Exercise 6

1) Neural Network Classifier from Scratch (10p.)

In this exercise we will implement a small neural network from scratch, i.e., only using numpy. This is nothing you would do "in real life" but it is a good exercise to deepen understanding.

The network will consist of an arbitrary number of hidden layers with ReLU activation, a sigmoid output layer (as we are doing binary classification) and we will train it using the binary cross entropy (negative bernoulli likelihood). Ok, so lets start by importing and loading what we need.

```
import numpy as np
import matplotlib.pyplot as plt
from typing import List, Tuple

# Load our two moons (I promise we will get a new dataset in the next exercise)
train_data = dict(np.load("two_moons.npz", allow_pickle=True))
test_data = dict(np.load("two_moons_test.npz", allow_pickle=True))
# we need to reshape our labels so that they are [N, 1] and not [N] anymore
train_samples, train_labels = train_data["samples"], train_data["labels"][:, Non
test_samples, test_labels = test_data["samples"], test_data["labels"][:, None]
```

1.1.) Auxillary Functions (3 p.)

We start with implementing some auxillary functions we are going to need later. The sigmoid and relu activation functions, the binary cross entropy loss as well as their derviatives.

The binary cross entropy loss is given as $-\frac{1}{N} \sum_{i=1}^N (y_i \log (p_i) + (1 - y_i) \log (1 - p_i))$ where y_i denotes the ground truth label and p_i the network prediction for sample i.

Hint all derivatives where derived/implemented during the lecture or previous exercise - so feel free to borrow them from there.

```
....
   elementwise gradient of relu activation function
   :param x: input to function [shape: arbitrary]
   :return : d relu(x) / dx [shape: same as x]
   x[x \le 0] = 0
   x[x>0] = 1
   return x
   def sigmoid(x: np.ndarray) -> np.ndarray:
   elementwise sigmoid activation function
   :param x: input to function [shape: arbitrary]
   :return : d sigmoid(x) /dx [shape: same as x]
   return (1/(1+np \cdot exp(-x)))
   def d sigmoid(x: np.ndarray) -> np.ndarray:
   elementwise sigmoid activation function
   :param x: input to function [shape: arbitrary]
   :return : sigmoid(x) [shape: same as x]
   # --- Is this correct?
   # --- Yes, seems so (https://towardsdatascience.com/derivative-of-the-sigmoi
   return sigmoid(x) * (1-sigmoid(x))
   def binary cross entropy(predictions: np.ndarray, labels: np.ndarray) -> float:
   binary cross entropy loss (negative bernoulli 11)
   :param predictions: predictions by model (shape [N])
   :param labels: class labels corresponding to train samples, (shape: [N])
   :return binary cross entropy
   N = labels.shape[0]
   loss = np.zeros((N,1))
   loss[labels == 1] = - np.log(predictions[labels == 1])
   loss[labels == 0] = - np.log(1-predictions[labels == 0])
   # optional: divide by number of predictions/ labels
   return 1/N * np.sum(loss)
   def d binary cross entropy(predictions: np.ndarray, labels: np.ndarray) -> np.nd
   gradient of the binary cross entropy loss
   :param predictions: predictions by model (shape [N])
   :param labels: class labels corresponding to train samples, (shape [N])
   :return gradient of binary cross entropy, w.r.t. the predictions (shape [N])
```

General Setup & Intialization

Next we are going to set up the Neural Network. We will represent it as a list of weight matrices and a list of bias vectors. Each list has one entry for each layer.

```
def init_weights(neurons_per_hidden_layer: List[int], input_dim: int, output_dim
In [28]:
                  -> Tuple[List[np.ndarray], List[np.ndarray]]:
              :param neurons_per_hidden_layer: list of numbers, indicating the number of n
              :param input dim: input dimension of the network
              :param output_dim: output dimension of the network
              :param seed: seed for random number generator
              return list of weights and biases as specified by dimensions and hidden lay
              # seed random number generator
              rng = np.random.RandomState(seed)
              scale factor = 1.0
              prev_n = input_dim
              weights = []
              biases = []
              # hidden layers
              for n in neurons per hidden layer:
                  # initialize weights with gaussian noise
                  weights.append(scale factor * rng.normal(size=[prev n, n]))
                  # initialize bias with zeros
                  biases.append(np.zeros([1, n]))
                  prev n = n
              # output layer
              weights.append(scale factor * rng.normal(size=[prev n, output dim]))
              biases.append(np.zeros([1, output dim]))
              return weights, biases
```

NOTE As NNs are non-convex, initialization plays a very important role in NN training and there is a lot of work into how to initialize them properly - this here is not a very good initialization, but sufficient for our small example.

1.2) Forward Pass (3 p.)

Next step is the forward pass, i.e., propagate a batch of samples through the network to get the final prediciton. But that's not all - to compute the gradietns later we also need to store all necessary quantities, here those are:

The input to every layer (here called h's)

• The "pre-activation" of every layer, i.e., the quntity that is fed into the non-linearity (here called z's)

```
In [29]:
         def forward_pass(x: np.ndarray, weights: List[np.ndarray], biases: List[np.ndarr
                 -> Tuple[np.ndarray, List[np.ndarray], List[np.ndarray]]:
             propagate input through network
             :param x: input: (shape, [N x input dim])
             :param weights: weight parameters of the layers
             :param biases: bias parameters of the layers
             :return: - Predictions of the network (shape, [N x out_put_dim])
                     - hs: output of each layer (input + all hidden layers) (length: len
                      - zs: preactivation of each layer (all hidden layers + output) (len
             0.00
             hs = [] # list to store all inputs
             zs = [] # list to store all pre-activations
             # input to first hidden layer is just the input to the network
             h = x
             hs.append(h)
             # pass "h" to all hidden layers
             # record all inputs and pre-activations in the lists
             for layer, w in enumerate(weights):
                 b = biases[layer]
                 # weight shape: [2, 64], [64,64], [64, 1]
                 # data shape: [100,2], [64,64], [64,64]
                 # bias shape: [1, 64], [1, 64], [1, 1]
                 print("Layer", layer, "Weights", w.shape, "Data", h.shape)
                 s = np.sum(w.T @ h.T,axis=0)
                 z = (s + b.T).T
                 print(s.shape, z.shape, b.shape)
                 zs.append(z)
                 h = relu(z)
                 print("H:", h.shape)
                 hs.append(h)
             # has to have same shape as labels, i.e. [N,1]
             y = sigmoid(z) # z denotes the pre-activation of the output layer here. Fe
             return y, hs[:-1], zs
```

1.3) Backward Pass (4 p.)

For training by gradient descent we need - well - gradients. Those are computed using backpropagation during the so called "backward pass". We will use the chain rule to propagate the gradient back through the network and at every layer, compute the gradients for the weights and biases at that layer. The initial gradient is given by the gradient of the loss function w.r.t. the network output.

```
weights: List[np.ndarray], biases: List[np.ndarray]) -> \
Tuple[List[np.ndarray], List[np.ndarray]]:
propagate gradient backwards through network
:param loss_grad: gradient of the loss function w.r.t. the network output (s
:param hs: values of all hidden layers during forward pass
:param zs: values of all preactivations during forward pass
:param weights: weight paramameters of the layers
:param biases: bias parameters of the layers
:return: d_weights: List of weight gradients - one entry with same shape for
         d_biases: List of bias gradients - one entry with same shape for ea
# return gradients as lists - we pre-initialize the lists as we iterate back
d_weights = [None] * len(weights)
d_biases = [None] * len(biases)
depth = len(weights)
hs_grad = [None] * (depth+1)
zs_grad = [None] * depth
print(f'Weights: {depth} with shapes: {[w.shape for w in weights]}')
print(f'Biases: {depth} with shapes: {[b.shape for b in biases ]}')
hs_grad[depth] = loss_grad # np.sum(loss_grad).reshape(-1,1)
# backwards trough network -- [2, 1, 0] for 3 layers
for layer in range(depth-1, -1, -1):
    print("values:", hs grad[layer+1].shape, "grad preact:", d sigmoid(zs[la
    zs_grad[layer] = hs_grad[layer+1] * d_relu(zs[layer])
    print("preactivation grad:", zs grad[layer].shape)
    d weights[layer] = np.outer(zs grad[layer],hs[layer])
    d_biases[layer] = zs_grad[layer]
    # update hs grad for next round -- like giving the loss to the subnetwor
    print("Weights:", weights[layer].shape, "Preact Grad:", zs_grad[layer].s
    hs grad[layer] = (weights[layer] @ zs grad[layer].T).T
print(f'Weight Grad: {depth} with shapes: {[w.shape for w in d weights]}')
print(f'Bias Grad: {depth} with shapes: {[b.shape for b in d biases]}')
######################################
return d weights, d biases
```

Tying Everything Together

Finally we can tie everything together and train our network.

```
In [31]: N = train_samples.shape[0]

# hyper parameters
layers = [64, 64]
learning_rate = 1e-2

# init model
weights, biases = init_weights(layers, input_dim=2, output_dim=1, seed=42)
```

```
#book keeping
train_losses = []
test_losses = []
# Here we work with a simple gradient descent implementation, using the whole da
# You can modify it to stochastic gradient descent or a batch gradient descent p
for i in range(1000):
    # predict network outputs and record intermediate quantities using the forwa
    prediction, hs, zs = forward pass(train samples, weights, biases)
    # print("Labels:", train_labels.shape, "vs. predictions", prediction.shape)
    train losses.append(binary cross entropy(prediction, train labels))
    # compute gradients
    loss_grad = d_binary_cross_entropy(prediction, train_labels)
    w_grads, b_grads = backward_pass(loss_grad, hs, zs, weights, biases)
    # apply gradients
    for i in range(len(w_grads)):
        weights[i] -= learning_rate * w_grads[i]
        biases[i] -= learning_rate * b_grads[i]
    test_losses.append(binary_cross_entropy(forward_pass(test_samples, weights,
# plotting
plt.title("Loss")
plt.semilogy(train_losses)
plt.semilogy(test losses)
plt.legend(["Train Loss", "Test Loss"])
def plt solution(samples, labels):
    plt range = np.arange(-1.5, 2.5, 0.01)
    plt grid = np.stack(np.meshgrid(plt range, plt range), axis=-1)
    plt_grid_shape = plt_grid.shape[:2]
    pred grid = np.reshape(forward pass(plt grid, weights, biases)[0], plt grid
    plt.contour(plt_grid[..., 0], plt_grid[..., 1], pred_grid, levels=[0.5], col
    plt.contourf(plt grid[..., 0], plt grid[..., 1], pred grid, levels=10)
    plt.colorbar()
    s0 = plt.scatter(x=samples[labels[:, 0] == 0, 0], y=samples[labels[:, 0] ==
                     label="c=0", c="blue")
    s1 = plt.scatter(x=samples[labels[:, 0] == 1, 0], y=samples[labels[:, 0] ==
                     label="c=1", c="orange")
    plt.legend([s0, s1], ["c0", "c1"])
    plt.xlim(-1.5, 2.5)
    plt.ylim(-1.5, 1.5)
plt.figure()
plt.title("Trained Network - with train samples")
plt solution(train samples, train labels)
plt.figure()
plt.title("Trained Network - with test samples")
plt solution(test samples, test labels)
plt.show()
```

```
Layer 0 Weights (2, 64) Data (100, 2) (100,) (100, 64) (1, 64) H: (100, 64)
```

```
Layer 1 Weights (64, 64) Data (100, 64)
        (100,) (100, 64) (1, 64)
        H: (100, 64)
        Layer 2 Weights (64, 1) Data (100, 64)
        (100,) (100, 1) (1, 1)
        H: (100, 1)
        Weights: 3 with shapes: [(2, 64), (64, 64), (64, 1)]
        Biases: 3 with shapes: [(1, 64), (1, 64), (1, 1)]
        values: (100, 1) grad preact: (100, 1)
        preactivation grad: (100, 1)
        Weights: (64, 1) Preact Grad: (100, 1)
        values: (100, 64) grad preact: (100, 64)
        preactivation grad: (100, 64)
        /home/vincent/.local/lib/python3.6/site-packages/ipykernel launcher.py:32: Runti
        meWarning: overflow encountered in exp
        /home/vincent/.local/lib/python3.6/site-packages/ipykernel_launcher.py:77: Runti
        meWarning: invalid value encountered in true divide
        Weights: (64, 64) Preact Grad: (100, 64)
        values: (100, 64) grad preact: (100, 64)
        preactivation grad: (100, 64)
        Weights: (2, 64) Preact Grad: (100, 64)
        Weight Grad: 3 with shapes: [(6400, 200), (6400, 6400), (100, 6400)]
        Bias Grad: 3 with shapes: [(100, 64), (100, 64), (100, 1)]
        ValueError
                                                  Traceback (most recent call last)
        <ipython-input-31-84f03f73ba91> in <module>
             28  # apply gradients
                  for i in range(len(w_grads)):
             29
        ---> 30
                        weights[i] -= learning_rate * w_grads[i]
             31
                        biases[i] -= learning rate * b grads[i]
        ValueError: operands could not be broadcast together with shapes (2,64) (6400,20
        0) (2,64)
In []: | a = np.ones((100,64))
         np.sum(a,axis=0).reshape(.shape
```

2.) MNIST Classifier with PyTorch (10 p.)

Modern deep learning approaches are mostly implemented using special libraries, providing functionality such as automatic differentiation, common SGD Optimiziers, easy usage of GPUs and so on. We will use PyTorch, at the moment the, arguably, most common framework (for research).

Getting Started

You can find a documentation of the PyTorch API here https://pytorch.org/docs/stable/torch.html# . Don't worry if it seems a lot, we will point out the relevant bits during the exercise as we go along

Installation You can find installation instructions here https://pytorch.org/. Take the most recent stable version (1.7.X). We won't use GPUs here so you can take the cuda-free installation.

We also don't need torchvision nor torchaudio so those don't need to be installed.

Data We finally use a new dataset. The classical MNIST Handwritten Digit Classification set. It consists of grayscale images of size 28x28 of handwritten digits. Let's load it and visualize some of the images. We also do some preprocessing.

```
import torch
In [ ]:
         import torch.nn as nn
         import numpy as np
         data dict = dict(np.load("mnist.npz"))
         # prepare data:
         # - images are casted to float 32 (from uint8) mapped in interval (0,1) and a "f
         # torch uses "NCHW"-layout for 2d convolutions. (i.e., a batch of images is re
         # where the first axis (N) is the batch dimension, the second the (color) **C*
         # and a **W**idth axis). As we have grayscale images there is only 1 color cha
         # - targets are mapped to one hot encoding - torch does that for us
         with torch.no_grad():
             # YTA: We don't need torch to calculate gradients here since we only want to
             # YTA: reshape() because of: https://pytorch.org/tutorials/beginner/blitz/ne
             train_samples = torch.from_numpy(data_dict["train_samples"].astype(np.float3)
             train labels = torch.nn.functional.one hot(torch.from numpy(data dict["train
             test_samples = torch.from_numpy(data_dict["test_samples"].astype(np.float32)
             test labels = torch.nn.functional.one hot(torch.from numpy(data dict["test 1
         # plot first 25 images in train setp
         plt.figure(figsize=(25, 1))
         for i in range(25):
            plt.subplot(1, 25, i + 1)
             # drop channel axis for plotting
             plt.imshow(train samples[i, 0], cmap="gray", interpolation="none")
             plt.gca().axis("off")
```

2.1) Specifiying Networks (4 p.)

The first step in training a neural network is specifying its architecture. Here we will actually build two networks

- classifier_fc: A classifier consisting only of fully connected layers
- classifier_conv: A classifier combining, convolutional layers, pooling and fully connected layers

In the torch API under torch.nn you can find everything you need. Take a look at the classes "Linear", "ReLU", "Softmax", "Conv2d", "MaxPool2d" and "Sequential"

```
# Hidden Layer 2: 128 neurons, Relu activation
    nn.Linear(256,128),
    nn.ReLU(),
    # Outputlayer: 10 neurons (one for each class), softmax activation
    nn.Linear(128,10),
    nn.Softmax()
    ##########
classifier_fc = torch.nn.Sequential(
    *layers fc # unpack layers
# YTA: THIS IS NOT DONE
layers_conv = [
    # Conv Layer 1: 8 filters of 3x3 size, ReLU, Max Pool with size 2x2 and stri
    nn.Conv2d(8, 33, 3, stride=2), # 1 auf 8
    nn.ReLU(),
    nn.MaxPool2d(22,2),
    # Conv Layer 2: 16 filters of 3x3 size, ReLU, Max Pool with size 2x2 and str
    nn.Conv2d(16, 33, 3, stride=2), # 8 auf 16
    nn.ReLU(),
    nn.MaxPool2d(22,2),
    # Flatten
   nn.Flatten(),
    # Fully Connected Layer 1: 64 Neurons, ReLU
   nn.Linear(400, 64),
    nn.ReLU(),
    # Outputlayer: 10 neurons (one for each class), softmax activation
    nn.Linear(64,10),
    nn.Softmax()
classifier_conv = torch.nn.Sequential(
    *layers conv
```

From now on we going to use both the classifiers interchangable, pick one here and the rest should work with both models

```
In [ ]: classifier = classifier_fc
#classifier = classifier_conv
```

2.2) Optimizer and Loss (2 p.)

Next we need to specify an optimizer and a loss function. For the optimizer we will use Adam (look at torch.optim) with default parameters and as a loss function we will use the cross-entropy

```
In [36]: from torch.optim import Adam
    from torch.nn import CrossEntropyLoss

optimizer:torch.optim.Adam = Adam(classifier.parameters(), lr=1e-4)
```

```
def cross_entropy_loss(labels: torch.Tensor, predictions: torch.Tensor) -> torch
    """ Cross entropy Loss:
    :param labels: Ground truth class labels (shape; [N, num_classes])
    :param predictions: predicted class labels (shape: [N, num_classes])
    :return: cross entropy (scalar)
    """

# YTA: I am ~80% sure we should implement this ourselves but I am learning P
    loss = CrossEntropyLoss()
    print(predictions.shape, labels.shape)
    return loss(predictions, labels)
```

2.3) Data Loader (2 p.)

TypeError: 'int' object is not callable

For batch gradient descent we need to shuffle and batch the data, PyTorch provdies some functionality for that in form of the "DataLoader" (Look at torch.utils.data). In the simplest form used here, it simply shuffles and batches the data but you can also build more complex preprocessing pipelines. We also need a loader for the test data.

```
In [37]: from torch.utils.data import DataLoader, TensorDataset

batch_size = 64

#TODO
train_data = TensorDataset(train_samples, train_labels)
train_loader = DataLoader(train_data, batch_size=batch_size, shuffle=True, num_w
test_data = TensorDataset(test_samples, test_labels)
test_loader = DataLoader(test_data, batch_size=batch_size, shuffle=True, num_wo
######
```

```
TypeError
                                          Traceback (most recent call last)
<ipython-input-37-9c783d532527> in <module>
      5 #TODO
---> 6 train data = TensorDataset(train samples, train labels)
     7 train loader = DataLoader(train data, batch size=batch size, shuffle=Tru
e, num workers=0)
      8 test data = TensorDataset(test samples, test labels)
~/.local/lib/python3.6/site-packages/torch/utils/data/dataset.py in init (sel
f, *tensors)
   164
            def init (self, *tensors: Tensor) -> None:
    165
--> 166
                assert all(tensors[0].size(0) == tensor.size(0) for tensor in te
nsors)
   167
               self.tensors = tensors
    168
~/.local/lib/python3.6/site-packages/torch/utils/data/dataset.py in <genexpr>(.
    164
           def __init__(self, *tensors: Tensor) -> None:
    165
--> 166
               assert all(tensors[0].size(0) == tensor.size(0) for tensor in te
nsors)
   167
               self.tensors = tensors
```

2.4) Training (2 p.)

We now have all ingredients and can implement our train loop and a evaluation procedure. You should get a test set accuracy of > 0.95 with both architectures in 2 epochs.

```
In [35]:
         epochs = 2 # small number of epochs should be sufficient to get descent perform
         train_losses = []
         test losses = []
         for i in range(epochs):
             print("Epoch {:03d}".format(i + 1))
             for batch in train_loader:
                 #TODO####################
                 # forward pass
                 samples, labels = batch
                 predictions = classifier(samples)
                 # backward pass
                 # YTA: note for the future: https://discuss.pytorch.org/t/runtimeerror-m
                 loss = cross_entropy_loss(labels, predictions)
                 optimizer.zero_grad() # clear gradient buffers
                 loss.backward()
                 # update step
                 optimizer.step()
                 ###########################
                 train losses.append(loss.detach().numpy())
         # Evaluate (we still need batching as evaluating all test points at once would p
         avg loss = avg acc = 0
         for batch in test loader:
             samples, labels = batch
             predictions = classifier(samples)
             loss = cross entropy loss(labels, predictions)
             acc = torch.count nonzero(predictions.argmax(dim=-1) == labels.argmax(dim=-1)
             avg acc += acc / len(test loader)
             avg loss += loss / len(test loader)
         print("Test Set Accuracy: {:.3f}, Test Loss {:.3f}".format(avg acc.detach().nump
         plt.figure()
         plt.semilogy(train losses)
         plt.show()
         Epoch 001
         torch.Size([64, 10]) torch.Size([64, 10])
         ______
         RuntimeError
                                                 Traceback (most recent call last)
         <ipython-input-35-7f29c3f5b91f> in <module>
             16
             17
                        # YTA: note for the future: https://discuss.pytorch.org/t/runtim
         eerror-multi-target-not-supported-newbie/10216/2
                        loss = cross_entropy_loss(labels, predictions)
         ---> 18
             19
                        optimizer.zero grad() # clear gradient buffers
```

```
<ipython-input-33-055bca1060a8> in cross entropy loss(labels, predictions)
             13
                    loss = CrossEntropyLoss()
             14
                    print(predictions.shape, labels.shape)
        ---> 15
                    return loss(predictions, labels)
        ~/.local/lib/python3.6/site-packages/torch/nn/modules/module.py in call impl(se
        lf, *input, **kwargs)
            725
                            result = self._slow_forward(*input, **kwargs)
            726
                        else:
        --> 727
                            result = self.forward(*input, **kwargs)
            728
                        for hook in itertools.chain(
            729
                                _global_forward_hooks.values(),
        ~/.local/lib/python3.6/site-packages/torch/nn/modules/loss.py in forward(self, i
        nput, target)
            960
                    def forward(self, input: Tensor, target: Tensor) -> Tensor:
            961
                        return F.cross_entropy(input, target, weight=self.weight,
        --> 962
                                                ignore index=self.ignore index, reduction
        =self.reduction)
            963
            964
        ~/.local/lib/python3.6/site-packages/torch/nn/functional.py in cross entropy(inp
        ut, target, weight, size average, ignore index, reduce, reduction)
                    if size average is not None or reduce is not None:
           2466
           2467
                        reduction = _Reduction.legacy_get_string(size_average, reduce)
        -> 2468
                    return nll_loss(log_softmax(input, 1), target, weight, None, ignore_
        index, None, reduction)
           2469
           2470
        ~/.local/lib/python3.6/site-packages/torch/nn/functional.py in nll loss(input, t
        arget, weight, size average, ignore index, reduce, reduction)
           2262
                                          .format(input.size(0), target.size(0)))
           2263
                    if dim == 2:
        -> 2264
                        ret = torch. C. nn.nll loss(input, target, weight, Reduction.ge
        t enum(reduction), ignore index)
                    elif dim == 4:
           2265
                        ret = torch. C. nn.nll loss2d(input, target, weight, Reduction.
           2266
        get enum(reduction), ignore index)
        RuntimeError: 1D target tensor expected, multi-target not supported
In [ ]:
```

20

In []:

loss.backward()