

Graph Neural Networks for Particle Momentum Estimation in the CMS Trigger System Task-1

from google.colab import drive
drive.mount('/content/drive')

Mounted at /content/drive

▼ Installing Requirements

!pip install pyg_lib torch_scatter torch_sparse -f https://data.pyg.org/whl/torc
!pip install torch-geometric

```
Looking in indexes: https://pypi.org/simple, https://us-python.pkg.dev/cola
Looking in links: <a href="https://data.pyg.org/whl/torch-1.13.1+cu116.html">https://data.pyg.org/whl/torch-1.13.1+cu116.html</a>
Collecting pyg lib
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                                                  - 1.9/1.9 MB 13.1 MB/s eta 0:00
Collecting torch scatter
  Downloading <a href="https://data.pyg.org/whl/torch-1.13.0%2Bcu116/torch_scatter-2">https://data.pyg.org/whl/torch-1.13.0%2Bcu116/torch_scatter-2</a>
                                                 - 9.4/9.4 MB 82.6 MB/s eta 0:00
Collecting torch sparse
  Downloading <a href="https://data.pyg.org/whl/torch-1.13.0%2Bcu116/torch_sparse-0">https://data.pyg.org/whl/torch-1.13.0%2Bcu116/torch_sparse-0</a>.
                                                  4.5/4.5 MB 90.2 MB/s eta 0:00
Requirement already satisfied: scipy in /usr/local/lib/python3.8/dist-packa
Requirement already satisfied: numpy<1.27.0,>=1.19.5 in /usr/local/lib/pyth
Installing collected packages: torch scatter, pyg lib, torch sparse
Successfully installed pyg lib-0.1.0+pt113cu116 torch scatter-2.1.0+pt113cu
Looking in indexes: <a href="https://pypi.org/simple">https://us-python.pkg.dev/cola</a>
Collecting torch-geometric
  Downloading torch geometric-2.2.0.tar.gz (564 kB)
                                                 - 565.0/565.0 KB 9.7 MB/s eta 0:
  Preparing metadata (setup.py) ... done
Requirement already satisfied: tgdm in /usr/local/lib/python3.8/dist-packag
Requirement already satisfied: numpy in /usr/local/lib/python3.8/dist-packa
Requirement already satisfied: scipy in /usr/local/lib/python3.8/dist-packa
Requirement already satisfied: jinja2 in /usr/local/lib/python3.8/dist-pack
Requirement already satisfied: requests in /usr/local/lib/python3.8/dist-pa
Requirement already satisfied: pyparsing in /usr/local/lib/python3.8/dist-p
Requirement already satisfied: scikit-learn in /usr/local/lib/python3.8/dis
Collecting psutil>=5.8.0
  Downloading psutil-5.9.4-cp36-abi3-manylinux 2 12 x86 64.manylinux2010 x8
                                               - 280.2/280.2 KB 31.8 MB/s eta 0:
Requirement already satisfied: MarkupSafe>=2.0 in /usr/local/lib/python3.8/
Requirement already satisfied: idna<3,>=2.5 in /usr/local/lib/python3.8/dis
Requirement already satisfied: chardet<5,>=3.0.2 in /usr/local/lib/python3.
Requirement already satisfied: certifi>=2017.4.17 in /usr/local/lib/python3
Requirement already satisfied: urllib3<1.27,>=1.21.1 in /usr/local/lib/pyth
Requirement already satisfied: joblib>=1.1.1 in /usr/local/lib/python3.8/di
Requirement already satisfied: threadpoolctl>=2.0.0 in /usr/local/lib/pytho
Building wheels for collected packages: torch-geometric
  Building wheel for torch-geometric (setup.py) ... done
  Created wheel for torch-geometric: filename=torch geometric-2.2.0-py3-non
  Stored in directory: /root/.cache/pip/wheels/59/a3/20/198928106d3169865ae
Successfully built torch-geometric
Installing collected packages: psutil, torch-geometric
  Attempting uninstall: psutil
    Found existing installation: psutil 5.4.8
    Uninstalling psutil-5.4.8:
      Successfully uninstalled psutil-5.4.8
Successfully installed psutil-5.9.4 torch-geometric-2.2.0
```

▼ Importing Libraries

```
import random
import numpy as np
import tensorflow as tf
import h5py
from tqdm import tqdm
from sklearn.model_selection import train_test_split
from sklearn.metrics import accuracy_score, roc_curve, auc, f1_score
import matplotlib.pyplot as plt
# Modules for keras model
from keras.models import Model
from keras.layers import Input, Conv2D, BatchNormalization, Activation, Add, Max
from keras.callbacks import LearningRateScheduler
# Modules for pytorch model
import torch
import torch.nn as nn
import torch.nn.functional as F
from torch.utils.data import Dataset, DataLoader
from torchvision import transforms
import torch.optim as optim
from torch.optim.lr_scheduler import StepLR
seed = 3
random.seed(seed)
np.random.seed(seed)
tf.random.set_seed(seed)
```

Reading the dataset

```
with h5py.File('/content/drive/MyDrive/GSOC/task1/SingleElectronPt50_IMGCROPS_n2
  X_electron = f.get('X')[:]
  y_electron = f.get('y')[:]
with h5py.File('/content/drive/MyDrive/GSOC/task1/SinglePhotonPt50_IMGCROPS_n249
  X_photon = f.get('X')[:]
  y_photon = f.get('y')[:]
print(X_electron.shape, y_electron.shape)
print(X_photon.shape, y_photon.shape)
     (249000, 32, 32, 2) (249000,)
     (249000, 32, 32, 2) (249000,)
X = np.concatenate((X_electron, X_photon), axis = 0)
print(X.shape)
     (498000, 32, 32, 2)
y = np.concatenate((y_electron, y_photon), axis = 0)
y = y.reshape(-1,1)
print(y.shape)
     (498000, 1)
del(X_photon, X_electron, y_electron, y_photon)
# Using only the energy channel for classification
X = X.T[0].T
X.reshape(-1,32,32,1)
X. shape
     (498000, 32, 32)
```

▼ Train-Val-Test split for the dataset

Default ratio is set as 80/10/10 train-val-test

▼ Model - Keras CNN

Built ResNet-15 architecture after going through the paper 'End-to-End Physics Event Classification with CMS Open Data'.

Removed BatchNorm and replaced MeanPooling with MaxPooling.

```
def residual_block(x, filters, strides=(1, 1), kernel_size=(3, 3)):
    """Residual block for ResNet"""
    shortcut = x
    x = Conv2D(filters, kernel size=kernel size, strides=strides, padding='same'
    x = Activation('relu')(x)
    x = Conv2D(filters, kernel_size=kernel_size, strides=(1, 1), padding='same')
    if strides != (1, 1) or shortcut.shape[-1] != filters:
        shortcut = Conv2D(filters, kernel_size=(1, 1), strides=strides, padding=
    x = Add()([shortcut, x])
    x = Activation('relu')(x)
    return x
def resnet15(input_shape, num_classes):
    """ResNet15 architecture"""
    input_tensor = Input(shape=input_shape)
    x = Conv2D(16, kernel_size=(3, 3), strides=(1, 1), padding='same')(input_ten
    x = Activation('relu')(x)
    x = MaxPooling2D(pool size=(2, 2), strides=(2, 2), padding='same')(x)
    for i in range(3):
        filters = 16 * (2 ** i)
        strides = (2, 2) if i != 0 else (1, 1)
        x = residual_block(x, filters=filters, strides=strides)
    x = Flatten()(x)
    x = Dense(256, activation='relu')(x)
    x = Dense(64, activation='relu')(x)
    x = Dense(num_classes, activation='sigmoid')(x)
    model = Model(inputs=input_tensor, outputs=x)
    return model
model_keras = resnet15((32,32,1), 1)
model_keras.summary()
```

Model: "model 2"

Layer (type)	Output Shape	Param #	Connected
input_3 (InputLayer)	[(None, 32, 32, 1	.)]	[]

conv2d_18 (Conv2D)	(None, 32, 32, 16)	160	['input_3[
activation_14 (Activation)	(None, 32, 32, 16)	0	['conv2d_1
<pre>max_pooling2d_2 (MaxPooling2D)</pre>	(None, 16, 16, 16)	0	['activati
conv2d_19 (Conv2D)	(None, 16, 16, 16)	2320	['max_pool
activation_15 (Activation)	(None, 16, 16, 16)	0	['conv2d_1
conv2d_20 (Conv2D)	(None, 16, 16, 16)	2320	['activati
add_6 (Add)	(None, 16, 16, 16)	0	['max_pool 'conv2d_2
activation_16 (Activation)	(None, 16, 16, 16)	0	['add_6[0]
conv2d_21 (Conv2D)	(None, 8, 8, 32)	4640	['activati
activation_17 (Activation)	(None, 8, 8, 32)	0	['conv2d_2
conv2d_23 (Conv2D)	(None, 8, 8, 32)	544	['activati
conv2d_22 (Conv2D)	(None, 8, 8, 32)	9248	['activati
add_7 (Add)	(None, 8, 8, 32)	0	['conv2d_2 'conv2d_2
activation_18 (Activation)	(None, 8, 8, 32)	0	['add_7[0]
conv2d_24 (Conv2D)	(None, 4, 4, 64)	18496	['activati
activation_19 (Activation)	(None, 4, 4, 64)	0	['conv2d_2
conv2d_26 (Conv2D)	(None, 4, 4, 64)	2112	['activati
conv2d_25 (Conv2D)	(None, 4, 4, 64)	36928	['activati
add_8 (Add)	(None, 4, 4, 64)	0	['conv2d_2 'conv2d_2
<pre>activation_20 (Activation)</pre>	(None, 4, 4, 64)	0	['add_8[0]
flatten_2 (Flatten)	(None, 1024)	0	['activati
dense_6 (Dense)	(None, 256)	262400	['flatten_
dense_7 (Dense)	(None, 64)	16448	['dense_6[
dense_8 (Dense)	(None, 1)	65	['dense_7[

Total params: 355,681

Adding a learning rate scheduler which makes the learning rate half after every 10 epochs.

```
def scheduler(epoch, lr):
    if epoch % 10 == 0 and epoch != 0:
        lr = lr / 2
    return lr

lr_schedule = LearningRateScheduler(scheduler)
```

▼ Training the Model

Set the optimiser and loss function. Evalutation metric is the ROC-AUC.

```
optimizer = tf.keras.optimizers.Adam(learning_rate = 5e-4)
model_keras.compile(loss='binary_crossentropy', optimizer=optimizer, metrics=[tf
# Chose the epochs and batch_size according to the paper
model keras.fit(X train, Y train, validation data = (X val, Y val), epochs=60, b
 Epoch 29/60
 Epoch 30/60
 Epoch 31/60
 Epoch 32/60
 Epoch 33/60
 Epoch 34/60
 Epoch 35/60
 Epoch 36/60
 Epoch 37/60
 Epoch 38/60
 Epoch 39/60
 Epoch 40/60
```

```
LPUCII +1/00
Epoch 42/60
Epoch 43/60
Epoch 44/60
Epoch 45/60
Epoch 46/60
Epoch 47/60
Epoch 48/60
Epoch 49/60
Epoch 50/60
Epoch 51/60
Epoch 52/60
Epoch 53/60
Epoch 54/60
Epoch 55/60
Epoch 56/60
Epoch 57/60
Fnoch 58/60
```

▼ Testing the Model

Calculating few metrics

```
accuracy_keras = accuracy_score(Y_test, Y_abs)
f1_keras = accuracy_score(Y_test, Y_abs)
fpr_keras, tpr_keras, thresholds_keras = roc_curve(Y_test, Y_probas)
auc_keras = auc(fpr_keras, tpr_keras)

print('RESULTS\n')

print(f'Testing Accuracy : {accuracy_keras:.3f}')
print(f'F1 score : {f1_keras:.3f}')
print(f'ROC-AUC : {auc_keras:.4f}')

RESULTS

Testing Accuracy : 0.737
F1 score : 0.737
ROC-AUC : 0.8078
```

▼ Model - PyTorch CNN

Creating Custom Dataset

```
class MyDataset(Dataset):

"""

Custom dataset for Image dataset
"""

def __init__(self, X, y):

   X = torch.from_numpy(X)
   X = X.unsqueeze(-1)
   self.X = X.permute(0, 3, 1, 2)
   self.y = torch.from_numpy(y).squeeze().long()

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

def __getitem__(self, idx):
   return self.X[idx], self.y[idx]
```

```
train_dataset = MyDataset(X_train, Y_train)
val_dataset = MyDataset(X_val, Y_val)
test_dataset = MyDataset(X_test, Y_test)
```

▼ Data Loaders

```
def get_data_loaders(train_dataset, val_dataset, test_dataset, batch_size=32):
    .....
    Function to create the DataLoaders for train-val-test data.
    Can specify batch size. Default value is set to 32.
    # Shuffle=True for training data to get diversity in batches at each trainin
    train_loader = DataLoader(train_dataset, batch_size=batch_size, shuffle=True
    val_loader = DataLoader(val_dataset, batch_size=batch_size, shuffle=False)
    test_loader = DataLoader(test_dataset, batch_size=batch_size, shuffle=False)
    return train loader, val loader, test loader
train_loader, val_loader, test_loader = get_data_loaders(train_dataset, val_data
Set Device
def get_device():
    return torch.device('cuda' if torch.cuda.is_available() else 'cpu')
device = get_device()
print(device)
    cuda
```

▼ Model Architecture

```
class ResidualBlock(nn.Module):
    """Residual block for ResNet"""

def __init__(self, in_channels, out_channels, stride=(1, 1), kernel_size=(3, super(ResidualBlock, self).__init__()
    self.shortcut = nn.Identity()
```

```
if stride != (1, 1) or in_channels != out_channels:
            self.shortcut = nn.Conv2d(in_channels, out_channels, kernel_size=(1,
        self.conv1 = nn.Conv2d(in_channels, out_channels, kernel_size=kernel_siz
        self.conv2 = nn.Conv2d(out channels, out channels, kernel size=kernel si
   def forward(self, x):
        shortcut = self.shortcut(x)
       x = F.relu(self.conv1(x))
       x = self_conv2(x)
       x += shortcut
       x = F.relu(x)
        return x
class ResNet15(nn.Module):
   """ResNet15 architecture"""
   def init (self, in channels = 1, num classes = 2):
        super(ResNet15, self).__init__()
        self.conv1 = nn.Conv2d(in_channels, 16, kernel_size=(3, 3), stride=(1, 1
        self.pool1 = nn.MaxPool2d(kernel_size=(2, 2), stride=(2, 2))
        self.layer1 = nn.Sequential(
            ResidualBlock(16, 16),
            ResidualBlock(16, 32, stride=(2, 2)),
            ResidualBlock(32, 64, stride=(2, 2))
        )
        self.fc1 = nn.Linear(64 * 4 * 4, 256)
        self.fc2 = nn.Linear(256, 64)
        self.fc3 = nn.Linear(64, num_classes)
   def forward(self, x):
        x = F.relu(self.conv1(x))
        x = self.pool1(x)
       x = self.layer1(x)
       x = x.view(x.size(0), -1)
        x = F.relu(self.fc1(x))
```

```
x = F.relu(self.fc2(x))
x = self.fc3(x)
return x
```

Setup -

- 1. Model Creation
- 2. Setting Adam optimizer with learning rate scheduler
- 3. Defining CrossEntropyLoss function

```
# Model
model_pytorch = ResNet15()
model_pytorch = model_pytorch.to(device)

# Optimizer and Learning Rate Scheduler

optimizer = optim.Adam(model_pytorch.parameters(), lr=5e-4)
scheduler = StepLR(optimizer, step_size=10, gamma=0.5)

# Loss Function

criterion = torch.nn.CrossEntropyLoss()
```

```
print(model_pytorch)
                      ResNet15(
                                 (conv1): Conv2d(1, 16, kernel_size=(3, 3), stride=(1, 1), padding=(1, 1),
                                 (pool1): MaxPool2d(kernel_size=(2, 2), stride=(2, 2), padding=0, dilation
                                 (layer1): Sequential(
                                           (0): ResidualBlock(
                                                    (shortcut): Identity()
                                                    (conv1): Conv2d(16, 16, kernel_size=(3, 3), stride=(1, 1), padding=(1, 1),
                                                    (conv2): Conv2d(16, 16, kernel_size=(3, 3), stride=(1, 1), padding=(1, 1),
                                           )
                                           (1): ResidualBlock(
                                                    (shortcut): Conv2d(16, 32, kernel_size=(1, 1), stride=(2, 2), bias=Fa
                                                    (conv1): Conv2d(16, 32, kernel_size=(3, 3), stride=(2, 2), padding=(1
                                                    (conv2): Conv2d(32, 32, kernel_size=(3, 3), stride=(1, 1), padding=(1, 2)
                                           (2): ResidualBlock(
                                                    (shortcut): Conv2d(32, 64, kernel_size=(1, 1), stride=(2, 2), bias=Fa
                                                    (conv1): Conv2d(32, 64, kernel_size=(3, 3), stride=(2, 2), padding=(1
                                                    (conv2): Conv2d(64, 64, kernel_size=(3, 3), stride=(1, 1), padding=(1
                                 )
                                 (fc1): Linear(in_features=1024, out_features=256, bias=True)
                                 (fc2): Linear(in_features=256, out_features=64, bias=True)
                                 (fc3): Linear(in_features=64, out_features=2, bias=True)
                       )
```

▼ Training

```
def train(model, device, loader, optimizer, criterion, scheduler):
    model.train()
    for data in tqdm(loader): # Iterate in batches over the training dataset.
        X, y = data
        X = X_{\bullet} to(device)
        y = y_{\bullet}to(device)
        out = model(X) # Perform a single forward pass.
        loss = criterion(out, y) # Compute the loss.
        loss.backward() # Derive gradients.
        optimizer.step() # Update parameters based on gradients.
        optimizer.zero_grad() # Clear gradients.
    scheduler.step()
    lr = optimizer.param_groups[0]['lr']
```

```
print(f"learning rate: {lr:.6f}")
    return model
def evaluate(model, device, loader):
    model.eval()
    y_{true} = []
    y_probas = []
    with torch.no_grad():
        for data in tqdm(loader):
            X, y = data
            X = X_{\bullet} to(device)
            y = y.to(device)
            out = model(X)
            y true += y.cpu().numpy().tolist()
            y_probas += out[:, 1].cpu().numpy().tolist() # probability of class
    # Calculating few metrics
        fpr, tpr, thresholds = roc_curve(y_true, y_probas)
        roc_auc = auc(fpr, tpr)
        print(f'Val AUC : {roc_auc:.3f}\n')
# Training Loop
epochs = 60
for epoch in range(epochs):
  print(f'Epoch : {epoch+1} \n')
  model_pytorch = train(model_pytorch, device, train_loader, optimizer, criterio
  evaluate(model_pytorch, device, val_loader)
    LPOCH : TO
    100%| 100%| 1107/1107 [00:10<00:00, 102.50it/s]
```

learning rate: 0.000250

100% | 139/139 [00:00<00:00, 204.26it/s]

Val AUC : 0.806

Epoch: 19

100%| 100%| 1107/1107 [00:10<00:00, 101.63it/s]

learning rate: 0.000250

100%| 139/139 [00:00<00:00, 205.32it/s]

Val AUC : 0.806

Epoch: 20

100%| 100%| 1107/1107 [00:10<00:00, 100.71it/s]

learning rate: 0.000125

100% | 139/139 [00:00<00:00, 206.76it/s]

Val AUC: 0.807

Epoch: 21

100% | 1107/1107 [00:10<00:00, 101.02it/s]

learning rate: 0.000125

100%| 139/139 [00:00<00:00, 207.26it/s]

Val AUC : 0.808

Epoch: 22

100% | 1107/1107 [00:10<00:00, 102.89it/s]

learning rate: 0.000125

100% | 139/139 [00:00<00:00, 154.47it/s]

Val AUC: 0.808

Epoch: 23

100%| 100%| 1107/1107 [00:10<00:00, 102.35it/s]

learning rate: 0.000125

100% | 139/139 [00:00<00:00, 204.28it/s]

Val AUC : 0.808

Epoch: 24

100%| 100.62it/s]

learning rate: 0.000125

100%| 139/139 [00:00<00:00, 205.96it/s]

Val AUC : 0.808

Epoch: 25

100% | 1107/1107 [00:11<00:00, 99.88it/s]

learning rate: 0.000125

100% | 139/139 [00:00<00:00, 200.85it/s]

Val AUC : 0.807

Epoch: 26

__----

```
100%| 1107/1107 [00:10<00:00, 101.02it/s] learning rate: 0.000125
```

▼ Testing

```
def test(model, device, loader):
    model.eval()
    y_{true} = []
    y_probas = []
    y_pred = []
    with torch.no_grad():
        for data in tqdm(loader):
            X, y = data
            X = X_{\bullet} to(device)
            y = y.to(device)
            out = model(X)
            y_true += y.cpu().numpy().tolist()
            y_pred += out.argmax(dim=1).cpu().numpy().tolist() # absoulte predi
            y_probas += out[:, 1].cpu().numpy().tolist() # probability of class
    # Calculating few metrics
    acc = accuracy_score(y_true, y_pred)
    f1 = f1 score(y true, y pred)
    fpr, tpr, thresholds = roc_curve(y_true, y_probas)
    roc_auc = auc(fpr, tpr)
    print('\nResults\n')
    print(f'Testing Accuracy {acc:.3f}')
    print(f'F1 score: {f1:.3f}')
    print(f'ROC-AUC: {roc_auc:.4f}\n')
    return acc, f1, fpr, tpr, roc_auc
```

acc_pytorch, f1_pytorch, fpr_pytorch, tpr_pytorch, auc_pytorch = test(model_pyto

100%| 139/139 [00:00<00:00, 200.01it/s]

Results

Testing Accuracy 0.736

F1 score: 0.738 ROC-AUC: 0.8058

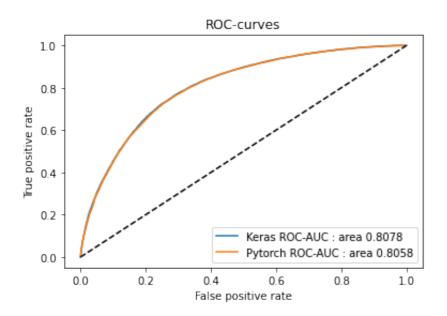
▼ Results

▼ 1. Plots

```
plt.plot(fpr_keras, tpr_keras, label=f'Keras ROC-AUC : area {auc_keras:.4f}')
plt.plot(fpr_pytorch, tpr_pytorch, label=f'Pytorch ROC-AUC : area {auc_pytorch:.

plt.plot([0, 1], [0, 1], 'k--')
plt.xlabel('False positive rate')
plt.ylabel('True positive rate')
plt.title('ROC-curves')

plt.legend()
plt.savefig('roc-auc.png')
plt.show()
```



▼ 2. Metrics

Keras Implementation

```
print(f'Testing Accuracy {accuracy_keras:.3f}')
print(f'F1 score: {f1_keras:.3f}')
print(f'ROC-AUC: {auc_keras:.4f}')

Testing Accuracy 0.737
  F1 score: 0.737
  ROC-AUC: 0.8078
```

Pytorch Implementation

```
print(f'Testing Accuracy {acc_pytorch:.3f}')
print(f'F1 score: {f1_pytorch:.3f}')
print(f'ROC-AUC: {auc_pytorch:.4f}')
```

Testing Accuracy 0.736

F1 score: 0.738 ROC-AUC: 0.8058

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