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1 ### md
2
3 PyTorch Lightning is a lightweight PyTorch wrapper
  that simplifies the process of training deep learning
  models. It provides a high-level interface for
  organizing and orchestrating training routines,
  making it easier for researchers and practitioners to
  focus on model development rather than low-level
  training details.
4
5 Advantages of using PyTorch Lightning to train models
  include:
6
7 ### Abstraction of Training Loop:
8 PyTorch Lightning abstracts away the boilerplate code
  for training loops, validation loops, and testing
  loops. This allows developers to focus more on
  designing and implementing the model architecture
  rather than writing repetitive training code.
9
10 ### Simplified Model Code:
11 By providing predefined hooks for common tasks such
  as forward passes, backward passes, and optimization
  steps, PyTorch Lightning reduces the complexity of
  model code. This results in cleaner, more organized
  code that is easier to understand and maintain.
12
13 ### Standardization:
14 PyTorch Lightning encourages a standardized structure
  for organizing deep learning projects. This makes it
  easier for developers to collaborate, share code,
  and reproduce results across different projects and
  teams.
15
16 ### Flexibility:
17 Despite providing a high-level interface, PyTorch
  Lightning remains flexible and customizable.
  Developers can override default behaviors and
  customize training routines according to their
  specific requirements.
18 ###
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```

19 !pip install pytorch-lightning
20 ###
21 import numpy as np
22 import h5py
23 import math
24 import os
25 import numpy as np
26 import matplotlib.pyplot as plt
27
28
29 import torch
30 import torchvision
31 import torch.nn.functional as F
32 from torch.utils.data import Dataset, DataLoader,
    random_split
33 import h5py
34 from torchvision import transforms
35 ###
36 from google.colab import drive
37 drive.mount('/content/drive')
38 ###
39 import numpy as np
40 import h5py
41
42 def load_h5(file_name, size):
43     # Load the dataset from the HDF5 file
44     with h5py.File(file_name, 'r') as f:
45         X = np.array(f['X_jets'][:size])
46         y = np.array(f['y'][:size])
47     return X, y
48
49 ###
50 file = '/content/drive/MyDrive/quark-gluon_data-
    set_n139306.hdf5'
51 size = 10000
52 X, y = load_h5(file, size)
53 ###
54 from skimage.transform import resize
55 def data_preprocess(X_jets):
56     #Normalizing the images
57

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58     # Resizing images from (125, 125, 3) to (128, 128
    , 3)
59     resized_images = np.zeros((X_jets.shape[0], 128,
    128, 3), dtype=np.float32)
60     for i in range(X_jets.shape[0]):
61         resized_images[i] = resize(X_jets[i], (128,
    128), anti_aliasing=True)
62
63     X_jets = resized_images
64     del resized_images
65
66     # Normalizing the entire image across all
    channels
67     mean = np.mean(X_jets)
68     std = np.std(X_jets)
69     X_jets = (X_jets - mean) / std
70
71     # Assuming X_jets is your image array
72     X_jets = np.clip(X_jets, 0, None)
73     # X_jets[:, :, :, 0] = X_jets[:, :, :, 0]/np.max(X_jets
    [:, :, :, 0])
74     # X_jets[:, :, :, 1] = X_jets[:, :, :, 1]/np.max(X_jets
    [:, :, :, 1])
75     # X_jets[:, :, :, 2] = X_jets[:, :, :, 2]/np.max(X_jets
    [:, :, :, 2])
76
77     return X_jets
78 ###
79 X_jets = data_preprocess(X)
80 ###
81 import matplotlib.pyplot as plt
82 import numpy as np
83
84 def plot_images_with_combined_channels(dataset):
85     # Extracting the initial 5 jet images from the
    dataset...
86     images = dataset[:5]
87
88     for i in range(5):
89         X_sample = images[i]
90         og_plot = plt.imshow(X_sample)

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91
92
93         fig, axs = plt.subplots(1, 3, figsize=(20,
94         20))
95         im1 = axs[0].imshow(X_sample[:, :, 0], cmap='
viridis', vmin=-0.5, vmax=2.0, interpolation='
nearest')
96         axs[0].set_title(f'Track for {i}th image')
97
98         im2 = axs[1].imshow(X_sample[:, :, 1], cmap=
'viridis', vmin=-0.5, vmax=2.0, interpolation='
nearest')
99         axs[1].set_title(f'ECAL for {i}th image')
100
101         im3 = axs[2].imshow(X_sample[:, :, 2], cmap='
viridis', vmin=-0.5, vmax=2.0, interpolation='
nearest')
102         axs[2].set_title(f'HCAL for {i}th image')
103
104         # Add colorbars
105         fig.colorbar(im1, ax=axs[0], shrink=0.25)
106         fig.colorbar(im2, ax=axs[1], shrink=0.25)
107         fig.colorbar(im3, ax=axs[2], shrink=0.25)
108
109         plt.show()
110     """
111     plot_images_with_combined_channels(X_jets)
112     """ md
113     * The supervised contrastive loss contrasts the set
      of all samples from the same class as positives
      against the negatives from the remainder of the
      given data batch in training.
114     * Taking class label information into account
      results in an embedding space where elements of the
      same class are more closely aligned than in the self-
      supervised case.
115     * Although we already know that the loss function is
      pushing to map the given pairs of positives close
      together, and the pair of negative and positive
      samples further apart.

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116 ### md
117 In a Supervised Contrastive Loss setting, label
    information is used to sample positives in addition
    to augmentations of the same image.
118 ###
119 # We can have an encoder, to which we pass the image
    (ResNet50 etc.), and obtain the underlying hidden
    representation of the specified dimension.
120 # Then, we apply a non-linear transformation on it
    to further apply contrastive layer.
121
122 # Then, normalize the obtained hidden
    representations and apply loss function.
123 ###
124 def nt_xent_loss(out_1, out_2, temperature):
125     out = torch.cat((out_1, out_2), dim=0)
126     n_samples = len(out)
127
128     #Full similarity matrix
129     cov = torch.mm(out, out.t().contiguous())
130     sim = torch.exp(cov/temperature)
131
132     mask = ~torch.eye(n_samples, device = sim.device).
    bool()
133     neg = sim.masked_select(mask).view(n_samples, -1).
    sum(dim=-1)
134
135     #Positive similarity
136     pos = torch.exp(torch.sum(out_1 * out_2, dim = -1
    ) / temperature)
137     pos = torch.cat([pos, pos], dim = 0)
138
139     loss = -(torch.log(pos/neg).mean())
140     return loss
141 ###
142 # class Projection(nn.Module):
143 #     def __init__(self, dim_in = 125*125, dim_hid
    = 125*125, dim_out = 128):
144 #         super(Projection, self).__init__()
145 #         self.dim_in = dim_in
146 #         self.dim_hid = dim_hid

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147 #         self.dim_out = dim_out
148 #         self.linear = nn.Linear(dim_in, dim_out)
149 #%%
150 import torch
151 import torch.nn as nn
152 import torch.nn.functional as F
153 import pytorch_lightning as pl
154 import torchvision.models as models
155
156 class SimCLR(pl.LightningModule):
157     def __init__(self, hidden_dim, lr, temperature,
158 weight_decay, max_epochs=500):
159         super().__init__()
160         self.save_hyperparameters()
161         assert self.hparams.temperature > 0.0, "The
temperature must be a positive float!"
162
163         # Base model for feature extraction
164         self.convnet = models.resnet18(pretrained=
True)
165         num_fters = self.convnet.fc.in_features
166         self.convnet.fc = nn.Linear(num_fters,
hidden_dim)
167         # self.lin1 = nn.Linear(self.convnet.fc.
in_features, hidden_dim)
168         # self.lin2 = nn.Linear(hidden_dim,
hidden_dim)
169         # self.relu = nn.ReLU(inplace=True)
170
171         # def forward(self, x):
172         #     x = self.convnet(x)
173         #     x = self.lin1(x)
174         #     x = self.relu(x)
175         #     x = self.lin2(x)
176
177     def configure_optimizers(self):
178         optimizer = torch.optim.AdamW(self.
parameters(), lr=self.hparams.lr, weight_decay=self.
hparams.weight_decay)
179         lr_scheduler = torch.optim.lr_scheduler.
CosineAnnealingLR(

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179         optimizer, T_max=self.hparams.max_epochs
    , eta_min=self.hparams.lr / 50
180     )
181     return [optimizer], [lr_scheduler]
182
183     def info_nce_loss(self, batch, mode="train"):
184         imgs, labels = batch
185         # print(imgs.shape)
186         # print(labels.shape)
187         # imgs = torch.cat(imgs, dim=0)
188
189         # Encode all images
190         feats = self.convnet(imgs)
191
192         # Normalize features
193         feats = F.normalize(feats, dim=1)
194
195         # Calculate cosine similarity
196         cos_sim = F.cosine_similarity(feats[:, None
    , :], feats[None, :, :], dim=-1)
197         # Mask out cosine similarity to itself
198         self_mask = torch.eye(cos_sim.shape[0],
    dtype=torch.bool, device=cos_sim.device)
199         cos_sim.masked_fill_(self_mask, -9e15)
200         # Find positive example -> batch_size//2
    away from the original example
201         pos_mask = self_mask.roll(shifts=cos_sim.
    shape[0] // 2, dims=0)
202         # InfoNCE loss
203         cos_sim = cos_sim / self.hparams.temperature
204         nll = -cos_sim[pos_mask] + torch.logsumexp(
    cos_sim, dim=-1)
205         nll = nll.mean()
206
207         # Supervised contrastive loss, calculating
    class similarity,
208         # class_sim = cos_sim[labels == labels[:,
    None]]
209         # class_sim = class_sim / self.hparams.
    temperature
210         # class_nll = -class_sim.diag() + torch.

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210 logsumexp(class_sim, dim = -1)
211         # class_nll = class_nll.mean()
212
213         #Combining both the losses,
214         total_loss = nll
215
216
217         # Logging loss
218         self.log(mode + "_loss", total_loss)
219         self.log(mode + "_nll", nll)
220     #         self.log(mode + "_class_nll", class_nll)
221     # Get ranking position of positive example
222     comb_sim = torch.cat(
223         [cos_sim[pos_mask][:, None], cos_sim.
masked_fill(pos_mask, -9e15)],
224         dim=-1,
225     )
226     sim_arg-sort = comb_sim.argsort(dim=-1,
descending=True).argmin(dim=-1)
227     # Logging ranking metrics
228     self.log(mode + "_acc_top1", (sim_arg-sort
== 0).float().mean())
229     self.log(mode + "_acc_top5", (sim_arg-sort <
5).float().mean())
230     self.log(mode + "_acc_mean_pos", 1 +
sim_arg-sort.float().mean())
231     return total_loss
232
233     def training_step(self, batch, batch_idx):
234         return self.info_nce_loss(batch, mode="train
")
235
236     def validation_step(self, batch, batch_idx):
237         self.info_nce_loss(batch, mode="val")
238
239     # def testing_step(self, batch, batch_idx):
240     #     self.info_nce_loss(batch, mode="test")
241
242     def on_epoch_end(self):
243         if self.current_epoch % 5 == 0:
244             print(f"Epoch: {self.current_epoch}

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244 , Train Loss: {self.trainer.callback_metrics['
    train_loss']}, Val Loss: {self.trainer.
    callback_metrics['val_loss']})"
245 #%%
246 from torch.utils.data import DataLoader, Dataset
247 from torchvision import transforms
248 from PIL import Image
249 from matplotlib import cm
250
251 class JetImageDataset(Dataset):
252     def __init__(self, images, labels, transform=
    None):
253         self.images = images
254         self.labels = labels
255         self.transform = transform
256
257     def __len__(self):
258         return len(self.images)
259
260     def __getitem__(self, idx):
261         image = self.images[idx]
262         # image = Image.fromarray(np.uint8(cm.
    gist_earth(image)*255))
263         label = self.labels[idx]
264         if self.transform:
265             image = self.transform(image)
266         return image, label
267
268 # Define your data augmentation pipeline
269 transform = transforms.Compose([
270     transforms.ToPILImage(),
271     transforms.RandomHorizontalFlip(),
272     transforms.RandomRotation(10),
273     transforms.ToTensor(),
274 ])
275
276 # Load your data
277 # Assuming `images` is a list of ndarrays and `
    labels` is a list of labels
278 dataset = JetImageDataset(X_jets, y, transform=
    transform)

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```

279 #dataloader = DataLoader(dataset, batch_size=32,
    shuffle=True)
280 #%%
281
282 #%%
283 print(dataset.labels[:20])
284 #%%
285 from torch.utils.data import random_split
286
287 # Splitting data as per the following scheme : 80%
    for training, 10% for validation, and 10% for
    testing
288 train_size = int(0.8 * len(dataset))
289 valid_size = int(0.1 * len(dataset))
290 test_size = len(dataset) - train_size - valid_size
291
292 # Splitting the dataset
293 train_dataset, valid_dataset, test_dataset =
    random_split(dataset, [train_size, valid_size,
    test_size])
294 #%%
295 train_loader = DataLoader(train_dataset, batch_size=
    256, shuffle=True)
296 valid_loader = DataLoader(valid_dataset, batch_size=
    256, shuffle=False)
297 test_loader = DataLoader(test_dataset, batch_size=
    256, shuffle=False)
298 #%%
299 from pytorch_lightning.loggers import import
    TensorBoardLogger
300
301 # Create a logger
302 logger = TensorBoardLogger('logs/', name='simclr')
303 model = SimCLR(hidden_dim=256, lr=0.001, temperature
    =10, weight_decay=0.1, max_epochs=50)
304 #%%
305 torch.cuda.device_count()
306 #%%
307 from pytorch_lightning import Trainer
308
309 logger = TensorBoardLogger('logs/', name='simclr')

```

```
310
311 trainer = Trainer(devices=1, accelerator="gpu",
    logger=logger, enable_checkpointing=True, max_time="
    00:00:45:00", max_epochs=100)
312 trainer.fit(model, train_loader, valid_loader)
313 #%%
314 %load_ext tensorboard
315 #%%
316 %tensorboard --logdir logs/simclr/
317 #%%
318
```