
    def __init__(self,ddf):
        self.data=ddf
        self.X= ddf['X_jets']
        self.y= ddf['y']
        self.pt= ddf['pt']
        self.m0= ddf['m0']

    def __len__(self):
        return (self.data.shape[0])
```

```
def __getitem__(self,idx):
    return torch.tensor(self.X[idx]/12,dtype=torch.float32), torch.
    tensor(self.y[idx],dtype=torch.float32)
```

```
[46]: train_data= QGdset(final_df)
```

# LETS SPLIT THE train\_data INTO TRAIN AND TEST SO THAT WE CAN VALIDATE OUR MODEL

```
[47]: 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])_u  

# split dataset into train and test
```

```
[48]: len(train_dataset),len(test_dataset)
```

[48]: (1160, 291)

#### Setting up the dataLoaders so that we can feed it to the loops further

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

## Creating architure as below

QGArchi( \* (conv1): Conv2d(3, 16, kernel\_size=(3, 3), stride=(1, 1), padding=(1, 1)) \* (bn1): BatchNorm2d(16, eps=1e-05, momentum=0.1, affine=True, track\_running\_stats=True) \* (relu1): ReLU() \* (pool1): MaxPool2d(kernel\_size=2, stride=2, padding=0, dilation=1, ceil\_mode=False) \* (conv2): Conv2d(16, 32, kernel\_size=(3, 3), stride=(1, 1), padding=(1, 1)) \* (bn2): BatchNorm2d(32, eps=1e-05, momentum=0.1, affine=True, track\_running\_stats=True) \* (relu2): ReLU() \* (pool2): MaxPool2d(kernel\_size=2, stride=2, padding=0, dilation=1, ceil\_mode=False) \* (conv3): Conv2d(32, 64, kernel\_size=(3, 3), stride=(1, 1), padding=(1, 1)) \* (bn3): BatchNorm2d(64, eps=1e-05, momentum=0.1, affine=True, track\_running\_stats=True) \* (relu3): ReLU() \* (pool3): MaxPool2d(kernel\_size=2, stride=2, padding=0, dilation=1, ceil\_mode=False) \* (fc1): Linear(in\_features=14400, out\_features=128, bias=True) \* (fc2): Linear(in\_features=14400, out\_features=128, bias=True) \* (fc2): Linear(in\_features=1, bias=True))\*\*

```
[50]: import torch.nn as nn

class QGArchi(nn.Module):
    def __init__(self):
        super(QGArchi, self).__init__()
        self.conv1 = nn.Conv2d(3, 16, kernel_size=3, stride=1, padding=1)
        self.bn1 = nn.BatchNorm2d(16)
        self.relu1 = nn.ReLU()
```

```
self.pool1 = nn.MaxPool2d(kernel_size=2, stride=2)
    self.conv2 = nn.Conv2d(16, 32, kernel_size=3, stride=1, padding=1)
    self.bn2 = nn.BatchNorm2d(32)
    self.relu2 = nn.ReLU()
    self.pool2 = nn.MaxPool2d(kernel_size=2, stride=2)
    self.conv3 = nn.Conv2d(32, 64, kernel_size=3, stride=1, padding=1)
    self.bn3 = nn.BatchNorm2d(64)
    self.relu3 = nn.ReLU()
    self.pool3 = nn.MaxPool2d(kernel size=2, stride=2)
    self.fc1 = nn.Linear(64 * 15 * 15, 128)
    self.fc2 = nn.Linear(128, 1)
def forward(self, x):
    out = self.conv1(x)
    out = self.bn1(out)
    out = self.relu1(out)
    out = self.pool1(out)
    out = self.conv2(out)
    out = self.bn2(out)
    out = self.relu2(out)
    out = self.pool2(out)
    out = self.conv3(out)
    out = self.bn3(out)
    out = self.relu3(out)
    out = self.pool3(out)
    out = out.view(out.size(0), -1)
    out = self.fc1(out)
    out = self.fc2(out)
    return nn.Sigmoid()(out.squeeze())
```

```
[51]: model=QGArchi()
```

```
[52]: # Define the loss function
    criterion = nn.CrossEntropyLoss()

# Define the learning rate and optimizer
    lr = 0.001
    optimizer = optim.Adam(QGArchi().parameters(), lr=lr)

# Define the scheduler
    scheduler = torch.optim.lr_scheduler.ReduceLROnPlateau(optimizer, factor=0.1, patience=2)
```

## Lets write the code to set the device that is the GPU

```
[53]: device=torch.device('cuda' if torch.cuda.is_available() else 'cpu')
```

```
[54]: device
                #checking if the device is on cuda...
[54]: device(type='cuda')
[55]: from sklearn.metrics import roc_auc_score, confusion_matrix_
       →,plot_confusion_matrix,roc_curve
      import matplotlib.pyplot as plt
      import seaborn as sns
      #we need to import these stuffs to validate our model and see the losses and \square
       \rightarrowaccuracy
[56]: # Set the number of epochs
      epochs = 150
      # Initialize the optimizer and the learning rate scheduler
      optimizer = torch.optim.Adam(model.parameters(), lr=0.001)
      scheduler = torch.optim.lr_scheduler.ReduceLROnPlateau(optimizer, patience=3,_
       ⇒factor=0.1, verbose=True)
      # Initialize the loss function
      criterion = nn.BCELoss()
      # Move the model and the loss function to the device
      model.to(device)
      criterion.to(device)
      # Initialize the lists to store the loss and accuracy values
      train losses = []
      test_losses = []
      train_accs = []
      test_accs = []
      # Iterate over the epochs
      for epoch in range(epochs):
          # Set the model to training mode
          model.train()
          running_loss = 0
          correct_train = 0
          total_train = 0
          # Iterate over the training set
          for X, y in train_loader:
              # Move the input and target tensors to the device
              X, y = X.to(device), y.to(device)
```

```
# Zero the gradients
    optimizer.zero_grad()
    # Forward
    outputs = model(X)
    # Compute the loss
    loss = criterion(outputs, y.float())
    # Backward and optimize
    loss.backward()
    optimizer.step()
    # Update the running loss
    running_loss += loss.item()
    # Compute the number of correct predictions
    predicted_train = torch.round(outputs)
    correct_train += (predicted_train == y).sum().item()
    total_train += y.size(0)
# Compute the training loss and accuracy
train_loss = running_loss / len(train_loader)
train_acc = 100 * correct_train / total_train
train_losses.append(train_loss)
train_accs.append(train_acc)
# Set the model to evaluation mode
model.eval()
running_loss = 0
correct_test = 0
total_test = 0
y_true = []
y_scores = []
# Disable gradient computation to save memory
with torch.no_grad():
    # Iterate over the test set
    for X, y in test_loader:
        # Move the input and target tensors to the device
        X, y = X.to(device), y.to(device)
        # Forward
        outputs = model(X)
        # Compute the loss
        loss = criterion(outputs, y.float())
```

```
# Update the running loss
                running_loss += loss.item()
                # Compute the number of correct predictions
                predicted_test = torch.round(outputs)
                correct_test += (predicted_test == y).sum().item()
                total_test += y.size(0)
                # Append the true and predicted target values
                y true += y.cpu().numpy().tolist()
                y_scores += outputs.cpu().numpy().tolist()
        # Compute the test loss, accuracy, and ROC-AUC score
        test_loss = running_loss / len(test_loader)
        test_acc = 100 * correct_test / total_test
        test_losses.append(test_loss)
        test_accs.append(test_acc)
        roc_auc = roc_auc_score(y_true, y_scores)
        # Print the loss and accuracy values
        if(epoch%30==0):print(f"Epoch {epoch + 1}/{epochs}, Train Loss: {train_loss:
      4.4f}, Train Acc: {train_acc:.2f}%, Test Loss: {test_loss:.4f}, Test Acc:
      # Update the learning
        scheduler.step(test_loss)
    Epoch 1/150, Train Loss: 2.4838, Train Acc: 55.60%, Test Loss: 0.7914, Test Acc:
    49.83%, ROC-AUC: 0.6149
    Epoch 00008: reducing learning rate of group 0 to 1.0000e-04.
    Epoch 00012: reducing learning rate of group 0 to 1.0000e-05.
    Epoch 00016: reducing learning rate of group 0 to 1.0000e-06.
    Epoch 00020: reducing learning rate of group 0 to 1.0000e-07.
    Epoch 00024: reducing learning rate of group 0 to 1.0000e-08.
    Epoch 31/150, Train Loss: 0.2793, Train Acc: 91.55%, Test Loss: 1.0932, Test
    Acc: 68.04%, ROC-AUC: 0.6929
    Epoch 61/150, Train Loss: 0.2783, Train Acc: 91.81%, Test Loss: 1.0568, Test
    Acc: 67.70%, ROC-AUC: 0.6925
    Epoch 91/150, Train Loss: 0.2778, Train Acc: 91.55%, Test Loss: 1.0672, Test
    Acc: 68.04%, ROC-AUC: 0.6930
    Epoch 121/150, Train Loss: 0.2748, Train Acc: 91.90%, Test Loss: 1.0541, Test
    Acc: 68.04%, ROC-AUC: 0.6927
[]:
```