Coursework: Self-supervised learning

Submission: You are asked to submit two versions of your notebook:

1. You should submit the raw notebook in `.ipynb` format with *all outputs cleared*. Please name your file `coursework.ipynb`.
2. Additionally, you will be asked to submit an exported version of your notebook in `.pdf` format, with *all outputs included*. We will primarily use this version for marking, but we will use the raw notebook to check for correct implementations. Please name this file `coursework_export.pdf`.

Your details

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Setup

In [ ]:
```
! pip install lightning medmnist tensorboard tensorboardX
```
In [2]:
```
import os
import numpy as np
import torch
import torch.nn as nn
import torch.nn.functional as F
import torchvision
import matplotlib.pyplot as plt

from torch.utils.data import DataLoader
from torchvision import models
# from torchvision import transforms
from torchvision.transforms import v2
from pytorch_lightning import LightningModule, LightningDataModule, Trainer, seed_everything
from pytorch_lightning.loggers import TensorBoardLogger
from pytorch_lightning.callbacks import ModelCheckpoint, TQDMProgressBar
from torchmetrics.functional import auroc
from PIL import Image
from medmnist.info import INFO
from medmnist.dataset import MedMNIST

# Set a random seed for reproducibility
torch.manual_seed(42)
np.random.seed(42)
```
In [3]:
```
device = torch.device('cuda:0' if torch.cuda.is_available() else 'cpu')
device
```
Out[3]:
```
device(type='cuda', index=0)
```

Part A: Implement a dataset suitable for contrastive learning.

Dataset: MedMNIST Pneumonia (chest X-ray images downsampled to 28 $\times$ 28 pixels), with binary labels indicating the presence of Pneumonia.

Task A-1: Complete the dataset implementation.

- implement a dataset class `SimCLRPneumoniaMNISTDataset`
- suitable for training a self-supervised model with a contrastive objective
- For each sample, your dataset class should return two 'views' of the corresponding image, forming the positive pairs for contrastive learning.
- It is up to you to design suitable augmentation pipeline for generating these views
- provide a short description

Once you have implemented your dataset class, you are asked to run the provided visualisation code to visualise one batch of your training dataloader.

Note: You can use the same data augmentation pipeline for training, validation, and testing.

In [4]:
```python
from typing import Any


class SimCLRPneumoniaMNISTDataset(MedMNIST):
    def __init__(self, split = 'train'):
        """Dataset class for PneumoniaMNIST.

        The provided init function will automatically download the necessary
        files at the first class initialization.

        Args:
            split (str, optional): select subset of the data: 'train', 'val' or 'test'. Defaults to 'train'.
        """

        self.flag = "pneumoniamnist"
        self.size = 28
        self.size_flag = ""
        self.root = './data/coursework/'
        self.info = INFO[self.flag]
        self.download()

        npz_file = np.load(os.path.join(self.root, "pneumoniamnist.npz"))

        self.split = split

        # Load all the images
        assert self.split in ['train','val','test']

        self.imgs = npz_file[f'{self.split}_images']
        self.labels = npz_file[f'{self.split}_labels']

        """
        The data augmentation follows a similar style as in the original paper's default settings with some minor adjustments for

            - random crop and resize:
                The original paper uses images from the ImageNet, with avg size of approx 400x400. They performed aggressive r

                For this coursework, we have pneumonia images that have been scaled down to a 28x28 resolution. I am inspired

            - random color-discoloration:
                The original paper uses random distortion composed by color jittering and color dropping. However, our images co

            - gaussian blur:
                In the paper, they blur the image 50% of the time using a Gaussian kernel. We randomly sample \sigma ∈ [0.1, 2.(
        """

        # Documentation: https://pytorch.org/vision/main/generated/torchvision.transforms.RandomResizedCrop.html

        random_crop = v2.RandomResizedCrop(size=self.size, scale=(0.0625, 1), ratio=(3/4, 4/3))

        # Documentation: http://pytorch.org/vision/master/generated/torchvision.transforms.RandomHorizontalFlip.html

        random_h_flip = v2.RandomHorizontalFlip(0.5)
```

```python
    # Documentation: https://pytorch.org/vision/main/generated/torchvision.transforms.ColorJitter.html
    # Why no hue: We want to keep the model strictly learning about black-and-white features from the black-and-white sca
    # Why no saturation: Increasing or decreasing saturation on a black and white image typically has no effect https://www

    strength = 1
    color_jitter = v2.ColorJitter(brightness=0.8*strength, contrast=0.8*strength)

    # Documentation: https://pytorch.org/vision/master/generated/torchvision.transforms.GaussianBlur.html
    # Custom Transforms: https://pytorch.org/tutorials/beginner/data_loading_tutorial.html#transforms

    class RandomGaussianBlur(object):
      def __init__(self, size, p=0.5):
        """Performs a GaussianBlur with a 50% chance. The unsuccessful times, the image is left as is.

        Args:
          p (float, optional): Probability of performing a gaussian blur. Defaults to 0.5.
        """

        self.size = size
        self.p = 0.5

      def __call__(self, x):
        """Stochastically performs a gaussian blur on the input defined by probability self.p

        Args:
          x (_type_): _description_
        """

        if (torch.rand(1).item() < self.p):
          # Gaussian filter size should be odd and positive
          kernel_size = int(0.1*self.size)
          kernel_size = kernel_size + 1 if kernel_size % 2 == 0 else kernel_size
          gaussian_blur = v2.GaussianBlur(kernel_size=kernel_size, sigma=(0.1, 2.0))
          return gaussian_blur(x)
        else:
          return x

    gaussian_blur = RandomGaussianBlur(size=self.size, p=0.5)

    # Define the data augmentation pipeline.

    self.augmentation_pipeline = v2.Compose([
      v2.ToImage(),
      v2.ToDtype(torch.float32, scale=True),
      random_crop,
      random_h_flip,
      color_jitter,
      gaussian_blur
    ])

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

  def __getitem__(self, index):
    # TASK: Fill in the blanks such that you return two tensors
    # of shape [1, 28, 28], img_view1 and img_view2, representing two augmented view of the images.

    # Get the image at the indexed position
    x = np.expand_dims(self.imgs[index], axis=0)

    x = torch.from_numpy(x)

    return self.augmentation_pipeline(x), self.augmentation_pipeline(x)
```

We use a LightningDataModule for handling your PneumoniaMNIST dataset. You do not need to make any modifications to the code below.

In [5]:

```
class SimCLRPneumoniaMNISTDataModule(LightningDataModule):
    def __init__(self, batch_size: int = 8):
        super().__init__()
        self.batch_size = batch_size
        self.train_set = SimCLRPneumoniaMNISTDataset(split='train')
        self.val_set = SimCLRPneumoniaMNISTDataset(split='val')
        self.test_set = SimCLRPneumoniaMNISTDataset(split='test')

    def train_dataloader(self):
        return DataLoader(dataset=self.train_set, batch_size=self.batch_size, shuffle=True)

    def val_dataloader(self):
        return DataLoader(dataset=self.val_set, batch_size=self.batch_size, shuffle=False)

    def test_dataloader(self):
        return DataLoader(dataset=self.test_set, batch_size=self.batch_size, shuffle=False)
```

Check dataset implementation.

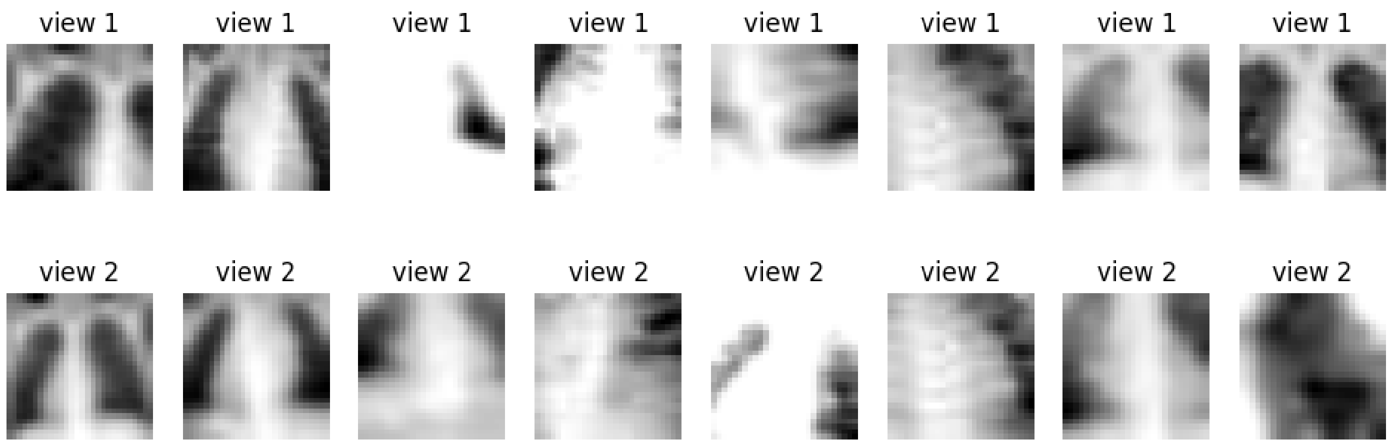
Run the below cell to visualise a batch of your training dataloader.

In [8]:

```
# DO NOT MODIFY THIS CELL! IT IS FOR CHECKING THE IMPLEMENTATION ONLY.

# Initialise data module
datamodule = SimCLRPneumoniaMNISTDataModule()
# Get train dataloader
train_dataloader = datamodule.train_dataloader()
# Get first batch
batch = next(iter(train_dataloader))
# Visualise the images
view1, view2 = batch
f, ax = plt.subplots(2, 8, figsize=(12,4))
for i in range(8):
  ax[0,i].imshow(view1[i, 0], cmap='gray')
  ax[1,i].imshow(view2[i, 0], cmap='gray')
  ax[0,i].set_title('view 1')
  ax[1,i].set_title('view 2')
  ax[0, i].axis("off")
  ax[1, i].axis("off")
```

```
Using downloaded and verified file: ./data/coursework/pneumoniamnist.npz
Using downloaded and verified file: ./data/coursework/pneumoniamnist.npz
Using downloaded and verified file: ./data/coursework/pneumoniamnist.npz
```



Part B: Implement the SimCLR loss and training step.

In this part, we ask you to:

1. Implement the SimCLR loss function, as per the equation in the lecture notes (and the original paper).
2. Once you have implemented the loss, implement the training step function in the provided LightningModule.

Task B-1: SimCLR loss function.

For the implementation of the SimCLR loss, you should follow the 'recipe' from the lecture slides. We provide a code skeleton to get you started. Fill in all the blanks.

Hint: In PyTorch, to compute scalar products (also called dot products) between many elements efficiently, note that for two batches of d-dimensional feature vectors $v1$ and $v2$ of size $[N, d]$ (with N being the batch size) computing the matrix multiplication `torch.mm(v1, v2.t())` returns a matrix S of size $[N, N]$ where each element $S[i, j]$ is the scalar product of $v1_i$ and $v2_j$.

In [9]:
```
def simclr_loss(embedding_view1, embedding_view2, tau = 1.0):
  """This function implements the SimCLR loss function as described in the original paper.
  See lecture notes for formulas.

  It takes as input the embeddings from both views and returns the loss value for that batch.

  Args:
     embedding_view1 (torch.tensor): shape [batch_size, embedding_dimension]
     embedding_view2 (torch.tensor): shape [batch_size, embedding_dimension]
     tau (float, optional): temperature parameter. Defaults to 1.0.

  Returns:
     torch.tensor: shape 1
  """

  # Step 1: normalize the embeddings with L_2 normalization over the embedding_dimension
  embedding_view1 = F.normalize(embedding_view1, dim=-1)
  embedding_view2 = F.normalize(embedding_view2, dim=-1)

  # Step 2: gather all embeddings into one big vector of size [2*N , feature_dim]
  embedding_combined = torch.cat((embedding_view1, embedding_view2), dim=0)

  # Step 3: compute all possible similarities, should be a matrix of size [2 * N, 2 * N]
  # all_similarities[i,j] will be the similarity between z_all_views[i] and z_all_views[j].
  # We don't need any further division by ||i|| * ||j|| because they are already normalized.
  all_similarities = torch.mm(embedding_combined, embedding_combined.T)

  # Step 4: Here we want to return a mask of size[2 * N, 2 * N] for which mask[i,j] = 1 if
  # z_all_views[i] and z_all_views[j] form a positive pair.
  # There should be exactly 2 * N non-zeros elements in this matrix.
  mask_self = torch.eye(all_similarities.size(0))
  mask_positive_pair = torch.roll(mask_self, shifts=embedding_view1.size(0), dims=1)

  # Step 5: self-mask. For computing the denominator term in the loss function,
  # we need to sum over all possible similarities except the self-similarity.
  # Create a mask of shape [2*N, 2*N] that is 1 for all valid pairs and 0 for all self-pairs (i = j).
  mask_negative = 1 - mask_self

  # Step 6: Computing all numerators for the loss function.
  # Should be vector of size [2 * N],
  # where element is exp(sim(i, j) / t) for each positive pair (i, j).
  # Re-use the computed quantities above.

  """
  print(mask_positive_pair.get_device()) # -1
  print(all_similarities.get_device())   # 0
  """

  mask_positive_pair = mask_positive_pair.to(embedding_view1.device)
  numerator = torch.exp(torch.sum(mask_positive_pair * all_similarities, dim=1)/tau)

  # Step 7: Computing all denominators for the loss function.
  # Should be a vector of size [2 * N].
  # Where each element should be the sum of exp(sim(i,k)/tau) for all k != i.
```

```
    """
    print(mask_negative.get_device())    # -1
    print(all_similarities.get_device()) # 0
    """

    mask_negative = mask_negative.to(embedding_view1.device)
    denominator = torch.sum(mask_negative * torch.exp(all_similarities/tau), dim=1)

    # Step 8: Return the final loss values, using the previously computing numerators and denominators.
    batch_loss = - torch.log(numerator / denominator)

    return torch.mean(batch_loss)
```

Check SimCLR loss function.

To check your implementation, please run the following tests. Note that we will also use other tests on different inputs to test your code.

In [10]:

```
# DO NOT MODIFY THIS CELL! IT IS FOR CHECKING THE IMPLEMENTATION ONLY.

seed_everything(33)

expected_results = [torch.tensor(1.7518), torch.tensor(1.6376), torch.tensor(4.194),  torch.tensor(4.1754)]
for i, (N, feature_dim) in enumerate(zip([3, 3, 33, 33], [5, 125, 5, 125])):
    embedding_view1 = torch.rand((N, feature_dim))#.to(device)
    embedding_view2 = torch.rand((N, feature_dim))#.to(device)
    loss = simclr_loss(embedding_view1.clone(), embedding_view2.clone(), tau=0.5)
    print(f"Expected loss: {expected_results[i]}, Computed loss: {loss}")
    assert torch.isclose(loss, expected_results[i], rtol=1e-3)
print("Passed all tests successfully !")
```

```
Seed set to 33
Expected loss: 1.7517999410629272, Computed loss: 1.7518142461776733
Expected loss: 1.6375999450683594, Computed loss: 1.637643814086914
Expected loss: 4.193999767303467, Computed loss: 4.194351673126221
Expected loss: 4.1753997802734375, Computed loss: 4.175372123718262
Passed all tests successfully !
```

Task B-2: SimCLR training step.

In this next task you are asked to complete the blanks in the provided LightningModule.

We provide the implementation of an image encoder (the CNN backbone that will act as feature extractor). No changes are needed for this part.

In [11]:

```
class ImageEncoder(torch.nn.Module):
    def __init__(self) -> None:
        super().__init__()
        self.net = models.resnet50(weights=None)
        del self.net.fc
        self.net.conv1 = torch.nn.Conv2d(1, 64, kernel_size=7, stride=2, padding=3, bias=False)

    def forward(self, x: torch.Tensor) -> torch.Tensor:
        x = self.net.conv1(x)
        x = self.net.bn1(x)
        x = self.net.relu(x)
        x0 = self.net.maxpool(x)
        x1 = self.net.layer1(x0)
        x2 = self.net.layer2(x1)
        x3 = self.net.layer3(x2)
        x4 = self.net.layer4(x3)
        x4 = self.net.avgpool(x4)
        x4 = torch.flatten(x4, 1)
        return x4
```

Next, you will need to complete the implementation of the SimCLR model. In order to make the training step work correctly, you will need to implement the `process_batch` function.

In [12]:

```python
class SimCLRModel(LightningModule):
    def __init__(self, learning_rate: float = 0.001):
        super().__init__()
        self.learning_rate = learning_rate

        self.encoder = ImageEncoder()

        self.projector = torch.nn.Sequential(
            torch.nn.Linear(2048, 1024),
            torch.nn.ReLU(),
            torch.nn.Linear(1024, 128),
        )

    def configure_optimizers(self):
        optimizer = torch.optim.Adam(self.parameters(), lr=self.learning_rate)
        return optimizer

    def process_batch(self, batch):
        # Process the 'left' and 'right' execution graph separately

        x1 = self.encoder(batch[0].float())
        x1 = self.projector(x1)

        x2 = self.encoder(batch[1].float())
        x2 = self.projector(x2)

        x1 = x1.float()
        x2 = x2.float()

        loss = simclr_loss(x1, x2)

        return loss

    def training_step(self, batch, batch_idx):
        loss = self.process_batch(batch)
        self.log('train_loss', loss, prog_bar=True)
        if batch_idx == 0:
            grid = torchvision.utils.make_grid(torch.cat((batch[0][0:4, ...], batch[1][0:4, ...]), dim=0), nrow=4, normalize=True)
            self.logger.experiment.add_image('train_images', grid, self.global_step)
        return loss

    def validation_step(self, batch, batch_idx):
        loss = self.process_batch(batch)
        self.log('val_loss', loss, prog_bar=True)
```

Check SimCLR training step.

Here you can test that your code runs fine by training the model for 5 epochs using the cell below.

Report the training and validation loss at the end of 5 epochs.

In [13]:

```python
# DO NOT MODIFY THIS CELL! IT IS FOR CHECKING THE IMPLEMENTATION ONLY.

seed_everything(33, workers=True)

data = SimCLRPneumoniaMNISTDataModule(batch_size=32)

model = SimCLRModel()

trainer = Trainer(
    max_epochs=5,
    accelerator='auto',
    devices=1,
    logger=TensorBoardLogger(save_dir='./lightning_logs/coursework/', name='simclr'),
    callbacks=[ModelCheckpoint(monitor='val_loss', mode='min'), TQDMProgressBar(refresh_rate=10)],
)
trainer.fit(model=model, datamodule=data)
```

```
Seed set to 33
Using downloaded and verified file: ./data/coursework/pneumoniamnist.npz
Using downloaded and verified file: ./data/coursework/pneumoniamnist.npz
Using downloaded and verified file: ./data/coursework/pneumoniamnist.npz
GPU available: True (cuda), used: True
TPU available: False, using: 0 TPU cores
IPU available: False, using: 0 IPUs
HPU available: False, using: 0 HPUs
You are using a CUDA device ('NVIDIA GeForce RTX 4070 Laptop GPU') that has Tensor Cores. To properly utilize them, you should set `torch.set_floa
t32_matmul_precision('medium' | 'high')` which will trade-off precision for performance. For more details, read https://pytorch.org/docs/stable/generated/t
orch.set_float32_matmul_precision.html#torch.set_float32_matmul_precision
LOCAL_RANK: 0 - CUDA_VISIBLE_DEVICES: [0]

  | Name      | Type         | Params
-------------------------------------------
0 | encoder   | ImageEncoder | 23.5 M
1 | projector | Sequential   | 2.2 M
-------------------------------------------
25.7 M    Trainable params
0         Non-trainable params
25.7 M    Total params
102.925   Total estimated model params size (MB)
Sanity Checking DataLoader 0:   0%|          | 0/2 [00:00<?, ?it/s]
/home/avzh1/Documents/imperial/year4/lectures/.venv/lib/python3.10/site-packages/pytorch_lightning/trainer/connectors/data_connector.py:441: The 'val
_dataloader' does not have many workers which may be a bottleneck. Consider increasing the value of the `num_workers` argument` to
`num_workers=31` in the `DataLoader` to improve performance.

/home/avzh1/Documents/imperial/year4/lectures/.venv/lib/python3.10/site-packages/pytorch_lightning/trainer/connectors/data_connector.py:441: The 'trai
n_dataloader' does not have many workers which may be a bottleneck. Consider increasing the value of the `num_workers` argument` to `num_workers=
31` in the `DataLoader` to improve performance.
Epoch 4: 100%|██████████| 148/148 [00:09<00:00, 15.58it/s, v_num=24, train_loss=1.920, val_loss=4.110]
`Trainer.fit` stopped: `max_epochs=5` reached.
Epoch 4: 100%|██████████| 148/148 [00:09<00:00, 14.88it/s, v_num=24, train_loss=1.920, val_loss=4.110]
```

Part C: Linear probing and model finetuning.

Implementation of transfer learning strategies (linear probing and finetuning) for model evaluation.

In this part, you are given two different image encoders that were pre-trained with different datasets and training strategies. The objective for this task is to assess the performance of these two encoders in a downstream classification task. For this task, you are asked to implement evaluation routines seen in the lecture: linear probing and model finetuning. The downstream task is the prediction of Pneumonia in the (small) chest X-ray images from the PneumoniaMNIST dataset.

This part can be broken down into the following tasks:

1. Adapt your PneunomiaMNIST dataset for the image classification task.
2. Implement a classification model with a linear layer attached to a pre-trained image encoder.
3. For both pre-trained encoders:
   - a) Train the classifier on top of the frozen encoder (linear probing)
   - b) Finetune the entire model (including the encoder).
4. Evaluate all models on the test set, and provide a brief summary (no more than 300 words) with an analysis of your findings.

Task C-1: Adapt your PneunomiaMNIST dataset for the image classification task.

We can base our implementation largely on the `SimCLRPneumoniaMNISTDataset` and adapt it to make it suitable for image classification. Think about a suitable data augmentation pipeline. Check previous tutorials for inspiration.

In [27]:

```python
class PneumoniaMNISTDataset(MedMNIST):
    def __init__(self, split = 'train', augmentation: bool = False):
        ''' Dataset class for Pneumonia MNST.
        The provided init function will automatically download the necessary
        files at the first class initialistion.

        :param split: 'train', 'val' or 'test', select subset

        '''
        self.flag = "pneumoniamnist"
        self.size = 28
        self.size_flag = ""
        self.root = './data/coursework/'
        self.info = INFO[self.flag]
        self.download()

        npz_file = np.load(os.path.join(self.root, "pneumoniamnist.npz"))

        self.split = split

        # Load all the images
        assert self.split in ['train','val','test']

        self.imgs = npz_file[f'{self.split}_images']
        self.labels = npz_file[f'{self.split}_labels']

        self.do_augment = augmentation

        # define the augmentation pipeline for classification
        self.augmentation_pipeline = v2.Compose([
            # I don't rotate because this introduces black artifacts into the image which may be misrepresented.
            v2.CenterCrop((26,26)),
            # We can flip because at this resolution there is no difference between the left and right lung
            v2.RandomHorizontalFlip(),
        ])

        self.default_augmentation = v2.Compose([
            v2.ToImage(),
            v2.ToDtype(torch.float32, scale=True)
        ])

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

    def __getitem__(self, index):
        # TASK: Implement the __getitem__ function to return the image and its class label.

        # Get the image at the indexed position
        x = np.expand_dims(self.imgs[index], axis=0)
        x = torch.from_numpy(x)

        if self.do_augment:
            x = self.augmentation_pipeline(x)

        return self.default_augmentation(x), self.labels[index]
```

Again, we use a LightningDataModule for handling your PneumoniaMNIST dataset. No changes needed for this part.

In [28]:

```
class PneumoniaMNISTDataModule(LightningDataModule):
    def __init__(self, batch_size: int = 32):
        super().__init__()
        self.batch_size = batch_size
        self.train_set = PneumoniaMNISTDataset(split='train', augmentation=True)
        self.val_set = PneumoniaMNISTDataset(split='val', augmentation=False)
        self.test_set = PneumoniaMNISTDataset(split='test', augmentation=False)

    def train_dataloader(self):
        return DataLoader(dataset=self.train_set, batch_size=self.batch_size, shuffle=True)

    def val_dataloader(self):
        return DataLoader(dataset=self.val_set, batch_size=self.batch_size, shuffle=False)

    def test_dataloader(self):
        return DataLoader(dataset=self.test_set, batch_size=self.batch_size, shuffle=False)
```

Check dataset implementation.

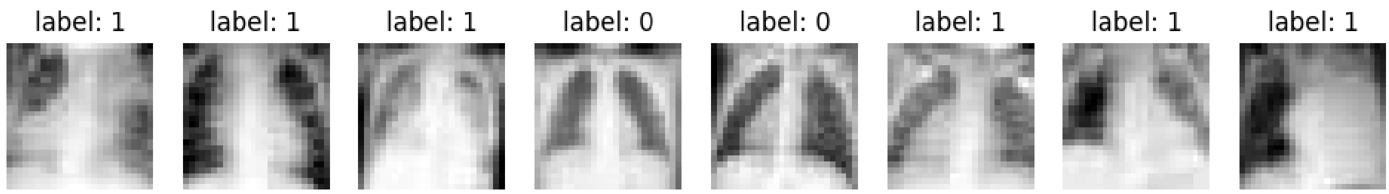
Run the below cell to visualise a batch of your training dataloader.

In [29]:

```
# DO NOT MODIFY THIS CELL! IT IS FOR CHECKING THE IMPLEMENTATION ONLY.

# Initialise data module
datamodule = PneumoniaMNISTDataModule()
# Get train dataloader
train_dataloader = datamodule.train_dataloader()
# Get first batch
batch = next(iter(train_dataloader))
# Visualise the images
images, labels = batch
f, ax = plt.subplots(1, 8, figsize=(12,4))
for i in range(8):
  ax[i].imshow(images[i, 0], cmap='gray')
  ax[i].set_title('label: ' + str(labels[i].item()))
  ax[i].axis("off")
```

```
Using downloaded and verified file: ./data/coursework/pneumoniamnist.npz
Using downloaded and verified file: ./data/coursework/pneumoniamnist.npz
Using downloaded and verified file: ./data/coursework/pneumoniamnist.npz
```



Task C-2: Implement a classification model with a linear layer attached to a pre-trained image encoder.

We first download the weights of the two pre-trained image encoders. One of them has been trained with the self-supervised SimCLR objective on a large publicly available chest X-ray dataset (different from PneunomiaMNIST). The other encoder is a standard ImageNet backbone that has been trained with a supervised classification objective on the ImageNet dataset.

In [30]:

```
# ! wget https://www.doc.ic.ac.uk/~bglocker/teaching/mli/coursework.zip
# ! unzip coursework.zip
```

We provide the function for loading the encoders. No changes needed here.

In [31]:

```
def load_encoder_from_checkpoint(checkpoint_path):
  ckpt = torch.load(checkpoint_path, map_location='cpu')
  simclr_module = SimCLRModel()
  print(simclr_module.load_state_dict(state_dict=ckpt))
  return simclr_module.encoder.eval()

imagenet_model = './data/coursework/model_imagenet.ckpt'
chestxray_model = './data/coursework/model_chestxray.ckpt'
```

Now, implement a classification model as a LightningModule for image classification using a pre-trained image encoder.

The model should have a flag in the init function `freeze_encoder` that if set to true freezes all the weights in the encoder (used for linear probing), and if set to false all weights are trainable (used for model finetuning).

Hint: Check out previous tutorials for inspiration on how to implement a classification model as LightningModule. For the coursework, we recommend using the Area Under the Receiver Operating Characteristic Curve (ROC-AUC) performance metric (instead of accuracy). ROC-AUC is measure of the overall discriminative power of a classification model. You can use the readily available implementation in torchmetrics. You should log the ROC-AUC similar to how we logged accuracy in previous tutorials.

In [36]:

```
# TASK: Implement the ImageClassifier class
# Check previous tutorials for inspiration on how to implement an `ImageClassifier`

class ImageClassifier(LightningModule):
    def __init__(self,
                 pretrained_encoder: torch.nn.Module,
                 freeze_encoder: bool = True,
                 output_dim: int = 2,
                 learning_rate: float = 0.001):
        super().__init__()

        self.pretrained_encoder = pretrained_encoder
        self.freeze_encoder = freeze_encoder
        self.output_dim = output_dim
        self.learning_rate = learning_rate

        # pre-trained image encoder
        for param in self.pretrained_encoder.parameters():
            param.requires_grad = not self.freeze_encoder

        # classification linear layer
        # in the paper, they implemented an MLP with one hidden layer z_i = g(h_i) = W_2*σ(W_1*h_i) where σ is a ReLU non-
        self.lin_layer = nn.Sequential(
            nn.Linear(2048, 1024),
            nn.ReLU(),
            nn.Linear(1024, output_dim),
        )

    def forward(self, x):
        x = self.pretrained_encoder(x)
        x = self.lin_layer(x)
        return x

    def configure_optimizers(self):
        optimizer = torch.optim.Adam(self.parameters(), lr=self.learning_rate)
        return optimizer

    def process_batch(self, batch):
        x, y = batch
        y = y.squeeze(dim=1)

        logits = self(x)
        loss = F.cross_entropy(logits, y)

        probs = torch.softmax(logits, dim=1)
        preds = torch.argmax(probs, dim=1).float()
        auroc_metric = auroc(preds, y, task='binary')
```

```
        return loss, auroc_metric

    def validation_step(self, batch, batch_idx):
        loss, acc = self.process_batch(batch)
        self.log('val_loss', loss, prog_bar=True)
        self.log('val_acc', acc, prog_bar=True)

    def test_step(self, batch, batch_idx):
        loss, acc = self.process_batch(batch)
        self.log('test_loss', loss)
        self.log('test_acc', acc)

    def training_step(self, batch, batch_idx):
        # training_step defines the train loop.
        # it is independent of forward
        loss, auroc_metric = self.process_batch(batch)
        self.log('train_loss', loss, prog_bar=True)
        self.log('train_acc', auroc_metric, prog_bar=True)
        # if batch_idx == 0:
        #     grid = torchvision.utils.make_grid(batch[0][0:16, ...], nrow=4, normalize=True)
        #     self.logger.experiment.add_image('train_images', grid, self.global_step)
        return loss
```

Task C-3a: Implement training and testing for linear probing.

Train two classification models using **linear probing**, one for each of the two provided image encoders. Evaluate on both the validation and test sets.

Note: Training for 25 epochs should be sufficient.

In [37]:

```
seed_everything(33, workers=True)

data = PneumoniaMNISTDataModule(batch_size=32)

# TASK: Implement the linear probing training and testing routines.

classifier_imageNet_linprob = ImageClassifier(pretrained_encoder = load_encoder_from_checkpoint(imagenet_model), freez
classifier_chestxray_linprob = ImageClassifier(pretrained_encoder= load_encoder_from_checkpoint(chestxray_model), freez
```

```
Seed set to 33
Using downloaded and verified file: ./data/coursework/pneumoniamnist.npz
Using downloaded and verified file: ./data/coursework/pneumoniamnist.npz
Using downloaded and verified file: ./data/coursework/pneumoniamnist.npz
<All keys matched successfully>
<All keys matched successfully>
```

In [39]:

```
# Linear Probing for classifier_imageNet_finetuned

trainer = Trainer(
    max_epochs=25,
    accelerator='auto',
    devices=1,
    logger=TensorBoardLogger(save_dir='./lightning_logs/classification/', name='classifier_imageNet_linprob'),
    callbacks=[ModelCheckpoint(monitor='val_loss', mode='min'), TQDMProgressBar(refresh_rate=10)],
)

trainer.fit(model=classifier_imageNet_linprob, datamodule=data)

print("Validation performance for ImageNet")
trainer.validate(model=classifier_imageNet_linprob, datamodule=data, ckpt_path=trainer.checkpoint_callback.best_model_pa

print("Test performance for ImageNet")
trainer.test(model=classifier_imageNet_linprob, datamodule=data, ckpt_path=trainer.checkpoint_callback.best_model_path)
```

```
GPU available: True (cuda), used: True
TPU available: False, using: 0 TPU cores
IPU available: False, using: 0 IPUs
HPU available: False, using: 0 HPUs
LOCAL_RANK: 0 - CUDA_VISIBLE_DEVICES: [0]

  | Name               | Type         | Params
----------------------------------------------------
0 | pretrained_encoder | ImageEncoder | 23.5 M
1 | lin_layer          | Sequential   | 2.1 M
----------------------------------------------------
2.1 M     Trainable params
23.5 M    Non-trainable params
25.6 M    Total params
102.408   Total estimated model params size (MB)
Epoch 24: 100%|██████████| 148/148 [00:01<00:00, 88.57it/s, v_num=4, train_loss=0.0266, train_acc=1.000, val_loss=0.214, val_acc=0.885]
`Trainer.fit` stopped: `max_epochs=25` reached.
Epoch 24: 100%|██████████| 148/148 [00:01<00:00, 78.24it/s, v_num=4, train_loss=0.0266, train_acc=1.000, val_loss=0.214, val_acc=0.885]
Restoring states from the checkpoint path at ./lightning_logs/classification/classifier_imageNet_linprob/version_4/checkpoints/epoch=24-step=3700.ckpt
LOCAL_RANK: 0 - CUDA_VISIBLE_DEVICES: [0]
Loaded model weights from the checkpoint at ./lightning_logs/classification/classifier_imageNet_linprob/version_4/checkpoints/epoch=24-step=3700.ckpt
Validation performance for ImageNet
Validation DataLoader 0: 100%|██████████| 17/17 [00:00<00:00, 130.47it/s]
Restoring states from the checkpoint path at ./lightning_logs/classification/classifier_imageNet_linprob/version_4/checkpoints/epoch=24-step=3700.ckpt
────────────────────────────────────────────────────────────────────────────────
     Validate metric           DataLoader 0
────────────────────────────────────────────────────────────────────────────────
         val_acc            0.8852105140686035
        val_loss            0.21388152241706848
────────────────────────────────────────────────────────────────────────────────
Test performance for ImageNet
LOCAL_RANK: 0 - CUDA_VISIBLE_DEVICES: [0]
Loaded model weights from the checkpoint at ./lightning_logs/classification/classifier_imageNet_linprob/version_4/checkpoints/epoch=24-step=3700.ckpt
Testing DataLoader 0: 100%|██████████| 20/20 [00:00<00:00, 115.07it/s]
────────────────────────────────────────────────────────────────────────────────
       Test metric             DataLoader 0
────────────────────────────────────────────────────────────────────────────────
        test_acc            0.768621563911438
        test_loss           0.4545881450176239
────────────────────────────────────────────────────────────────────────────────
```

Out[39]:

```
[{'test_loss': 0.4545881450176239, 'test_acc': 0.768621563911438}]
```

In [40]:

```python
# Linear Probing for classifier_chestxray_finetuned

trainer = Trainer(
    max_epochs=25,
    accelerator='auto',
    devices=1,
    logger=TensorBoardLogger(save_dir='./lightning_logs/classification/', name='classifier_chestxray_linprob'),
    callbacks=[ModelCheckpoint(monitor='val_loss', mode='min'), TQDMProgressBar(refresh_rate=10)],
)

trainer.fit(model=classifier_chestxray_linprob, datamodule=data)

print("Validation performance for ChestXRay")
trainer.validate(model=classifier_chestxray_linprob, datamodule=data, ckpt_path=trainer.checkpoint_callback.best_model_pa

print("Test performance for ChestXRay")
trainer.test(model=classifier_chestxray_linprob, datamodule=data, ckpt_path=trainer.checkpoint_callback.best_model_path)
```

```
GPU available: True (cuda), used: True
TPU available: False, using: 0 TPU cores
IPU available: False, using: 0 IPUs
HPU available: False, using: 0 HPUs
LOCAL_RANK: 0 - CUDA_VISIBLE_DEVICES: [0]

  | Name               | Type         | Params
----------------------------------------------------
0 | pretrained_encoder | ImageEncoder | 23.5 M
1 | lin_layer          | Sequential   | 2.1 M
----------------------------------------------------
2.1 M     Trainable params
23.5 M    Non-trainable params
25.6 M    Total params
102.408   Total estimated model params size (MB)
Epoch 24: 100%|██████████| 148/148 [00:01<00:00, 107.03it/s, v_num=3, train_loss=0.0723, train_acc=1.000, val_loss=0.509, val_acc=0.83
6]
`Trainer.fit` stopped: `max_epochs=25` reached.
Epoch 24: 100%|██████████| 148/148 [00:01<00:00, 106.96it/s, v_num=3, train_loss=0.0723, train_acc=1.000, val_loss=0.509, val_acc=0.83
6]
Restoring states from the checkpoint path at ./lightning_logs/classification/classifier_chestxray_linprob/version_3/checkpoints/epoch=6-step=1036.ckpt
LOCAL_RANK: 0 - CUDA_VISIBLE_DEVICES: [0]
Validation performance for ChestXRay
Loaded model weights from the checkpoint at ./lightning_logs/classification/classifier_chestxray_linprob/version_3/checkpoints/epoch=6-step=1036.ckpt
Validation DataLoader 0: 100%|██████████| 17/17 [00:00<00:00, 100.06it/s]
────────────────────────────────────────────────────────
    Validate metric           DataLoader 0
────────────────────────────────────────────────────────
        val_acc            0.8541482090950012
        val_loss           0.28128740191459656
────────────────────────────────────────────────────────
Restoring states from the checkpoint path at ./lightning_logs/classification/classifier_chestxray_linprob/version_3/checkpoints/epoch=6-step=1036.ckpt
LOCAL_RANK: 0 - CUDA_VISIBLE_DEVICES: [0]
Test performance for ChestXRay
Loaded model weights from the checkpoint at ./lightning_logs/classification/classifier_chestxray_linprob/version_3/checkpoints/epoch=6-step=1036.ckpt
Testing DataLoader 0: 100%|██████████| 20/20 [00:00<00:00, 107.60it/s]
────────────────────────────────────────────────────────
      Test metric             DataLoader 0
────────────────────────────────────────────────────────
        test_acc           0.7554169297218323
        test_loss          0.4647181034088135
────────────────────────────────────────────────────────
```

Out[40]:

```
[{'test_loss': 0.4647181034088135, 'test_acc': 0.7554169297218323}]
```

Task C-3b: Implement training and testing for model finetuning.

Repeat the experiments, but this time using model finetuning instead of linear probing. Evaluate on both the validation and test sets.

In [41]:

```python
seed_everything(33, workers=True)

data = PneumoniaMNISTDataModule(batch_size=32)

classifier_imageNet_finetuned = ImageClassifier(pretrained_encoder = load_encoder_from_checkpoint(imagenet_model), fre
classifier_chestxray_finetuned = ImageClassifier(pretrained_encoder= load_encoder_from_checkpoint(chestxray_model), fre
```

```
Seed set to 33
Using downloaded and verified file: ./data/coursework/pneumoniamnist.npz
Using downloaded and verified file: ./data/coursework/pneumoniamnist.npz
Using downloaded and verified file: ./data/coursework/pneumoniamnist.npz
<All keys matched successfully>
<All keys matched successfully>
```

In [42]:

```
# Fine-tuning for classifier_imageNet_finetuned

trainer = Trainer(
    max_epochs=25,
    accelerator='auto',
    devices=1,
    logger=TensorBoardLogger(save_dir='./lightning_logs/classification/', name='classifier_imageNet_finetuned'),
    callbacks=[ModelCheckpoint(monitor='val_loss', mode='min'), TQDMProgressBar(refresh_rate=10)],
)

trainer.fit(model=classifier_imageNet_finetuned, datamodule=data)

print("Validation performance for ImageNet")
trainer.validate(model=classifier_imageNet_finetuned, datamodule=data, ckpt_path=trainer.checkpoint_callback.best_model_

print("Test performance for ImageNet")
trainer.test(model=classifier_imageNet_finetuned, datamodule=data, ckpt_path=trainer.checkpoint_callback.best_model_path
```

```
GPU available: True (cuda), used: True
TPU available: False, using: 0 TPU cores
IPU available: False, using: 0 IPUs
HPU available: False, using: 0 HPUs
LOCAL_RANK: 0 - CUDA_VISIBLE_DEVICES: [0]

  | Name               | Type         | Params
----------------------------------------------------
0 | pretrained_encoder | ImageEncoder | 23.5 M
1 | lin_layer          | Sequential   | 2.1 M
----------------------------------------------------
25.6 M    Trainable params
0         Non-trainable params
25.6 M    Total params
102.408   Total estimated model params size (MB)
Epoch 24: 100%|██████████████████| 148/148 [00:03<00:00, 38.03it/s, v_num=2, train_loss=0.300, train_acc=0.500, val_loss=0.146, val_acc=0.962]
`Trainer.fit` stopped: `max_epochs=25` reached.
Epoch 24: 100%|██████████████████| 148/148 [00:03<00:00, 38.01it/s, v_num=2, train_loss=0.300, train_acc=0.500, val_loss=0.146, val_acc=0.962]
Restoring states from the checkpoint path at ./lightning_logs/classification/classifier_imageNet_finetuned/version_2/checkpoints/epoch=17-step=2664.ck
pt
Validation performance for ImageNet
LOCAL_RANK: 0 - CUDA_VISIBLE_DEVICES: [0]
Loaded model weights from the checkpoint at ./lightning_logs/classification/classifier_imageNet_finetuned/version_2/checkpoints/epoch=17-step=2664.c
kpt
Validation DataLoader 0: 100%|██████████████████| 17/17 [00:00<00:00, 127.52it/s]
Restoring states from the checkpoint path at ./lightning_logs/classification/classifier_imageNet_finetuned/version_2/checkpoints/epoch=17-step=2664.ck
pt
────────────────────────────────────────────────────────────
     Validate metric           DataLoader 0
────────────────────────────────────────────────────────────
         val_acc            0.9474622011184692
        val_loss            0.10434147715568542
────────────────────────────────────────────────────────────
Test performance for ImageNet
LOCAL_RANK: 0 - CUDA_VISIBLE_DEVICES: [0]
Loaded model weights from the checkpoint at ./lightning_logs/classification/classifier_imageNet_finetuned/version_2/checkpoints/epoch=17-step=2664.c
kpt
Testing DataLoader 0: 100%|██████████████████| 20/20 [00:00<00:00, 115.62it/s]
────────────────────────────────────────────────────────────
       Test metric             DataLoader 0
────────────────────────────────────────────────────────────
        test_acc            0.7693948745727539
        test_loss           0.5829694867134094
────────────────────────────────────────────────────────────
```

Out[42]:

```
[{'test_loss': 0.5829694867134094, 'test_acc': 0.7693948745727539}]
```

In [43]:

```
# Fine-tuning for classifier_chestxray_finetuned

trainer = Trainer(
    max_epochs=25,
    accelerator='auto',
    devices=1,
    logger=TensorBoardLogger(save_dir='./lightning_logs/classification/', name='classifier_chestXRay_finetuned'),
    callbacks=[ModelCheckpoint(monitor='val_loss', mode='min'), TQDMProgressBar(refresh_rate=10)],
)

trainer.fit(model=classifier_chestxray_finetuned, datamodule=data)

print("Validation performance for ImageNet")
trainer.validate(model=classifier_chestxray_finetuned, datamodule=data, ckpt_path=trainer.checkpoint_callback.best_model_

print("Test performance for ImageNet")
trainer.test(model=classifier_chestxray_finetuned, datamodule=data, ckpt_path=trainer.checkpoint_callback.best_model_path
```

```
GPU available: True (cuda), used: True
TPU available: False, using: 0 TPU cores
IPU available: False, using: 0 IPUs
HPU available: False, using: 0 HPUs
LOCAL_RANK: 0 - CUDA_VISIBLE_DEVICES: [0]

  | Name               | Type         | Params
----------------------------------------------------
0 | pretrained_encoder | ImageEncoder | 23.5 M
1 | lin_layer          | Sequential   | 2.1 M
----------------------------------------------------
25.6 M    Trainable params
0         Non-trainable params
25.6 M    Total params
102.408   Total estimated model params size (MB)
Epoch 24: 100%|██████████| 148/148 [00:03<00:00, 42.02it/s, v_num=2, train_loss=2.68e-7, train_acc=1.000, val_loss=0.117, val_acc=0.962
]
`Trainer.fit` stopped: `max_epochs=25` reached.
Epoch 24: 100%|██████████| 148/148 [00:03<00:00, 42.01it/s, v_num=2, train_loss=2.68e-7, train_acc=1.000, val_loss=0.117, val_acc=0.962
]
Restoring states from the checkpoint path at ./lightning_logs/classification/classifier_chestXRay_finetuned/version_2/checkpoints/epoch=10-step=1628.c
kpt
Validation performance for ImageNet
LOCAL_RANK: 0 - CUDA_VISIBLE_DEVICES: [0]
Loaded model weights from the checkpoint at ./lightning_logs/classification/classifier_chestXRay_finetuned/version_2/checkpoints/epoch=10-step=1628.
ckpt
Validation DataLoader 0: 100%|██████████| 17/17 [00:00<00:00, 131.48it/s]
Restoring states from the checkpoint path at ./lightning_logs/classification/classifier_chestXRay_finetuned/version_2/checkpoints/epoch=10-step=1628.c
kpt
─────────────────────────────────────────────────────────────
   Validate metric          DataLoader 0
─────────────────────────────────────────────────────────────
       val_acc           0.9695884585380554
      val_loss           0.05485376715660095
─────────────────────────────────────────────────────────────
Test performance for ImageNet
LOCAL_RANK: 0 - CUDA_VISIBLE_DEVICES: [0]
Loaded model weights from the checkpoint at ./lightning_logs/classification/classifier_chestXRay_finetuned/version_2/checkpoints/epoch=10-step=1628.
ckpt
Testing DataLoader 0: 100%|██████████| 20/20 [00:00<00:00, 119.97it/s]
─────────────────────────────────────────────────────────────
     Test metric            DataLoader 0
─────────────────────────────────────────────────────────────
      test_acc           0.8175238966941833
      test_loss          0.42045509815216064
─────────────────────────────────────────────────────────────
```

Out[43]:

```
[{'test_loss': 0.42045509815216064, 'test_acc': 0.8175238966941833}]
```

Task C-4: Your evaluation report.

Provide a brief summary (no more than 300 words) with an analysis of your findings. Try explaining the observed performance.

I've re-ran the model since, but these were the numbers I was referring to (they're similar to the ones above)

copying over the performance for convenience:

- Linear Probing
  - imageNet
    - val_acc 0.883340060710907
    - val_loss 0.20424185693264008
    - test_acc 0.785427451133728
    - test_loss 0.41231027245521545
  - chestxray
    - val_acc 0.8496582508087158
    - val_loss 0.26481953263282776
    - test_acc 0.7455279231071472
    - test_loss 0.5827047228813171
- FineTuning
  - imageNet
    - val_acc 0.9408426880836487
    - val_loss 0.12713123857975006
    - test_acc 0.745345950126648
    - test_loss 0.7334343791007996
  - chestxray
    - val_acc 0.9651557207107544
    - val_loss 0.05536622926592827
    - test_acc 0.7902529239654541
    - test_loss 0.948483407497406

In the fine tuning approach, layers are not frozen in the encoder. This allows for the gradient from learning the simple classifier head to trickle into the encoder. This allows for better performance when compared to the linear probing approach because the encoder may also learn how to complement with the decoder more. This is why we see an overall improvement in the validation accuracy between the two approaches. However, when we consider the test data, the results are very similar, only varying at most 5% (When compared to the validation accuracy whose accuracy varies by 10%).

In the linear probing approach, we note that the layers have been frozen. This forces the simple decoder layer to learn more about the encoder's representation to provide the correct output. However, since this decoder layer is a very primitive linear layer, it cannot learn enough detail to fully learn the hidden representation. This is why we see that when compared to fine tuning the approach, the validation accuracy varies by approximately 10% in both cases.

Other observations include the increase of test loss when fine tuning when compared to the linear probing. This is perhaps due to there being more trainable layers present in the fine tuning approach, which may explain the bigger number.

Logging

In [44]:

```
%load_ext tensorboard
%tensorboard --logdir './lightning_logs/coursework/'
```