ltck7jivp

April 5, 2024

[1]:
```
!pip -q install torch-geometric -f https://data.pyg.org/whl/torch-1.11.0+cu113.
↪html
import numpy as np
import pandas as pd
import torch
import matplotlib.pyplot as plt
import torch.nn as nn
from torch.utils.data import Dataset,DataLoader
import time
import h5py
from sklearn.model_selection import train_test_split
import torch.nn.functional as F
from tqdm import tqdm
from sklearn.metrics import roc_auc_score
import gc
from torch.optim import AdamW
import torch.optim as optim
import torchvision
from sklearn.feature_extraction.image import grid_to_graph
import pytorch_lightning as pl
import os
```

[ ]:
```
```

[3]:
```
import warnings
warnings.filterwarnings('ignore')
```

[4]:
```
class CFG:
    train_batch_size=32
    val_batch_size=64
    k_neighbours=10
    n_epochs = 40
    train_size = 16000
    val_size = 2000
    test_size = 2000
    c_out = 2
    lr = 5e-4
```

[5]:
```
%%time
f = h5py.File('/kaggle/input/quark-gluon-dataset/dataset.hdf5')
X = np.array(f['/X_jets'][:20000])
labels = np.array(f['/y'][:20000])
sz = len(X)
```

```
CPU times: user 8.67 s, sys: 4.93 s, total: 13.6 s
Wall time: 14.4 s
```

[ ]:
```
```

1 Construction of graph

[6]:
```
from sklearn.neighbors import kneighbors_graph
from sklearn.model_selection import train_test_split
from torch_geometric.data import Data, Batch
from torch_geometric.loader import DataLoader
from torch_geometric.nn import SAGEConv
from torch_geometric.nn import global_mean_pool
```

[8]:
```
data = X.reshape((-1,X.shape[1]*X.shape[2],3))
non_zero_mask = np.any(data!=[0.0,0.0,0.0],axis=-1)
node_list = []
start_time = time.time()
for i,x in tqdm(enumerate(data)):
    node_list.append(x[non_zero_mask[i]])
print(time.time()-start_time)
start_time = time.time()
dataset = []
for i,nodes in tqdm(enumerate(node_list)):
    edges = kneighbors_graph(nodes,CFG.
 ↪k_neighbours,mode='connectivity',include_self=True)
    c = edges.tocoo()
    edge_list = torch.from_numpy(np.vstack((c.row,c.col))).type(torch.long)
    edge_weight = torch.from_numpy(c.data.reshape(-1,1))
    y = torch.tensor([int(labels[i])],dtype=torch.long)
    data = Data(x=torch.from_numpy(nodes), edge_index=edge_list,␣
 ↪edge_attr=edge_weight, y=y)
    dataset.append(data)
print(time.time()-start_time)
train_loader = DataLoader(dataset[:16000], batch_size=CFG.train_batch_size,␣
 ↪shuffle=True,num_workers=2)
test_loader = DataLoader(dataset[16000:18000], batch_size=32,␣
 ↪shuffle=False,num_workers=2)
val_loader = DataLoader(dataset[18000:], batch_size=CFG.val_batch_size,␣
 ↪shuffle=False,num_workers=2)
```

```
20000it [00:01, 16615.42it/s]
1.2061340808868408
20000it [01:09, 286.29it/s]
69.91259169578552
```

[ ]:

[9]:
```
data = dataset[0]
print(f'Number of nodes: {data.num_nodes}')
print(f'Number of edges: {data.num_edges}')
print(f'Number of node features: {data.num_node_features}')
print(f'Number of edges features: {data.num_edge_features}')

print(dataset[0])
```

```
Number of nodes: 884
Number of edges: 8840
Number of node features: 3
Number of edges features: 1
Data(x=[884, 3], edge_index=[2, 8840], edge_attr=[8840, 1], y=[1])
```

[ ]:

[10]:
```
del X
del labels
gc.collect()
```

[10]: 1053

2 Model

[11]:
```
import torch.utils.data as data
class GraphSAGE(nn.Module):
    def __init__(self,c_in,c_hidden_conv,c_hidden_lin,c_out,dp_rate_linear=0.3):
        super(GraphSAGE,self).__init__()
        self.conv = nn.ModuleDict()
        self.len_conv = len(c_hidden_conv)+1
        self.len_lin = len(c_hidden_lin)
        self.conv[str(0)] = SAGEConv(c_in,c_hidden_conv[0])

        self.bn  =  nn.ModuleDict()
        self.bn[str(0)] = nn.BatchNorm1d(c_hidden_conv[0])
        for k in range(1,len(c_hidden_conv)):
            self.conv[str(k)] = SAGEConv(c_hidden_conv[k-1],c_hidden_conv[k])
```

```
            self.bn[str(k)] = nn.BatchNorm1d(c_hidden_conv[k])
        self.conv[str(len(c_hidden_conv))] =␣
↪SAGEConv(c_hidden_conv[-1],c_hidden_lin[0])
        self.bn[str(len(c_hidden_conv))] = nn.BatchNorm1d(c_hidden_lin[0])
        self.lin = nn.ModuleDict()
        for k in range(1,len(c_hidden_lin)):
            self.lin[str(k)] = nn.Linear(c_hidden_lin[k-1],c_hidden_lin[k])
        self.out = nn.Linear(c_hidden_lin[-1],c_out)
        self.dp_rate_linear = dp_rate_linear
    def forward(self,x,edge_index,batch):
        for i in range(self.len_conv):
            x = self.conv[str(i)](x,edge_index)
            x =self.bn[str(i)](x)
            x = x.relu()
        x = global_mean_pool(x,batch)
        for i in range(1,self.len_lin):
            x = self.lin[str(i)](x)
            x = x.relu()
        x = self.out(x)
        return x
```

[12]:

```
"""model = GraphSAGE(c_in=3, c_hidden_conv=[32,64,128],c_hidden_lin␣
↪=[1024,512,256] ,c_out=2)
optimizer = optim.AdamW(model.parameters(), lr=1e-3, weight_decay=0) # High lr␣
↪because of small dataset and small model
device = torch.device('cuda' if torch.cuda.is_available() else 'cpu')
loss_module = nn.BCEWithLogitsLoss() if CFG.c_out == 1 else nn.
↪CrossEntropyLoss()
logs = {'training_loss':[],'training_accuracy':[],\
        'validation_loss':[],'validation_accuracy':[],\
        'batch_wise_trainloss':[],'batch_wise_val_loss':[]}
model.to(device)
for epoch in range(2):#range(CFG.n_epochs):
    #Training Loop
    ep_acc = 0
    for data in tqdm(iter(train_loader)):
        optimizer.zero_grad()
        data.to(device)
        x, edge_index, batch_idx = data.x, data.edge_index, data.batch
        ##Forward Pass
        x = model(x,edge_index,batch_idx)
        x = x.squeeze(dim=-1)

        if CFG.c_out == 1:
            preds = (x > 0).float()
            data.y = data.y.float()
        else:
```

```
            preds = x.argmax(dim=-1)
        loss = loss_module(x, data.y)
        ep_acc += (preds == data.y).sum().float().detach().cpu()# / preds.
↪shape[0]

        ##Backprop
        loss.backward()
        optimizer.step()

        ###Logging
        logs['training_loss'].append(loss.detach().cpu().item())
        data=data.cpu()
        del data
        gc.collect()
    logs['training_accuracy'].append((ep_acc/CFG.train_size))
    ##Validation Loop
    ep_acc = 0
    model.eval()
    for data in tqdm(iter(val_loader)):
        optimizer.zero_grad()
        data.to(device)
        x, edge_index, batch_idx = data.x, data.edge_index, data.batch
        ##Forward Pass
        with torch.no_grad():
            x = model(x,edge_index,batch_idx)
            x = x.squeeze(dim=-1)

            if CFG.c_out == 1:
                preds = (x > 0).float()
                data.y = data.y.float()
            else:
                preds = x.argmax(dim=-1)
            loss = loss_module(x, data.y)
            ep_acc += (preds == data.y).sum().float().cpu()# / preds.shape[0]
        ###Logging
        logs['validation_loss'].append(loss.detach().cpu().item())
        data=data.cpu()
        del data
        gc.collect()
    logs['validation_accuracy'].append((ep_acc/CFG.val_size))
    print(f"Training Accuracy:{logs['training_accuracy'][-1]} Validation␣
↪Accuracy:{logs['validation_accuracy'][-1]}")"""
"""Taking too much time, shifted to pytorch lightning"""
```

[12]: 'Taking too much time, shifted to pytorch lightning'

[13]:
```
#plt.plot(logs['training_loss'],color='r',label='Training loss')
#plt.show()
```

[14]:
```
#plt.plot(logs['validation_loss'],color='g',label='Validation loss')
```

[15]:
```
#plt.plot(logs['validation_accuracy'],c='g',label='Validation Accuracy')
#plt.plot(logs['training_accuracy'],c='r',label='Training Accuracy')
#plt.legend()
#plt.show()
```

[16]:
```
class GraphLevelGNN(pl.LightningModule):
    def __init__(self, **model_kwargs):
        super(GraphLevelGNN,self).__init__()
        # Saving hyperparameters
        self.save_hyperparameters()
        self.model = GraphSAGE(**model_kwargs)
        self.loss_module = nn.BCEWithLogitsLoss() if self.hparams.c_out == 1␣
 ↪else nn.CrossEntropyLoss()

    def forward(self, data, mode="train"):
        x, edge_index, batch_idx = data.x, data.edge_index, data.batch
        # print(data.x.shape, data.edge_index.shape, data.batch.shape)
        device = torch.device('cuda' if torch.cuda.is_available() else 'cpu')
        data.to(device=device)
        self.model.to(device=device)
        x = self.model(x, edge_index, batch_idx)
        x = x.squeeze(dim=-1)

        if self.hparams.c_out == 1:
            preds = (x > 0).float()
            data.y = data.y.float()
        else:
            preds = x.argmax(dim=-1)

        loss = self.loss_module(x, data.y)
        acc = (preds == data.y).sum().float() / preds.shape[0]

        return loss, acc

    def configure_optimizers(self):
        optimizer = optim.AdamW(self.parameters(), lr=CFG.lr, weight_decay=0) #␣
 ↪High lr because of small dataset and small model
        return optimizer

    def training_step(self, batch, batch_idx):
        loss, acc = self.forward(batch, mode="train")
        self.log('train_loss', loss, prog_bar=True,logger=True)
```

```
        self.log('train_acc', acc, prog_bar=True,logger=True)

        return loss

    def validation_step(self, batch, batch_idx):
        loss, acc = self.forward(batch, mode="val")
        self.log('val_loss', loss, on_epoch=True, prog_bar=False,logger=True)
        self.log('val_acc', acc, on_epoch=True, prog_bar=False,logger=True)

    def test_step(self, batch, batch_idx):
        loss, acc = self.forward(batch, mode="test")
        self.log('test_loss', loss, on_epoch=True, prog_bar=False)
        self.log('test_acc', acc, on_epoch=True, prog_bar=False)

def train_graph_classifier(model_name,logger, **model_kwargs):
    pl.seed_everything(17)

    trainer = pl.Trainer(accelerator='auto',
                         max_epochs=CFG.n_epochs,logger=logger)

    # Check whether pretrained model exists. If yes, load it and skip training
    model = GraphLevelGNN(**model_kwargs)
    device = torch.device('cuda' if torch.cuda.is_available() else 'cpu')
    model.to(device)

    trainer.fit(model, train_loader, val_loader)
    model = GraphLevelGNN.load_from_checkpoint(trainer.checkpoint_callback.
 ↪best_model_path)
    model.to(device)
    # Test best model on validation and test set
    # train_result = trainer.test(model, dataloaders=train_loader,␣
 ↪verbose=False)
    val_result = trainer.test(model, dataloaders=val_loader, verbose=False)
    test_result = trainer.test(model, dataloaders=test_loader, verbose=False)
    result = {"test": test_result[0]['test_acc'], "valid":␣
 ↪val_result[0]['test_acc']}
    return trainer, model, result
```

[17]:
```
import os
device = torch.device('cuda' if torch.cuda.is_available() else 'cpu')
logger = pl.loggers.CSVLogger(save_dir='logs/', name='GraphSAGE')
trainer, model, result =␣
 ↪train_graph_classifier(model_name="GraphSAGE",logger=logger,c_in=3,␣
 ↪c_hidden_conv=[32,64,128],c_hidden_lin =[1024,512,256] ,c_out=2)
```

```
Sanity Checking: |          | 0/? [00:00<?, ?it/s]

Training: |          | 0/? [00:00<?, ?it/s]
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```

```
Validation: |          | 0/? [00:00<?, ?it/s]
Validation: |          | 0/? [00:00<?, ?it/s]
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Validation: |          | 0/? [00:00<?, ?it/s]
Testing: |          | 0/? [00:00<?, ?it/s]
Testing: |          | 0/? [00:00<?, ?it/s]
```
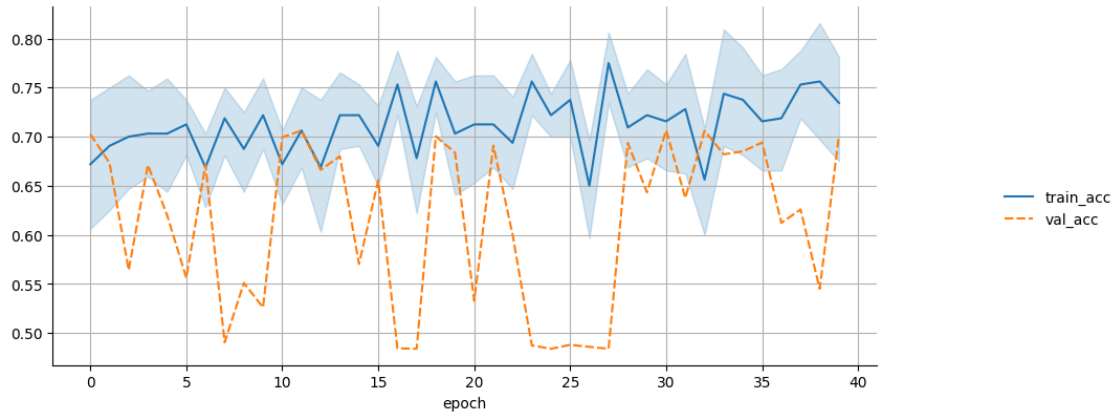
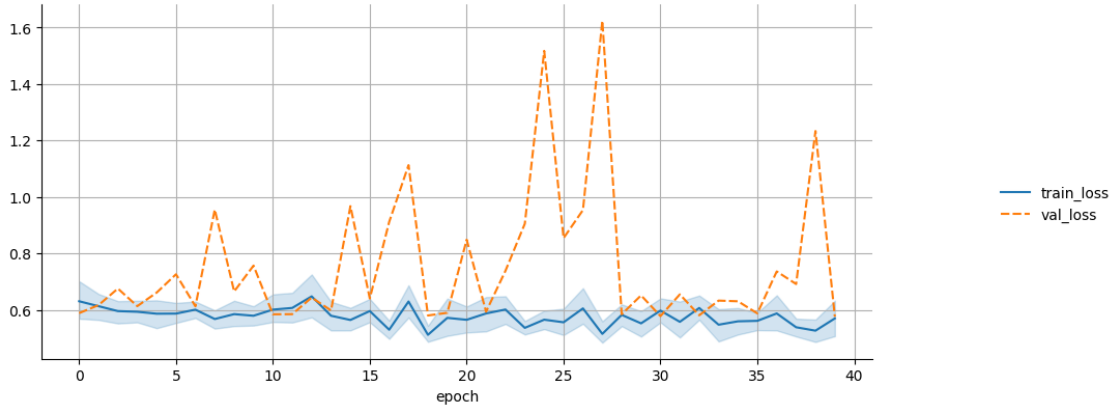

[18]:
```python
import seaborn as sn

metrics = pd.read_csv(f'{trainer.logger.log_dir}/metrics.csv')
del metrics["step"]
del metrics['test_loss']
del metrics['test_acc']
del metrics['train_loss']
del metrics['val_loss']
metrics.set_index("epoch", inplace=True)
# display(metrics.dropna(axis=1, how="all").head())
g = sn.relplot(data=metrics, kind="line")
plt.gcf().set_size_inches(12, 4)
# plt.gca().set_yscale('log')
plt.grid()
```



[19]:
```python
metrics = pd.read_csv(f'{trainer.logger.log_dir}/metrics.csv')
del metrics["step"]
```

```
del metrics['test_loss']
del metrics['test_acc']
del metrics['train_acc']
del metrics['val_acc']
metrics.set_index("epoch", inplace=True)
# display(metrics.dropna(axis=1, how="all").head())
g = sn.relplot(data=metrics, kind="line")
plt.gcf().set_size_inches(12, 4)
# plt.gca().set_yscale('log')
plt.grid()
```



3 Discussion

I have used K-nearest neighbours to construct the graph from the point cloud
I have used stack of GraphSAGEconv layers and the graphs above show the result
Learning rate, preprocessing can be explored more to improve the training
Different architectures like GAT can be explored and ablation studies can further help determine the depth and other choices of the architecture