Assignment 6: Neural Networks

1. Backpropagation - Essentials

As you examined in class, a simple layer in a feedforward neural network can be expressed as the following:

$$h = Wx + b$$

$$t = \sigma(h)$$

$$\mathcal{L} = \frac{1}{2}(y - t)^2$$

where x is the input, W is the weight matrix at this node, b is the bias added at the node, $\sigma(\cdot)$ is the activation function, y is the label, and $\mathcal{L}$ is the loss.

The activation function and the loss function (squared loss used here) are choices made when creating a neural network.

a. What are the unknowns in the problem?

The unknowns are the weight matrix W and the bias vector b.

b. What do we want minimize?

We want to minimize the loss function.

c. What method could we use to find the unknowns?

We can either use gradient descent or optimize with calculus (depending on the choice of loss).

d. Find the partial derivatives of L with respect to the unknowns.

Assume we use ReLU for the activation function.

Let $\mathbf{w}_i$ be the i-th row of the matrix W. Then, the gradient of $\mathcal{L}$ will be a vector, and we can calculate its i-th entry:

For $h \geq 0$: $t = h$, so

$$(\nabla_W \mathcal{L})_i = \frac{\delta \mathcal{L}}{\delta \mathbf{w}_i} = \frac{\delta \mathcal{L}}{\delta h}\frac{\delta h}{\delta \mathbf{w}_i} = -(y_i - h_i)x = -(y_i - \mathbf{w}_i \cdot x - b_i)x$$
$$\frac{\delta \mathcal{L}}{\delta b} = -(y - Wx - b)$$

For $h < 0$: $t = 0$, so

$$(\nabla_W \mathcal{L})_i = 0$$
$$\frac{\delta \mathcal{L}}{\delta b} = 0$$

2. Backpropagation

A neural network is regarded as compositional, in that the output of one layer feeds in as the input to the next layer. Using the the same notation as above but ignoring the bias b for simplicity:

$$t = \sigma_L(W_L \sigma_{L-1}(\ldots \sigma_2(W_2 \sigma_1(W_1 x))\ldots))$$

Here x is the original input data, and t is the output of the neural network.

Even more simply, we can look at each layer L:

$$N_1 \rightarrow N_2 \rightarrow N_3 \rightarrow \ldots N_{L-1} \rightarrow N_L$$

The idea here is the same - we will need to solve for partial derivatives for each layer to set the unknowns. As the previous layer feeds into the next, you can only solve for a Jacobian (vector of partials) one wrt one layer down e.g. we can first solve for

$$J_{N_L}(N_{L-1})$$

the Jacobian of N_L with respect to N_{L-1}

a. For the above simple representation, write out the Jacobian of the the final layer with respect to the first layer.

TODO:

b. Based on the equation you've described above, explain using time or space complexity why the best way to solve for the gradient in 2a. is to work backwards.

TODO:

3. Simple Neural Network

Here you'll try out writing a neural network for a simple classification problem. For full credit, the final test accuracy should be above 0.6.

The dataset is of cell images from thin blood smear slides of segmented cells, with labels indicating the presence of malaria.

Source: [https://lhncbc.nlm.nih.gov/publication/pub9932 (https://lhncbc.nlm.nih.gov/publication/pub9932)](https://lhncbc.nlm.nih.gov/publication/pub9932)

Paper: [https://www.ncbi.nlm.nih.gov/pmc/articles/PMC6544011/ (https://www.ncbi.nlm.nih.gov/pmc/articles/PMC6544011/)](https://www.ncbi.nlm.nih.gov/pmc/articles/PMC6544011/)

Some setup to start with:

In [ ]:
```python
import numpy as np
import matplotlib.pyplot as plt
import tensorflow as tf
import cv2
from tensorflow import keras
import tensorflow_datasets as tfds
from sklearn import model_selection
```

In [ ]:
```
malaria, info = tfds.load(name="malaria", split="train", with_info=Tru
malaria = malaria.shuffle(30000).prefetch(tf.data.experimental.AUTOTUN
info
```

Out[2]:
```
tfds.core.DatasetInfo(
    name='malaria',
    version=1.0.0,
    description='The Malaria dataset contains a total of 27,558 cell
images
with equal instances of parasitized and uninfected cells from the thi
n blood
smear slide images of segmented cells.',
    homepage='https://lhncbc.nlm.nih.gov/publication/pub9932',
    features=FeaturesDict({
        'image': Image(shape=(None, None, 3), dtype=tf.uint8),
        'label': ClassLabel(shape=(), dtype=tf.int64, num_classes=2),
    }),
    total_num_examples=27558,
    splits={
        'train': 27558,
    },
    supervised_keys=('image', 'label'),
    citation="""@article{rajaraman2018pre,
      title={Pre-trained convolutional neural networks as feature ext
ractors toward
      improved malaria parasite detection in thin blood smear images}
,
      author={Rajaraman, Sivaramakrishnan and Antani, Sameer K and Po
ostchi, Mahdieh
      and Silamut, Kamolrat and Hossain, Md A and Maude, Richard J an
d Jaeger,
      Stefan and Thoma, George R},
      journal={PeerJ},
      volume={6},
      pages={e4568},
      year={2018},
      publisher={PeerJ Inc.}
    }""",
    redistribution_info=,
)
```

In [ ]:
```
info
```

Out[3]:
```
tfds.core.DatasetInfo(
    name='malaria',
    version=1.0.0,
    description='The Malaria dataset contains a total of 27,558 cell
images
with equal instances of parasitized and uninfected cells from the thi
n blood
smear slide images of segmented cells.',
    homepage='https://lhncbc.nlm.nih.gov/publication/pub9932',
    features=FeaturesDict({
        'image': Image(shape=(None, None, 3), dtype=tf.uint8),
        'label': ClassLabel(shape=(), dtype=tf.int64, num_classes=2),
    }),
    total_num_examples=27558,
    splits={
        'train': 27558,
    },
    supervised_keys=('image', 'label'),
    citation="""@article{rajaraman2018pre,
      title={Pre-trained convolutional neural networks as feature ext
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,
      author={Rajaraman, Sivaramakrishnan and Antani, Sameer K and Po
ostchi, Mahdieh
      and Silamut, Kamolrat and Hossain, Md A and Maude, Richard J an
d Jaeger,
      Stefan and Thoma, George R},
      journal={PeerJ},
      volume={6},
      pages={e4568},
      year={2018},
      publisher={PeerJ Inc.}
    }""",
    redistribution_info=,
)
```
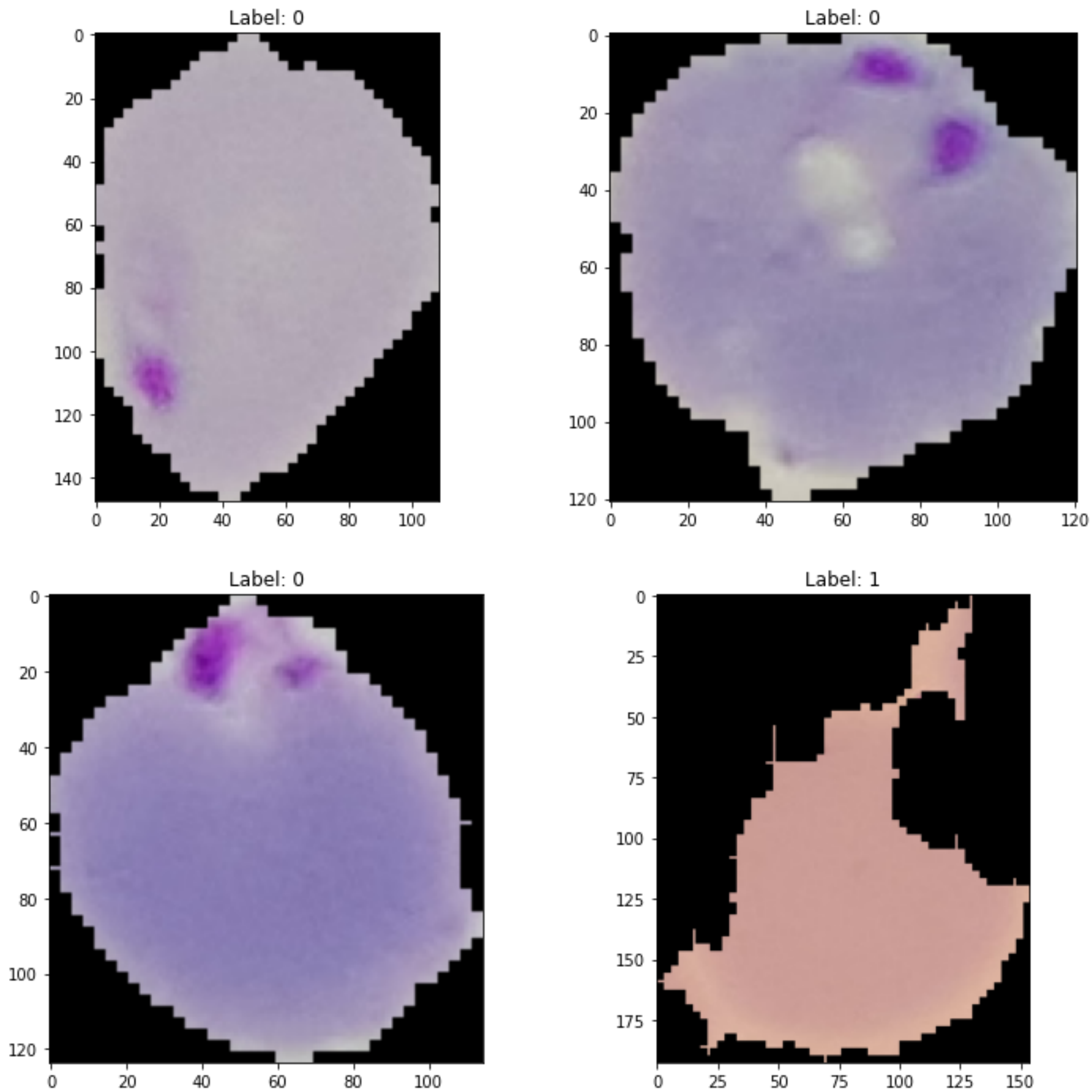

In [ ]:
```
# Visualize some images
plt.figure(figsize=(12,12))

for i, feature in enumerate(malaria.take(4)):
    image = feature["image"].numpy()
    label = feature["label"].numpy()

    plt.subplot(2, 2, i+1)
    plt.title("Label: "+str(label))
    plt.imshow(image)
    # i+=1
plt.show()
```



a. Extract some samples from the malaria dataset

Hints:

- Keep the total number of samples small (< 10000) - it largely depends on your memory (if your notebook starts to crash, reduce the number of samples and try again)
- The dimension of each image is height * width * 3, with the 3 representing the number of channels
- The height and width of the images aren't all the same, so resize all of them to be 133 by 133 (see [cv2.resize (https://medium.com/@manivannan_data/resize-image-using-opencv-python-d2cdbbc480f0)](https://medium.com/@manivannan_data/resize-image-using-opencv-python-d2cdbbc480f0))
- The possibles labels are 0s and 1s (scalars)
- Split into a training and testing set (a split like 80:20 train to test is reasonable)

In [ ]:
```
# TODO: Initialize to the correct shapes with zeros
malaria = tfds.load("malaria", split='train[:10000]')

images = []
labels = []
dim = (133, 133)
for feature in malaria:
    images.append(cv2.resize(feature["image"].numpy(), dim) / 255)
    labels.append(feature["label"].numpy())

images = np.array(images)
labels = np.array(labels)

train_images, test_images, train_labels, test_labels = model_selectior
```

b. Add some layers to the model

Hints:

- See examples of layers in the Keras documentation: [https://keras.io/layers/core/ (https://keras.io/layers/core/)](https://keras.io/layers/core/)
- For the first layer, provide an input_shape, which refers to the shape of an image from your dataset

See examples at [https://www.tensorflow.org/tutorials (https://www.tensorflow.org/tutorials)](https://www.tensorflow.org/tutorials)

In [ ]:
```
model = keras.Sequential([keras.Input(shape=(133, 133, 3))])

model.add(keras.layers.Conv2D(16, 3, activation='relu', padding='same'
model.add(keras.layers.MaxPool2D())
model.add(keras.layers.BatchNormalization())
model.add(keras.layers.Conv2D(32, 3, activation='relu', padding='same'
model.add(keras.layers.BatchNormalization())
model.add(keras.layers.MaxPool2D())
model.add(keras.layers.Conv2D(64, 3, activation='relu', padding='same'
model.add(keras.layers.BatchNormalization())
model.add(keras.layers.MaxPool2D())

model.add(keras.layers.Flatten())

model.add(keras.layers.Dense(256, activation='relu'))
model.add(keras.layers.BatchNormalization())

model.add(keras.layers.Dense(128, activation='relu'))
model.add(keras.layers.BatchNormalization())

model.add(keras.layers.Dense(64, activation='relu'))
model.add(keras.layers.BatchNormalization())

model.add(keras.layers.Dense(32, activation='relu'))
model.add(keras.layers.BatchNormalization())
model.add(keras.layers.Dropout(0.5))

model.add(keras.layers.Dense(1, activation='sigmoid'))
```

c. Choose how to train the above model

Pick an optimizer, loss function, and metric. If you choose something not covered in class, give a brief explanation and an advantage of your choice.

- Optimizers: [https://keras.io/optimizers/ (https://keras.io/optimizers/)](https://keras.io/optimizers/)
- Losses: [https://keras.io/losses/ (https://keras.io/losses/)](https://keras.io/losses/)
- Metrics: [https://keras.io/metrics/ (https://keras.io/metrics/)](https://keras.io/metrics/)

Reasoning:

Chose the Adam optimizer since it is "well suited for problems that are large in terms of data/parameters".

Chose binary cross entropy since we are performing binary classification -- we would not want to use loss functions better suited for regression such as mean squared error or multi-class classification losses such as general cross-entropy.

Chose AUC as the metric since it was the first listed metric under classification, wasn't sure how to distinguish between other metrics.

In [ ]:
```
# TODO:
opt = 'adam'
loss_func = 'binary_crossentropy'
metric = keras.metrics.AUC(name='auc')
```

In [ ]:
```
model.compile(optimizer=opt,
              loss=loss_func,
              metrics=metric)
```

d. Train the model

Choose an appropriate number of epochs (Hint: try some different values)

In [ ]:
```
# TODO:
num_epochs = 5

model.fit(train_images, train_labels, epochs=num_epochs)
```

```
Epoch 1/5
250/250 [==============================] - 161s 635ms/step - loss: 0.
7604 - auc: 0.6915
Epoch 2/5
250/250 [==============================] - 157s 627ms/step - loss: 0.
2841 - auc: 0.9506
Epoch 3/5
250/250 [==============================] - 154s 617ms/step - loss: 0.
2060 - auc: 0.9722
Epoch 4/5
250/250 [==============================] - 155s 622ms/step - loss: 0.
2014 - auc: 0.9734
Epoch 5/5
250/250 [==============================] - 155s 618ms/step - loss: 0.
1556 - auc: 0.9834
```

Out[7]:
```
<tensorflow.python.keras.callbacks.History at 0x7faa0ef3d950>
```

e. Evaluate based on the testing set

Must be greater that 0.55 for full credit

In [ ]:
```
test_loss, test_acc = model.evaluate(test_images, test_labels, verbose

print('\nTest accuracy:', test_acc)
```

```
63/63 - 11s - loss: 0.3282 - auc: 0.9684

Test accuracy: 0.9683736562728882
```

f. Based on the above accuracies between the testing and training sets, did you overfit while training?

It seems like the model was overfit while training since the accuracy for the last epoch was slightly higher than the accuracy for the training set.

g. (Extra Credit) Improve your model to achieve an accuracy of greater than 0.70 on the testing set.