linear_probing_with_pretraining

April 5, 2024

[ ]:
```
!pip install einops
```

[3]:
```
import os
import gc
import torch
import torch.nn as nn
import torch.nn.functional as F
import pandas as pd
import numpy as np
import h5py
import copy
import matplotlib.pyplot as plt
from torch.utils.data import Dataset, DataLoader, TensorDataset,␣
  ↪SubsetRandomSampler, ConcatDataset
from torchvision import transforms, utils, datasets
from torchmetrics import Accuracy
from sklearn.model_selection import KFold, StratifiedKFold, train_test_split
from torchvision.datasets import ImageFolder
from PIL import Image
import cv2
import pyarrow.parquet as pq
import seaborn as sns
from tqdm import tqdm
from statistics import mean
from sklearn.metrics import accuracy_score, roc_auc_score
from sklearn.preprocessing import StandardScaler
import csv
import torchvision
import ctypes
import torch.optim as optim
from torch.optim import Adam
from functools import partial
from einops import repeat, rearrange
from einops.layers.torch import Rearrange
from timm.models.vision_transformer import PatchEmbed, Block
from torch.optim import AdamW
```

```
from torch.optim.lr_scheduler import CosineAnnealingWarmRestarts,␣
 ↪CosineAnnealingLR, StepLR, ReduceLROnPlateau
from torch.cuda.amp import autocast, GradScaler
from transformers import AutoModel, AutoTokenizer
from torch.utils.data.sampler import BatchSampler, Sampler
from skimage import io, transform
from torch.nn.utils import clip_grad_norm_


torch.manual_seed(42)
np.random.seed(42)
torch.cuda.manual_seed(42)

import warnings
warnings.filterwarnings("ignore")
```

[3]:

```
<torch._C.Generator at 0x7b066d371550>
```

[4]:

```
with h5py.File('/kaggle/input/autoencoders-labelled/Dataset_Specific_labelled.
 ↪h5', 'r') as file:

    print("Groups in the HDF5 file:")
    for group in file:
        print(group)

    dataset = file['jet']
    print("Dataset shape:", dataset.shape)
    print("Dataset dtype:", dataset.dtype)

    dataset = file['Y']
    print("Dataset shape:", dataset.shape)
    print("Dataset dtype:", dataset.dtype)

    print("Dataset attributes:")
    for attr_name, attr_value in dataset.attrs.items():
        print(f"{attr_name}: {attr_value}")

    X = np.array(file['jet'][:])
    Y = np.array(file['Y'][:])
```

```
Groups in the HDF5 file:

Y

jet

Dataset shape: (10000, 125, 125, 8)
```

```
Dataset dtype: float32

Dataset shape: (10000, 1)

Dataset dtype: float32

Dataset attributes:
```

[5]:
```
X.shape
```

[5]:
```
(10000, 125, 125, 8)
```

[6]:
```
def get_2d_sincos_pos_embed(embed_dim, grid_size, cls_token=False):

    grid_h = np.arange(grid_size, dtype=np.float32)
    grid_w = np.arange(grid_size, dtype=np.float32)
    grid = np.meshgrid(grid_w, grid_h)  # here w goes first
    grid = np.stack(grid, axis=0)

    grid = grid.reshape([2, 1, grid_size, grid_size])
    pos_embed = get_2d_sincos_pos_embed_from_grid(embed_dim, grid)
    if cls_token:
        pos_embed = np.concatenate([np.zeros([1, embed_dim]), pos_embed],␣
↪axis=0)
    return pos_embed


def get_2d_sincos_pos_embed_from_grid(embed_dim, grid):
    assert embed_dim % 2 == 0

    emb_h = get_1d_sincos_pos_embed_from_grid(embed_dim // 2, grid[0])  # (H*W,␣
↪D/2)
    emb_w = get_1d_sincos_pos_embed_from_grid(embed_dim // 2, grid[1])  # (H*W,␣
↪D/2)

    emb = np.concatenate([emb_h, emb_w], axis=1) # (H*W, D)
    return emb


def get_1d_sincos_pos_embed_from_grid(embed_dim, pos):

    assert embed_dim % 2 == 0
    omega = np.arange(embed_dim // 2, dtype='float32')
    omega /= embed_dim / 2.
    omega = 1. / 10000**omega  # (D/2,)

    pos = pos.reshape(-1)  # (M,)
```

```
    out = np.einsum('m,d->md', pos, omega)  # (M, D/2), outer product

    emb_sin = np.sin(out) # (M, D/2)
    emb_cos = np.cos(out) # (M, D/2)

    emb = np.concatenate([emb_sin, emb_cos], axis=1)  # (M, D)
    return emb
```

[ ]:
```
class Encoder(nn.Module):
    def __init__(self, img_size=224, patch_size=16, in_chans=8,
                 embed_dim=1024, depth=24, num_heads=16,
                 decoder_embed_dim=512, decoder_depth=8, decoder_num_heads=16,
                 mlp_ratio=4., norm_layer=nn.LayerNorm, norm_pix_loss=False):
        super().__init__()

        self.mask_ratio = 0.75
        self.patch_embed = PatchEmbed(img_size, patch_size, in_chans, embed_dim)
        num_patches = self.patch_embed.num_patches
        self.cls_token = nn.Parameter(torch.zeros(1, 1, embed_dim))
        self.pos_embed = nn.Parameter(torch.zeros(1, num_patches + 1,␣
↪embed_dim), requires_grad=False)  # fixed sin-cos embedding
        self.blocks = nn.ModuleList([
            Block(embed_dim, num_heads, mlp_ratio, qkv_bias=True,␣
↪norm_layer=norm_layer)
            for i in range(depth)])
        self.norm = norm_layer(embed_dim)
        self.initialize_weights()

    def initialize_weights(self):
        pos_embed = get_2d_sincos_pos_embed(self.pos_embed.shape[-1], int(self.
↪patch_embed.num_patches**.5), cls_token=True)
        self.pos_embed.data.copy_(torch.from_numpy(pos_embed).float().
↪unsqueeze(0))
        w = self.patch_embed.proj.weight.data
        torch.nn.init.xavier_uniform_(w.view([w.shape[0], -1]))
        torch.nn.init.normal_(self.cls_token, std=.02)
        self.apply(self._init_weights)

    def _init_weights(self, m):
        if isinstance(m, nn.Linear):
            torch.nn.init.xavier_uniform_(m.weight)
            if isinstance(m, nn.Linear) and m.bias is not None:
                nn.init.constant_(m.bias, 0)
        elif isinstance(m, nn.LayerNorm):
            nn.init.constant_(m.bias, 0)
            nn.init.constant_(m.weight, 1.0)
```

```
    def patchify(self, imgs):
        p = self.patch_embed.patch_size[0]
        assert imgs.shape[2] == imgs.shape[3] and imgs.shape[2] % p == 0
        h = w = imgs.shape[2] // p
        x = imgs.reshape(shape=(imgs.shape[0], 8, h, p, w, p))
        x = torch.einsum('nchpwq->nhwpqc', x)
        x = x.reshape(shape=(imgs.shape[0], h * w, p**2 * 8))
        return x

    def unpatchify(self, x):
        p = self.patch_embed.patch_size[0]
        h = w = int(x.shape[1]**.5)
        assert h * w == x.shape[1]
        x = x.reshape(shape=(x.shape[0], h, w, p, p, 8))
        x = torch.einsum('nhwpqc->nchpwq', x)
        imgs = x.reshape(shape=(x.shape[0], 8, h * p, h * p))
        return imgs

    def random_masking(self, x, mask_ratio):
        N, L, D = x.shape  # batch, length, dim
        len_keep = int(L * (1 - mask_ratio))
        noise = torch.rand(N, L, device=x.device)
        ids_shuffle = torch.argsort(noise, dim=1)  # ascend: small is keep,
↪large is remove
        ids_restore = torch.argsort(ids_shuffle, dim=1)
        ids_keep = ids_shuffle[:, :len_keep]
        x_masked = torch.gather(x, dim=1, index=ids_keep.unsqueeze(-1).
↪repeat(1, 1, D))
        mask = torch.ones([N, L], device=x.device)
        mask[:, :len_keep] = 0
        mask = torch.gather(mask, dim=1, index=ids_restore)
        return x_masked, mask, ids_restore

    def forward(self, x):
        imgs = self.patchify(x)
        x = self.patch_embed(x)
        x = x + self.pos_embed[:, 1:, :]
        x, mask, ids_restore = self.random_masking(x, self.mask_ratio)
        cls_token = self.cls_token + self.pos_embed[:, :1, :]
        cls_tokens = cls_token.expand(x.shape[0], -1, -1)
        x = torch.cat((cls_tokens, x), dim=1)
        for blk in self.blocks:
            x = blk(x)
        x = self.norm(x)
        return x, mask, ids_restore, imgs

class Decoder(nn.Module):
```

```python
    def __init__(self, img_size=224, patch_size=16, in_chans=8,
                 embed_dim=1024, depth=24, num_heads=16,
                 decoder_embed_dim=512, decoder_depth=8, decoder_num_heads=16,
                 mlp_ratio=4., norm_layer=nn.LayerNorm, norm_pix_loss=False):
        super().__init__()

        self.num_patches = (img_size//patch_size)**2
        self.decoder_embed = nn.Linear(embed_dim, decoder_embed_dim, bias=True)
        self.mask_token = nn.Parameter(torch.zeros(1, 1, decoder_embed_dim))
        self.decoder_pos_embed = nn.Parameter(torch.zeros(1, self.num_patches + 1, decoder_embed_dim), requires_grad=False)  # fixed sin-cos embedding
        self.decoder_blocks = nn.ModuleList([
            Block(decoder_embed_dim, decoder_num_heads, mlp_ratio, qkv_bias=True, norm_layer=norm_layer)
            for i in range(decoder_depth)])

        self.decoder_norm = norm_layer(decoder_embed_dim)
        self.decoder_pred = nn.Linear(decoder_embed_dim, patch_size**2 * in_chans, bias=True)
        self.norm_pix_loss = norm_pix_loss

        self.initialize_weights()

    def initialize_weights(self):
        decoder_pos_embed = get_2d_sincos_pos_embed(self.decoder_pos_embed.shape[-1], int(self.num_patches**.5), cls_token=True)
        self.decoder_pos_embed.data.copy_(torch.from_numpy(decoder_pos_embed).float().unsqueeze(0))
        torch.nn.init.normal_(self.mask_token, std=.02)
        self.apply(self._init_weights)

    def _init_weights(self, m):
        if isinstance(m, nn.Linear):
            torch.nn.init.xavier_uniform_(m.weight)
            if isinstance(m, nn.Linear) and m.bias is not None:
                nn.init.constant_(m.bias, 0)
        elif isinstance(m, nn.LayerNorm):
            nn.init.constant_(m.bias, 0)
            nn.init.constant_(m.weight, 1.0)

    def patchify(self, imgs):
        p = self.patch_embed.patch_size[0]
        assert imgs.shape[2] == imgs.shape[3] and imgs.shape[2] % p == 0

        h = w = imgs.shape[2] // p
        x = imgs.reshape(shape=(imgs.shape[0], 8, h, p, w, p))
        x = torch.einsum('nchpwq->nhwpqc', x)
```

```python
        x = x.reshape(shape=(imgs.shape[0], h * w, p**2 * 8))
        return x

    def unpatchify(self, x):
        p = self.patch_embed.patch_size[0]
        h = w = int(x.shape[1]**.5)
        assert h * w == x.shape[1]
        x = x.reshape(shape=(x.shape[0], h, w, p, p, 8))
        x = torch.einsum('nhwpqc->nchpwq', x)
        imgs = x.reshape(shape=(x.shape[0], 8, h * p, h * p))
        return imgs

    def forward(self, x, ids_restore):
        x = self.decoder_embed(x)
        mask_tokens = self.mask_token.repeat(x.shape[0], ids_restore.shape[1] + 1 - x.shape[1], 1)
        x_ = torch.cat([x[:, 1:, :], mask_tokens], dim=1)  # no cls token
        x_ = torch.gather(x_, dim=1, index=ids_restore.unsqueeze(-1).repeat(1, 1, x.shape[2]))  # unshuffle
        x = torch.cat([x[:, :1, :], x_], dim=1)
        x = x + self.decoder_pos_embed
        for blk in self.decoder_blocks:
            x = blk(x)
        x = self.decoder_norm(x)
        x = self.decoder_pred(x)
        x = x[:, 1:, :]
        return x

class Masked_VIT(nn.Module):
    def __init__(self, encoder, decoder, mask_ratio):
        super().__init__()

        self.encoder = encoder
        self.decoder = decoder
        self.mask_ratio = mask_ratio

    def forward(self, x):
        x, mask, ids_restore, imgs = self.encoder(x)
        pred = self.decoder(x, ids_restore)

        return imgs, pred, mask

def mae_vit_base_patch16_dec512d8b(img_size=125, mask_ratio = 0.75, **kwargs):
    encoder = Encoder(
        img_size=img_size, patch_size=5, embed_dim=768, depth=8, num_heads=12,
        decoder_embed_dim=512, decoder_depth=4, decoder_num_heads=16,
        mlp_ratio=4, norm_layer=partial(nn.LayerNorm, eps=1e-6), **kwargs)
```

```
    decoder = Decoder(
        img_size=img_size, patch_size=5, embed_dim=768, depth=8, num_heads=12,
        decoder_embed_dim=512, decoder_depth=4, decoder_num_heads=16,
        mlp_ratio=4, norm_layer=partial(nn.LayerNorm, eps=1e-6), **kwargs)

    model = Masked_VIT(encoder, decoder, mask_ratio)

    return model

model = mae_vit_base_patch16_dec512d8b(img_size=125, mask_ratio = 0.75)
model = torch.load('/kaggle/input/pretrained-weights-autoencoder/model.pth')
```

[10]:

```
class VIT_classifier(nn.Module):
    def __init__(self, encoder, num_classes):
        super().__init__()
        self.encoder = encoder
        self.patch_embed = encoder.patch_embed
        self.cls_token = encoder.cls_token
        self.pos_embed = encoder.pos_embed
        self.patchify = encoder.patchify
        self.transformer = encoder.blocks
        self.layer_norm = encoder.norm
        self.head = torch.nn.Linear(self.pos_embed.shape[-1], num_classes)
        self.blocks = encoder.blocks

        self.avg_pool = nn.AdaptiveAvgPool1d((1))
        self.flatten = nn.Flatten()
        self.fc = nn.Linear(in_features=625, out_features=64)
        self.fc_1 = nn.Linear(in_features=64, out_features=1)
        self.sigmoid = nn.Sigmoid()

    def forward(self, x):

        x = self.patch_embed(x)
        x = x + self.pos_embed[:, 1:, :]
        cls_token = self.cls_token + self.pos_embed[:, :1, :]
        cls_tokens = cls_token.expand(x.shape[0], -1, -1)
        x = torch.cat((cls_tokens, x), dim=1)
        for blk in self.blocks:
            x = blk(x)
        x = self.layer_norm(x)
        x = x[:,1:,:]
        x = self.avg_pool(x)
        x = self.flatten(x)
        x = self.fc(x)
        x = self.fc_1(x)
```

```
        x = self.sigmoid(x)

        return x

encoder = model.encoder
classifier = VIT_classifier(encoder, 2)
```

[13]:
```
for _z in range(8):
    X[:,:,:,_z] = (X[:,:,:,_z] - X[:,:,:,_z].mean()) / (X[:,:,:,_z].std())
```

[14]:
```
class Custom_Dataset(Dataset):
    def __init__(self, x, y, transform):
        self.x = x
        self.y = y
        self.transform = transform

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

    def __getitem__(self,idx):
        if torch.is_tensor(idx):
            idx = idx.tolist()
        img_1 = self.x[idx]
        label = self.y[idx]

        if self.transform:
            img_1 = self.transform(img_1)
        sample = {'img' : img_1, 'label' : label}
        return sample

transform = torchvision.transforms.Compose([torchvision.transforms.ToTensor()])

dataset = Custom_Dataset(X, Y, transform = transform)
sample = dataset.__getitem__(0)
print((sample['img']).shape)
print(sample['label'].shape)
```

```
torch.Size([8, 125, 125])

(1,)
```

[15]:
```
device = torch.device("cuda:0" if torch.cuda.is_available() else "cpu")
```

[16]:
```
def model_train(fold, model, epochs, train_dataloader, test_dataloader):

    criterion = nn.BCELoss()
    optimizer = optim.AdamW(model.parameters(), lr=1.5e-5)
```

```python
best_acc = -np.inf
best_weights = None
accuracy = Accuracy(task = 'binary').to(device)

train_losses = []
val_losses = []
train_accuracies = []
val_accuracies = []

for epoch in range(epochs):
    train_pred = []
    val_pred = []

    model.train()
    for batch in tqdm(train_dataloader):
        images, labels = batch['img'], batch['label']
        images = images.to(device)
        labels = labels.to(device)

        optimizer.zero_grad()
        outputs = model(images)
        loss = criterion(outputs, labels)
        loss.backward()
        optimizer.step()

        train_pred.append(loss.item())

        # Calculate training accuracy
        train_acc = accuracy(outputs, labels)
        train_accuracies.append(train_acc.item())

    train_loss = np.mean(train_pred)
    model.eval()
    with torch.no_grad():
        for val_batch in tqdm(test_dataloader):
            val_images, val_labels = val_batch['img'], val_batch['label']
            val_images = val_images.to(device)
            val_labels = val_labels.to(device)

            val_outputs = model(val_images)
            val_loss = criterion(val_outputs, val_labels)
            val_pred.append(val_loss.item())

            val_acc = accuracy(val_outputs, val_labels)
            val_accuracies.append(val_acc.item())

    val_loss = np.mean(val_pred)
```

```
        print(f'Epoch {epoch+1}/{epochs}, Train Loss: {train_loss:.4f}, Train␣
↪Accuracy: {np.mean(train_accuracies):.4f}, Valid Loss: {val_loss:.4f}, Valid␣
↪Accuracy: {np.mean(val_accuracies):.4f}')
        train_losses.append(train_loss)
        val_losses.append(val_loss)

        # Save best model
        if max(train_accuracies) > best_acc:
            best_acc = max(train_accuracies)
            best_weights = copy.deepcopy(model.state_dict())

    # Save the best model
    torch.save(best_weights, f'./best_model_{fold}.pth')

    return train_losses, val_losses, train_accuracies, val_accuracies
```

[17]:
```
del classifier
gc.collect()
torch.cuda.empty_cache()
```

[19]:
```
train_size = int(0.8 * len(dataset))
val_size = len(dataset) - train_size
train_dataset, val_dataset = torch.utils.data.random_split(dataset,␣
 ↪[train_size, val_size])
training_loss = []
validation_loss = []
train_dataloader = DataLoader(train_dataset, batch_size=64, shuffle=True)
val_dataloader = DataLoader(val_dataset, batch_size=64, shuffle=False)
classifier = VIT_classifier(model.encoder, 2)
NUM_GPU = torch.cuda.device_count()
if NUM_GPU > 1:
    classifier = nn.DataParallel(classifier)
classifier = classifier.to(device)
train_losses, val_losses, train_accuracies, val_accuracies =␣
 ↪model_train(1,classifier, 8, train_dataloader, val_dataloader)
```

```
100%|      | 125/125 [05:24<00:00,  2.59s/it]

100%|      | 32/32 [00:26<00:00,  1.20it/s]

Epoch 1/8, Train Loss: 0.6876, Train Accuracy: 0.5116, Valid Loss: 0.6572, Valid
Accuracy: 0.8130

100%|      | 125/125 [05:33<00:00,  2.67s/it]

100%|      | 32/32 [00:26<00:00,  1.20it/s]

Epoch 2/8, Train Loss: 0.6066, Train Accuracy: 0.6817, Valid Loss: 0.5604, Valid
Accuracy: 0.8342
```

```
100%|          | 125/125 [05:32<00:00,  2.66s/it]

100%|          | 32/32 [00:26<00:00,  1.21it/s]

Epoch 3/8, Train Loss: 0.5186, Train Accuracy: 0.7469, Valid Loss: 0.4897, Valid
Accuracy: 0.8447

100%|          | 125/125 [05:32<00:00,  2.66s/it]

100%|          | 32/32 [00:26<00:00,  1.20it/s]

Epoch 4/8, Train Loss: 0.4522, Train Accuracy: 0.7807, Valid Loss: 0.4434, Valid
Accuracy: 0.8486

100%|          | 125/125 [05:32<00:00,  2.66s/it]

100%|          | 32/32 [00:26<00:00,  1.21it/s]

Epoch 5/8, Train Loss: 0.3829, Train Accuracy: 0.8050, Valid Loss: 0.4104, Valid
Accuracy: 0.8499

100%|          | 125/125 [05:32<00:00,  2.66s/it]

100%|          | 32/32 [00:26<00:00,  1.20it/s]

Epoch 6/8, Train Loss: 0.3303, Train Accuracy: 0.8234, Valid Loss: 0.3832, Valid
Accuracy: 0.8523

100%|          | 125/125 [05:32<00:00,  2.66s/it]

100%|          | 32/32 [00:26<00:00,  1.21it/s]

Epoch 7/8, Train Loss: 0.2872, Train Accuracy: 0.8378, Valid Loss: 0.3744, Valid
Accuracy: 0.8541

100%|          | 125/125 [05:32<00:00,  2.66s/it]

100%|          | 32/32 [00:26<00:00,  1.20it/s]

Epoch 8/8, Train Loss: 0.2604, Train Accuracy: 0.8494, Valid Loss: 0.3750, Valid
Accuracy: 0.8548
```

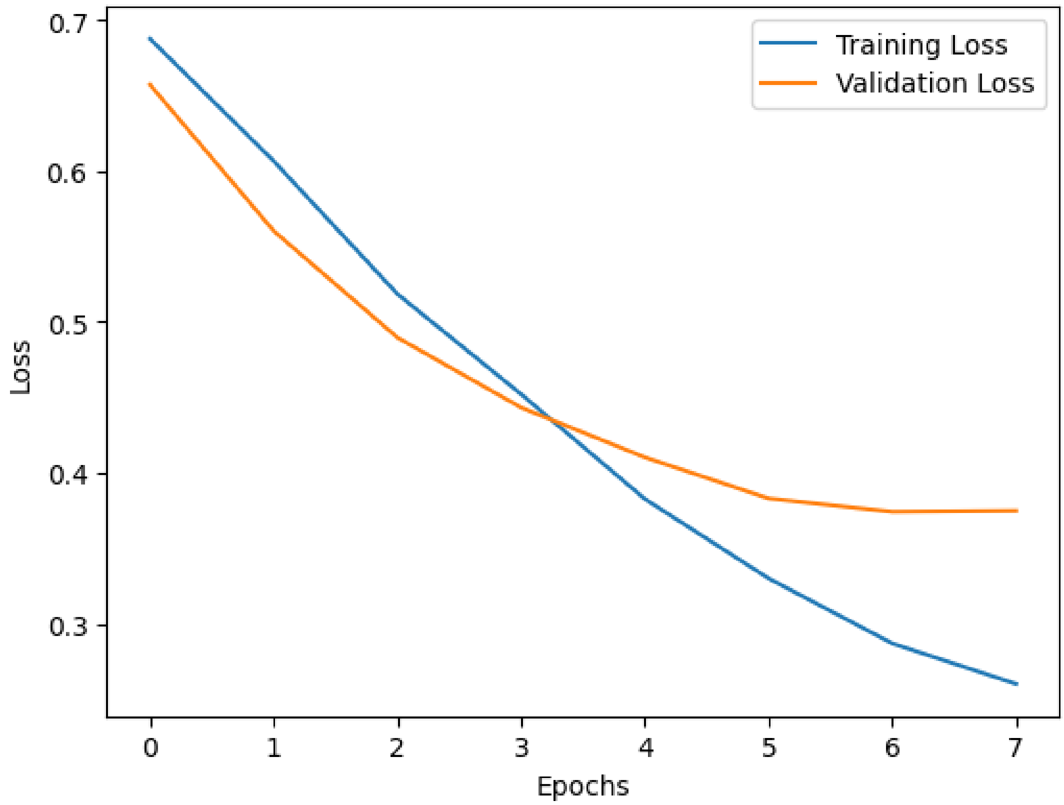
[21]:
```
encoder = classifier.module.encoder
```

[22]:
```
torch.save(encoder, 'encoder.pth')
```

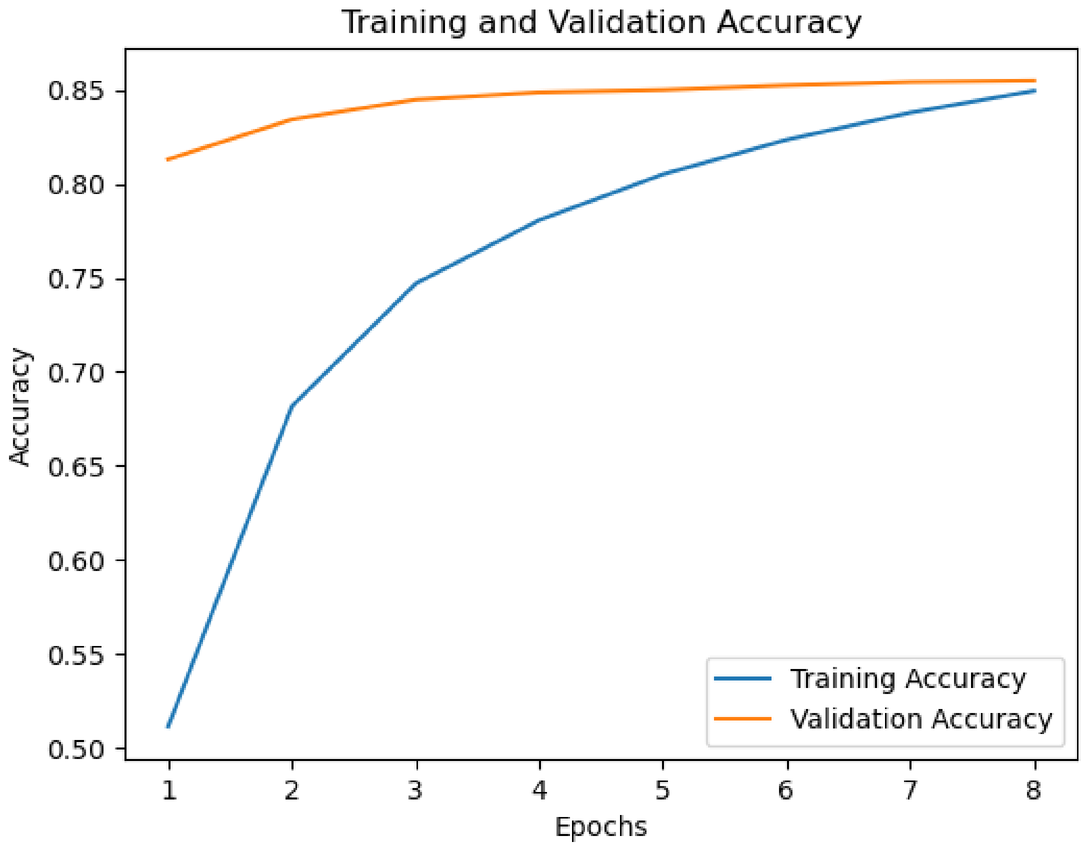
[23]:
```
torch.save(classifier.module, 'model.pth')
```

[24]:
```
plt.plot(train_losses, label='Training Loss')
plt.plot(val_losses, label='Validation Loss')
plt.xlabel('Epochs')
plt.ylabel('Loss')
plt.legend()
```

```
plt.show()
```



[25]:
```
plt.plot(epochs, train_accuracy, label='Training Accuracy')
plt.plot(epochs, valid_accuracy, label='Validation Accuracy')
plt.title('Training and Validation Accuracy')
plt.xlabel('Epochs')
plt.ylabel('Accuracy')
plt.legend()
plt.show()
```


Training and Validation Accuracy
0.85
0.80
0.75
0.70
0.65
0.60
0.55
0.50
Accuracy
1
2
3
4
5
6
7
8
Epochs
Training Accuracy
Validation Accuracy