BIOSTAT823 Final Project

December 12, 2022

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In this notebook, we explore different neural network architectures to predict for in-hospital mortality using the "In Hospital Mortality Prediction" data set, which is taken from https://www.kaggle.com/datasets/saurabhshahane/in-hospital-mortality-prediction. This dataset was derived from the MIMIC III dataset, and includes demographic characteristics (age, sex, ethnicity, weight, and height), vital signs (all continuous variables), comorbidities (all binary variables), and laboratory variables (all continuous variables).

The demographic characteristics and vital signs were taken once during the first 24 hours of ICU admission, laboratory variables were measured throughout the entire ICU stay, and comorbidities were determined via ICD-9 codes. The mean value was reported if there were multiple measurements of a variable recorded throughout the ICU stay. The primary outcome was in-hospital mortality, defined as the vital status of the patient at the time of discharge.

Training and validation epoch outputs are not shown as to limit the number of pages in the notebook.

1 Set-Up

1.1 Library Import

[ ]:
```
# Library import
import os
import numpy as np
import math
import random
import matplotlib.pyplot as plt
import pandas as pd
import tensorflow as tf

from sklearn.impute import SimpleImputer
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import MinMaxScaler
from sklearn.metrics import mean_squared_error
from sklearn import metrics
from sklearn.utils import compute_class_weight
from tensorflow import keras
from tensorflow.keras import Sequential
from tensorflow.keras import layers
from tensorflow.keras.layers import Dense, Dropout
from tensorflow.keras import optimizers
from tensorflow.keras import regularizers
from tensorflow.keras import callbacks
from tensorflow.keras.callbacks import EarlyStopping
from sklearn.metrics import confusion_matrix
from sklearn.metrics import roc_curve
from sklearn.metrics import roc_auc_score
from sklearn.metrics import auc
from sklearn.metrics import precision_recall_curve
from sklearn.metrics import f1_score
```

1.2 Importing Data

The imported dataset had a size of 1177 x 51.

[ ]:
```
# Set Seed
tf.random.set_seed(1)
```

[ ]:
```
# All data
df = pd.read_csv("data01.csv")
print(df.shape)
df.head(5)
```

```
(1177, 51)
```

[ ]:
```
   group      ID  outcome  age  gendera        BMI  hypertensive  \
0      1  125047      0.0   72        1  37.588179             0
1      1  139812      0.0   75        2        NaN             0
2      1  109787      0.0   83        2  26.572634             0
3      1  130587      0.0   43        2  83.264629             0
4      1  138290      0.0   75        2  31.824842             1

   atrialfibrillation  CHD with no MI  diabetes  …  Blood sodium  \
0                   0               0         1  …    138.750000
1                   0               0         0  …    138.888889
2                   0               0         0  …    140.714286
3                   0               0         0  …    138.500000
4                   0               0         0  …    136.666667

   Blood calcium    Chloride  Anion gap  Magnesium ion     PH  Bicarbonate  \
0       7.463636  109.166667  13.166667       2.618182  7.230    21.166667
1       8.162500   98.444444  11.444444       1.887500  7.225    33.444444
2       8.266667  105.857143  10.000000       2.157143  7.268    30.571429
```

```
3       9.476923   92.071429  12.357143       1.942857  7.370     38.571429
4       8.733333  104.500000  15.166667       1.650000  7.250     22.000000

   Lactic acid  PCO2  EF
0          0.5  40.0  55
1          0.5  78.0  55
2          0.5  71.5  35
3          0.6  75.0  55
4          0.6  50.0  55

[5 rows x 51 columns]
```

2 Data Pre-processing

2.1 Data Scaling

We must first scale the continuous variables to be in range [0, 1] to standardize the image inputs for neural networks.

[ ]:
```
# Scale continuous vars
noncont_cols = ["group", "ID", "outcome", "gendera", "hypertensive",␣
 ↪"atrialfibrillation", "CHD with no MI", "diabetes",
                 "deficiencyanemias","depression","Hyperlipemia","Renal␣
 ↪failure","COPD"]
all_cols = list(df.columns.values)
cont_df = df.drop(noncont_cols, axis = 1)
scaled_df = (cont_df-cont_df.min())/(cont_df.max()-cont_df.min())
clean_df = pd.concat((df[noncont_cols], scaled_df), 1)
print(clean_df.shape)
clean_df.head(5)
```

```
(1177, 51)

<ipython-input-27-a57081da2b61>:7: FutureWarning: In a future version of pandas
all arguments of concat except for the argument 'objs' will be keyword-only
  clean_df = pd.concat((df[noncont_cols], scaled_df), 1)
```

[ ]:
```
   group      ID  outcome  gendera  hypertensive  atrialfibrillation  \
0      1  125047      0.0        1             0                   0
1      1  139812      0.0        2             0                   0
2      1  109787      0.0        2             0                   0
3      1  130587      0.0        2             0                   0
4      1  138290      0.0        2             1                   0

   CHD with no MI  diabetes  deficiencyanemias  depression  …  Blood sodium  \
0               0         1                  1           0  …      0.601029
```

```
1              0         0                  1           0  …       0.604495
2              0         0                  1           0  …       0.650050
3              0         0                  0           0  …       0.594790
4              0         0                  1           0  …       0.549037

   Blood calcium  Chloride  Anion gap  Magnesium ion        PH  Bicarbonate  \
0       0.179679  0.683867   0.346185       0.455782  0.285714     0.238714
1       0.344118  0.430145   0.254886       0.182398  0.275510     0.591427
2       0.368627  0.605553   0.178313       0.283285  0.363265     0.508892
3       0.653394  0.279339   0.303270       0.203110  0.571429     0.738714
4       0.478431  0.573439   0.452209       0.093537  0.326531     0.262654

   Lactic acid      PCO2        EF
0     0.000000  0.266124  0.666667
1     0.000000  0.742016  0.666667
2     0.000000  0.660614  0.333333
3     0.012766  0.704446  0.666667
4     0.012766  0.391359  0.666667

[5 rows x 51 columns]
```

2.2 Missing Values

We then check for missing values. One observation had a missing value for outcome. That individual was removed. We then performed mean imputation for those with missing laboratory values.

[ ]:
```
# Get number of NAs
clean_df.isna().sum()
```

[ ]:
```
group                         0
ID                            0
outcome                       1
gendera                       0
hypertensive                  0
atrialfibrillation            0
CHD with no MI                0
diabetes                      0
deficiencyanemias             0
depression                    0
Hyperlipemia                  0
Renal failure                 0
COPD                          0
age                           0
BMI                         215
heart rate                   13
Systolic blood pressure      16
```

```
Diastolic blood pressure     16
Respiratory rate             13
temperature                  19
SP O2                        13
Urine output                 36
hematocrit                    0
RBC                           0
MCH                           0
MCHC                          0
MCV                           0
RDW                           0
Leucocyte                     0
Platelets                     0
Neutrophils                 144
Basophils                   259
Lymphocyte                  145
PT                           20
INR                          20
NT-proBNP                     0
Creatine kinase             165
Creatinine                    0
Urea nitrogen                 0
glucose                      18
Blood potassium               0
Blood sodium                  0
Blood calcium                 1
Chloride                      0
Anion gap                     0
Magnesium ion                 0
PH                          292
Bicarbonate                   0
Lactic acid                 229
PCO2                        294
EF                            0
dtype: int64
```

[ ]:
```python
# Remove where outcome is unknown
clean_df2 = clean_df[~clean_df['outcome'].isna()]
print(clean_df2.shape)
clean_df2.head(5)
```

```
(1176, 51)
```

[ ]:
```
   group      ID  outcome  gendera  hypertensive  atrialfibrillation  \
0      1  125047      0.0        1             0                   0
1      1  139812      0.0        2             0                   0
2      1  109787      0.0        2             0                   0
```

```
3      1  130587      0.0        2            0                   0
4      1  138290      0.0        2            1                   0

   CHD with no MI  diabetes  deficiencyanemias  depression  …  Blood sodium  \
0               0         1                  1           0  …      0.601029
1               0         0                  1           0  …      0.604495
2               0         0                  1           0  …      0.650050
3               0         0                  0           0  …      0.594790
4               0         0                  1           0  …      0.549037

   Blood calcium  Chloride  Anion gap  Magnesium ion        PH  Bicarbonate  \
0       0.179679  0.683867   0.346185       0.455782  0.285714     0.238714
1       0.344118  0.430145   0.254886       0.182398  0.275510     0.591427
2       0.368627  0.605553   0.178313       0.283285  0.363265     0.508892
3       0.653394  0.279339   0.303270       0.203110  0.571429     0.738714
4       0.478431  0.573439   0.452209       0.093537  0.326531     0.262654

   Lactic acid      PCO2        EF
0     0.000000  0.266124  0.666667
1     0.000000  0.742016  0.666667
2     0.000000  0.660614  0.333333
3     0.012766  0.704446  0.666667
4     0.012766  0.391359  0.666667

[5 rows x 51 columns]
```

[ ]:
```
# Imput with mean
cont_df = clean_df2.drop(noncont_cols, axis = 1)
imputed_df = cont_df.fillna(cont_df.mean())
clean_df3 = pd.concat((clean_df2[noncont_cols], imputed_df), 1)
clean_df3.head(5)
```

```
<ipython-input-183-601ef2ee5cec>:4: FutureWarning: In a future version of pandas
all arguments of concat except for the argument 'objs' will be keyword-only
  clean_df3 = pd.concat((clean_df2[noncont_cols], imputed_df), 1)
```

[ ]:
```
   group      ID  outcome  gendera  hypertensive  atrialfibrillation  \
0      1  125047      0.0        1            0                   0
1      1  139812      0.0        2            0                   0
2      1  109787      0.0        2            0                   0
3      1  130587      0.0        2            0                   0
4      1  138290      0.0        2            1                   0

   CHD with no MI  diabetes  deficiencyanemias  depression  …  Blood sodium  \
0               0         1                  1           0  …      0.601029
1               0         0                  1           0  …      0.604495
2               0         0                  1           0  …      0.650050
```

```
3              0        0                  0           0  …       0.594790
4              0        0                  1           0  …       0.549037

   Blood calcium  Chloride  Anion gap  Magnesium ion        PH  Bicarbonate  \
0       0.179679  0.683867   0.346185       0.455782  0.285714     0.238714
1       0.344118  0.430145   0.254886       0.182398  0.275510     0.591427
2       0.368627  0.605553   0.178313       0.283285  0.363265     0.508892
3       0.653394  0.279339   0.303270       0.203110  0.571429     0.738714
4       0.478431  0.573439   0.452209       0.093537  0.326531     0.262654

   Lactic acid      PCO2        EF
0     0.000000  0.266124  0.666667
1     0.000000  0.742016  0.666667
2     0.000000  0.660614  0.333333
3     0.012766  0.704446  0.666667
4     0.012766  0.391359  0.666667

[5 rows x 51 columns]
```

2.3 Data types

We then looked at the data types of the variables. The outcome variable was shown to be of float64. We converted it to int64. We also saw that gender was coded as 1 or 2. We converted gender to be coded as 0 or 1.

```
[ ]: # Get info
     print(clean_df3.info(verbose = True))
```

```
<class 'pandas.core.frame.DataFrame'>
Int64Index: 1176 entries, 0 to 1176
Data columns (total 51 columns):
 #   Column                    Non-Null Count  Dtype
---  ------                    --------------  -----
 0   group                     1176 non-null   int64
 1   ID                        1176 non-null   int64
 2   outcome                   1176 non-null   float64
 3   gendera                   1176 non-null   int64
 4   hypertensive              1176 non-null   int64
 5   atrialfibrillation        1176 non-null   int64
 6   CHD with no MI            1176 non-null   int64
 7   diabetes                  1176 non-null   int64
 8   deficiencyanemias         1176 non-null   int64
 9   depression                1176 non-null   int64
 10  Hyperlipemia              1176 non-null   int64
 11  Renal failure             1176 non-null   int64
 12  COPD                      1176 non-null   int64
 13  age                       1176 non-null   float64
 14  BMI                       1176 non-null   float64
 15  heart rate                1176 non-null   float64
 16  Systolic blood pressure   1176 non-null   float64
 17  Diastolic blood pressure  1176 non-null   float64
 18  Respiratory rate          1176 non-null   float64
 19  temperature               1176 non-null   float64
 20  SP O2                     1176 non-null   float64
 21  Urine output              1176 non-null   float64
 22  hematocrit                1176 non-null   float64
 23  RBC                       1176 non-null   float64
 24  MCH                       1176 non-null   float64
 25  MCHC                      1176 non-null   float64
 26  MCV                       1176 non-null   float64
 27  RDW                       1176 non-null   float64
 28  Leucocyte                 1176 non-null   float64
 29  Platelets                 1176 non-null   float64
 30  Neutrophils               1176 non-null   float64
 31  Basophils                 1176 non-null   float64
 32  Lymphocyte                1176 non-null   float64
 33  PT                        1176 non-null   float64
 34  INR                       1176 non-null   float64
 35  NT-proBNP                 1176 non-null   float64
 36  Creatine kinase           1176 non-null   float64
 37  Creatinine                1176 non-null   float64
 38  Urea nitrogen             1176 non-null   float64
 39  glucose                   1176 non-null   float64
 40  Blood potassium           1176 non-null   float64
 41  Blood sodium              1176 non-null   float64
 42  Blood calcium             1176 non-null   float64
 43  Chloride                  1176 non-null   float64
 44  Anion gap                 1176 non-null   float64
 45  Magnesium ion             1176 non-null   float64
 46  PH                        1176 non-null   float64
 47  Bicarbonate               1176 non-null   float64
 48  Lactic acid               1176 non-null   float64
 49  PCO2                      1176 non-null   float64
 50  EF                        1176 non-null   float64
dtypes: float64(39), int64(12)
memory usage: 477.8 KB
None
```

[ ]:
```
# Change dtype of outcome
clean_df3.outcome = clean_df3.outcome.astype(int)
print(clean_df3.info(verbose = True))
```

```
<class 'pandas.core.frame.DataFrame'>
Int64Index: 1176 entries, 0 to 1176
Data columns (total 51 columns):
 #   Column                    Non-Null Count  Dtype
---  ------                    --------------  -----
 0   group                     1176 non-null   int64
 1   ID                        1176 non-null   int64
 2   outcome                   1176 non-null   int64
 3   gendera                   1176 non-null   int64
 4   hypertensive              1176 non-null   int64
 5   atrialfibrillation        1176 non-null   int64
 6   CHD with no MI            1176 non-null   int64
 7   diabetes                  1176 non-null   int64
 8   deficiencyanemias         1176 non-null   int64
 9   depression                1176 non-null   int64
 10  Hyperlipemia              1176 non-null   int64
 11  Renal failure             1176 non-null   int64
 12  COPD                      1176 non-null   int64
 13  age                       1176 non-null   float64
 14  BMI                       1176 non-null   float64
 15  heart rate                1176 non-null   float64
 16  Systolic blood pressure   1176 non-null   float64
 17  Diastolic blood pressure  1176 non-null   float64
 18  Respiratory rate          1176 non-null   float64
 19  temperature               1176 non-null   float64
 20  SP O2                     1176 non-null   float64
 21  Urine output              1176 non-null   float64
 22  hematocrit                1176 non-null   float64
 23  RBC                       1176 non-null   float64
 24  MCH                       1176 non-null   float64
 25  MCHC                      1176 non-null   float64
 26  MCV                       1176 non-null   float64
 27  RDW                       1176 non-null   float64
 28  Leucocyte                 1176 non-null   float64
 29  Platelets                 1176 non-null   float64
 30  Neutrophils               1176 non-null   float64
 31  Basophils                 1176 non-null   float64
 32  Lymphocyte                1176 non-null   float64
 33  PT                        1176 non-null   float64
 34  INR                       1176 non-null   float64
 35  NT-proBNP                 1176 non-null   float64
 36  Creatine kinase           1176 non-null   float64
 37  Creatinine                1176 non-null   float64
 38  Urea nitrogen             1176 non-null   float64
 39  glucose                   1176 non-null   float64
 40  Blood potassium           1176 non-null   float64
 41  Blood sodium              1176 non-null   float64
 42  Blood calcium             1176 non-null   float64
 43  Chloride                  1176 non-null   float64
 44  Anion gap                 1176 non-null   float64
 45  Magnesium ion             1176 non-null   float64
 46   PH                         1176 non-null   float64
 47   Bicarbonate                1176 non-null   float64
 48   Lactic acid                1176 non-null   float64
 49   PCO2                       1176 non-null   float64
 50   EF                         1176 non-null   float64
dtypes: float64(38), int64(13)
memory usage: 477.8 KB
None
```

[ ]:
```
# Change gender to be binary, 0 or 1
clean_df4 = clean_df3.copy()
clean_df4['gendera'] = clean_df4['gendera'].replace([1,2],[0, 1])
clean_df4.gendera.head(5)
```

[ ]:
```
0    1017
1     159
Name: outcome, dtype: int64
```

3 Dataset Splitting

The dataset was split to be in a 80:10:10 ratio (training, validation, testing). The split data was then converted to tensors, with the predictor tensors of the training, validation, and testing datasets being of respective size (940, 48), (118, 48), and (118, 48). Class imbalance was checked and in-hospital mortality was shown to have a prevalence of 0.135. To address this, class weights were calculated to give more weight to those observations with an observed in-hospital mortality.

[ ]:
```
# Split train, val, and test in 80:10:10
x = clean_df4.drop(["group","ID", "outcome"], axis = 1).copy()
y = clean_df4['outcome']
X_train, X_rem, y_train, y_rem = train_test_split(x,y, train_size=0.8)
X_valid, X_test, y_valid, y_test = train_test_split(X_rem,y_rem, test_size=0.5)

print(X_train.shape), print(y_train.shape)
print(X_valid.shape), print(y_valid.shape)
print(X_test.shape), print(y_test.shape)
```

```
(940, 48)
(940,)
(118, 48)
(118,)
(118, 48)
(118,)
```

[ ]:
```
(None, None)
```

[ ]:
```
# Convert to tensors
train_x = tf.stack(X_train)
train_y = tf.stack(y_train)
val_x = tf.stack(X_valid)
val_y = tf.stack(y_valid)
test_x = tf.stack(X_test)
test_y = tf.stack(y_test)
test_y
```

[ ]:
```
<tf.Tensor: shape=(118,), dtype=int64, numpy=
array([0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 1, 0, 0, 0, 0, 0,
       1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0,
       0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 1, 0, 0, 1, 0, 0, 0,
       1, 0, 1, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 1, 1, 0, 0, 0, 0, 0,
       0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1,
       0, 0, 1, 0, 0, 0, 0, 0])>
```

[ ]:
```
# Examine class imbalance
clean_df4['outcome'].value_counts()
```

[ ]:
```
0    1017
1     159
Name: outcome, dtype: int64
```

[ ]:
```
class_weights = compute_class_weight(class_weight = "balanced",
                                     classes = np.unique(y_train),
                                     y = y_train
                                    )
class_weights = dict(zip(np.unique(y_train), class_weights))
class_weights
```

[ ]:
```
{0: 0.5752753977968176, 1: 3.821138211382114}
```

4 First Model

4.1 Architecture

[ ]:
```
model = Sequential([
                    tf.keras.Input(48),
                    tf.keras.layers.Flatten(),
                    tf.keras.layers.Dense(128, activation=tf.nn.relu),
                    tf.keras.layers.Dense(1, activation=tf.nn.sigmoid)
                    ]
                   )
model.summary()
```

```
Model: "sequential_33"
_________________________________________________________________
 Layer (type)                Output Shape              Param #
=================================================================
 flatten_34 (Flatten)        (None, 48)                0

 dense_68 (Dense)            (None, 128)               6272

 dense_69 (Dense)            (None, 1)                 129

=================================================================
Total params: 6,401
Trainable params: 6,401
Non-trainable params: 0
_________________________________________________________________
```

The model has an input layer, flatten layer, and two dense layers. The first input layers takes in the shape of (48) as that is the shape of the number of predictors. Inputs are flattened and passed to a dense layer with 128 hidden units and a ReLU activation function. The final output layer has 1 hidden unit with activation function sigmoid to return a predicted probability for in-hospital mortality from 0 to 1.

[ ]:
```
# Define path to store callback
cp_path = "model1.ckpt"
cp_dir = os.path.dirname(cp_path)

# Callback that saves the models weights at the best validation accuracy
cp_weights = tf.keras.callbacks.ModelCheckpoint(filepath=cp_path,
                                       save_weights_only=False,
                                       monitor='val_accuracy',
                                       mode='max',
                                       save_best_only=True)

# Compile model
model.compile(optimizer = optimizers.Adam(0.001), loss = 'binary_crossentropy',␣
 ↪metrics = ['accuracy'])
```

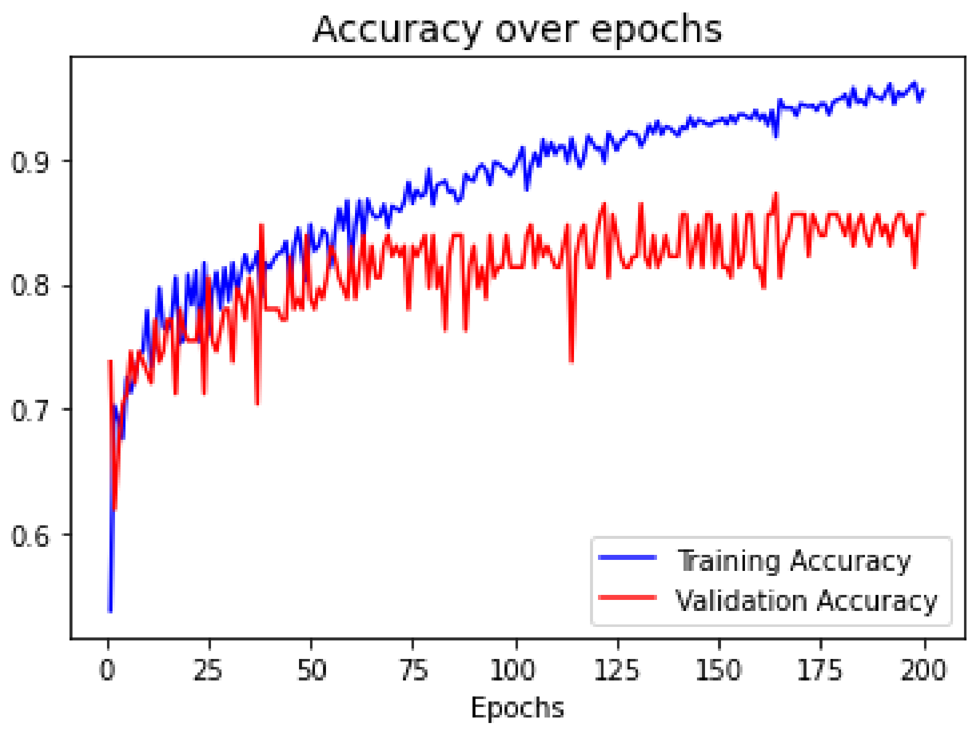
The model was compiled with an Adam optimizer with learning rate = 0.001, loss calculated through the binary cross entropy, and the evaluated metric to be accuracy.

4.2 Training and Validation

[ ]:
```
history = model.fit(train_x, train_y, epochs = 200, batch_size=64,␣
 ↪validation_data=(val_x, val_y), callbacks=[cp_weights],␣
 ↪class_weight=class_weights, verbose=1)
```

4.3 Training Evaluation

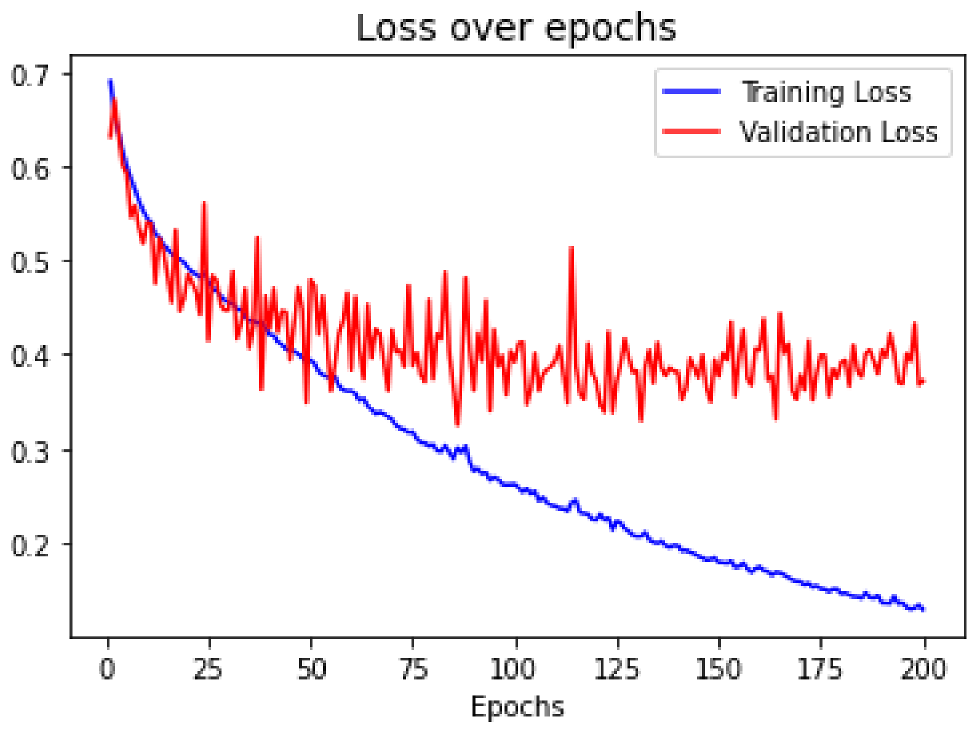
```
[ ]: # Obtain training and validation metrics
train_acc = history.history['accuracy']
val_acc = history.history['val_accuracy']
train_loss = history.history['loss']
val_loss = history.history['val_loss']
epochs = range(1, len(train_acc) + 1)

# Accuracy over epochs
plt.plot(epochs, train_acc, color='blue', label='Training Accuracy')
plt.plot(epochs, val_acc, color='red', label='Validation Accuracy')
plt.title("Accuracy over epochs", fontsize=14)
plt.xlabel('Epochs')
plt.legend(loc='lower right')
plt.show()

# Print best validation accuracy and epoch
print("Best validation accuracy was %5.3f at epoch %2.f" % (np.max(val_acc), np.
 ↪argmax(val_acc)+1))
```



```
Best validation accuracy was 0.873 at epoch 164
```

The best validation accuracy was observed to be 0.873 at epoch 164. The Accuracy vs Epoch plot shows that there is overfitting observed beginning at epoch 70 because following that epoch, the validation accuracy plateaus while the training accuracy continues to increase.

```
[ ]: # Loss over epochs
plt.plot(epochs, train_loss, color='blue', label='Training Loss')
plt.plot(epochs, val_loss, color='red', label='Validation Loss')
plt.title("Loss over epochs", fontsize=14)
plt.xlabel('Epochs')
plt.legend(loc='upper right')
plt.show()
```



Overfitting is observed with the Loss vs Epoch plot. At around epoch 20, the validation loss begins to plateau while the training loss continues to decrease.

5 Second Model

5.1 Architecture

```
[ ]: model2 = Sequential([
                      tf.keras.Input(48),
                      tf.keras.layers.Dropout(0.05),
                      tf.keras.layers.Flatten(),
                      tf.keras.layers.Dense(128, activation=tf.nn.relu),
                      tf.keras.layers.Dense(1, activation=tf.nn.sigmoid)
                      ]
                     )
  model2.summary()
```

```
Model: "sequential_35"

_________________________________________________________________
 Layer (type)                Output Shape              Param #
=================================================================
 dropout_23 (Dropout)        (None, 48)                0

 flatten_36 (Flatten)        (None, 48)                0

 dense_72 (Dense)            (None, 128)               6272

 dense_73 (Dense)            (None, 1)                 129

=================================================================
Total params: 6,401
Trainable params: 6,401
Non-trainable params: 0
_________________________________________________________________
```

As the model was overfitting, adding a dropout layer would help. A dropout layer was added before flattening to drop out observations with a rate of 0.05.

```
[ ]: # Define path to store callback
cp_path = "model2.ckpt"
cp_dir = os.path.dirname(cp_path)

# Callback that saves the models weights at the best validation accuracy
cp_weights = tf.keras.callbacks.ModelCheckpoint(filepath=cp_path,
                                       save_weights_only=False,
                                       monitor='val_accuracy',
                                       mode='max',
                                       save_best_only=True)

# Compile model
model2.compile(optimizer = optimizers.Adam(0.0001), loss =␣
 ↪'binary_crossentropy', metrics = ['accuracy'])
```

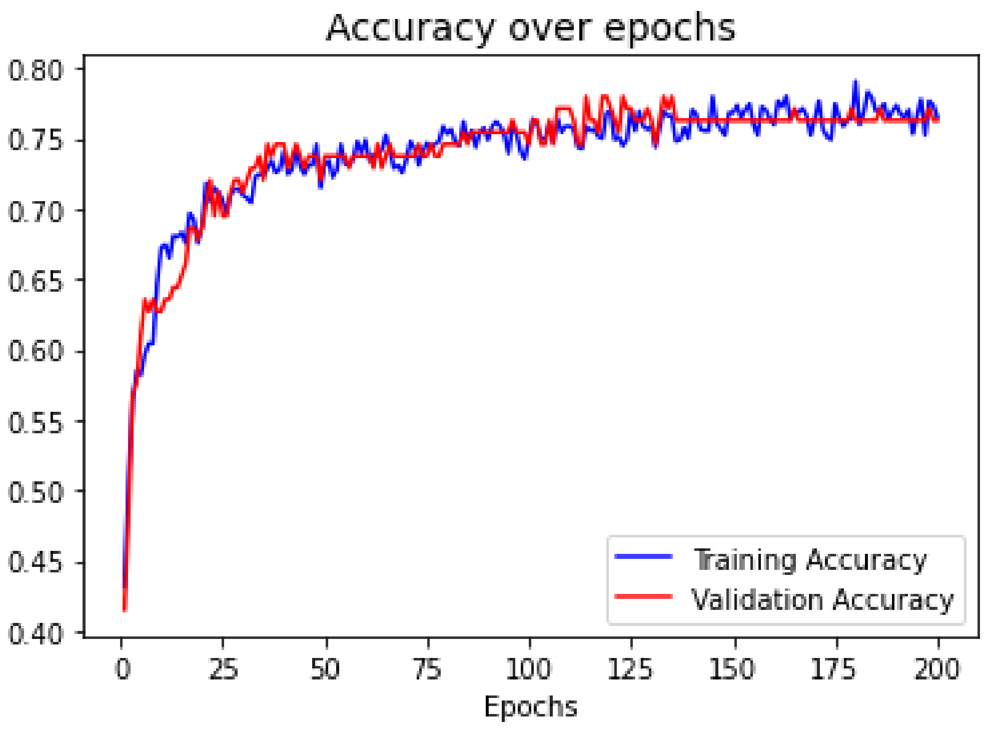
The learning rate was decreased from 0.001 to 0.0001 to slow the learning of the model, since within 50 epochs the model already began to overfit.

5.2 Training and Validation

```
[ ]: history2 = model2.fit(train_x, train_y, epochs = 200, batch_size=64,␣
      ↪validation_data=(val_x, val_y), callbacks=[cp_weights],␣
      ↪class_weight=class_weights, verbose=1)
```

5.3 Training Evaluation

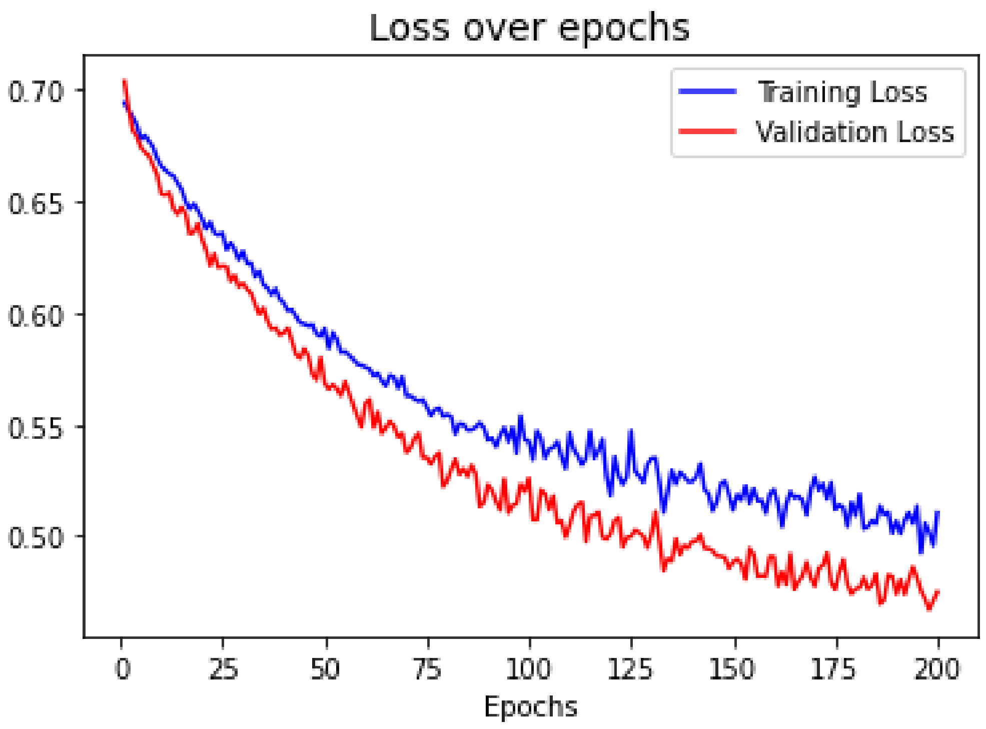
```
[ ]: # Obtain training and validation metrics
     train_acc = history2.history['accuracy']
     val_acc = history2.history['val_accuracy']
     train_loss = history2.history['loss']
     val_loss = history2.history['val_loss']
     epochs = range(1, len(train_acc) + 1)

     # Accuracy over epochs
     plt.plot(epochs, train_acc, color='blue', label='Training Accuracy')
     plt.plot(epochs, val_acc, color='red', label='Validation Accuracy')
     plt.title("Accuracy over epochs", fontsize=14)
     plt.xlabel('Epochs')
     plt.legend(loc='lower right')
     plt.show()

     # Print best validation accuracy and epoch
     print("Best validation accuracy was %5.3f at epoch %2.f" % (np.max(val_acc), np.
      ↪argmax(val_acc) + 1))
```



```
Best validation accuracy was 0.780 at epoch 114
```

The best accuracy for the validation set was 0.780 at epoch 114. This validation accuracy is worse than the first validation accuracy of 0.873 which occurred at epoch 164. It appears that the training and validation accuracy have plateaud around 0.750.

[ ]:
```
# Loss over epochs
plt.plot(epochs, train_loss, color='blue', label='Training Loss')
plt.plot(epochs, val_loss, color='red', label='Validation Loss')
plt.title("Loss over epochs", fontsize=14)
plt.xlabel('Epochs')
plt.legend(loc='upper right')
plt.show()
```



Slight underfitting is observed. Both losses are still decreasing (although validation is decreasing at a slower rate), indicating that there is underfitting and more training can be done to reach the optimum solution.

6 Third Model

6.1 Architecture

```
[ ]: model3 = Sequential([
                         tf.keras.Input(48),
                         tf.keras.layers.Dropout(0.1),
                         tf.keras.layers.Flatten(),
                         tf.keras.layers.Dense(128, activation=tf.nn.relu),
                         tf.keras.layers.Dense(64, activation=tf.nn.relu),
                         tf.keras.layers.Dense(32, activation=tf.nn.relu),
                         tf.keras.layers.Dense(1, activation=tf.nn.sigmoid)
                         ]
                        )
     model3.summary()
```

```
Model: "sequential_43"
_________________________________________________________________
```

```
 Layer (type)                Output Shape              Param #
=================================================================
 dropout_31 (Dropout)        (None, 48)                0

 flatten_44 (Flatten)        (None, 48)                0

 dense_100 (Dense)           (None, 128)               6272

 dense_101 (Dense)           (None, 64)                8256

 dense_102 (Dense)           (None, 32)                2080

 dense_103 (Dense)           (None, 1)                 33

=================================================================
Total params: 16,641
Trainable params: 16,641
Non-trainable params: 0
_________________________________________________________________
```

Due to some slight potential for underfitting, a third and fourth dense layer were added, with 64 and 32 hidden units. This was done to increase complexity of the model to address the slight potential for underfitting. To slightly offset the added complexity of the model, the dropout rate was increased from 0.05 to 0.1.

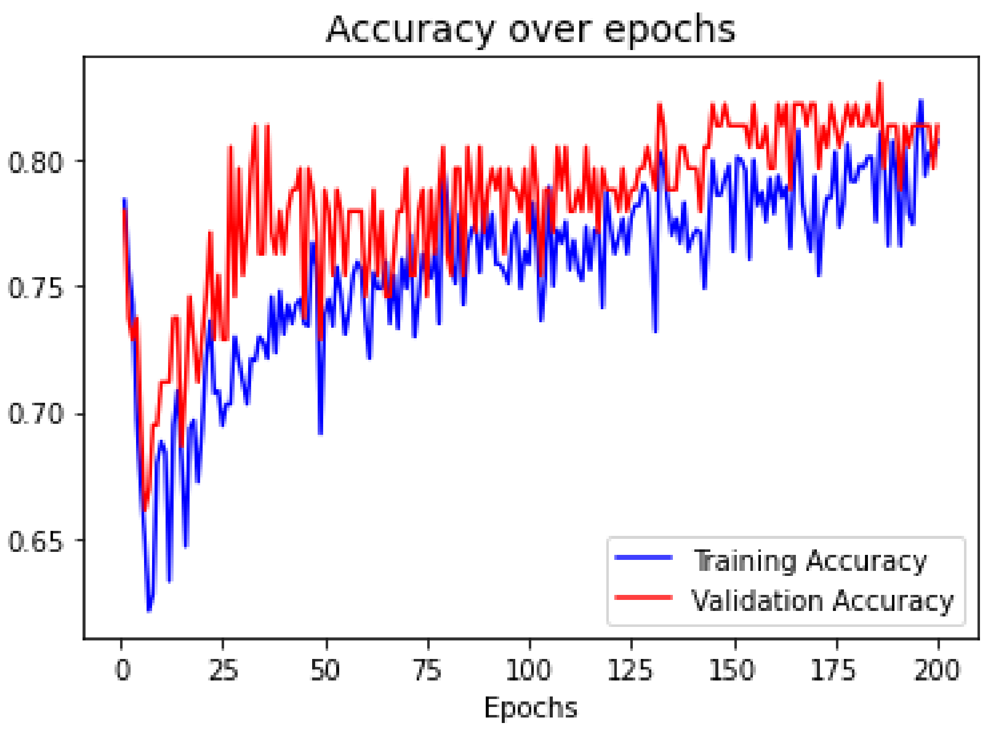
```
[ ]: # Define path to store callback
cp_path = "model3.ckpt"
cp_dir = os.path.dirname(cp_path)

# Callback that saves the models weights at the best validation accuracy
cp_weights = tf.keras.callbacks.ModelCheckpoint(filepath=cp_path,
                                               save_weights_only=False,
                                               monitor='val_accuracy',
                                               mode='max',
                                               save_best_only=True)

# Compile model
model3.compile(optimizer = optimizers.Adam(0.0001), loss =␣
 ↪'binary_crossentropy', metrics = ['accuracy'])
```

6.2 Training and Validation

```
[ ]: history3 = model3.fit(train_x, train_y, epochs = 200, batch_size=64,␣
 ↪validation_data=(val_x, val_y), callbacks=[cp_weights],␣
 ↪class_weight=class_weights, verbose=1)
```

6.3 Training Evaluation

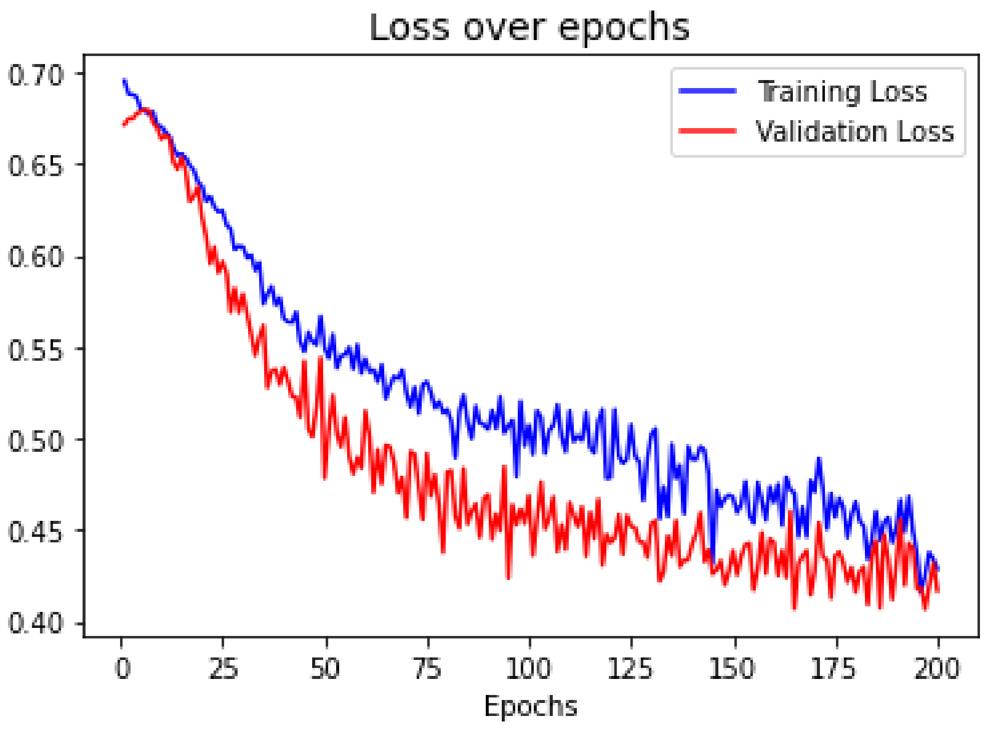
[ ]:
```python
# Obtain training and validation metrics
train_acc = history3.history['accuracy']
val_acc = history3.history['val_accuracy']
train_loss = history3.history['loss']
val_loss = history3.history['val_loss']
epochs = range(1, len(train_acc) + 1)

# Accuracy over epochs
plt.plot(epochs, train_acc, color='blue', label='Training Accuracy')
plt.plot(epochs, val_acc, color='red', label='Validation Accuracy')
plt.title("Accuracy over epochs", fontsize=14)
plt.xlabel('Epochs')
plt.legend(loc='lower right')
plt.show()

# Print best validation accuracy and epoch
print("Best validation accuracy was %5.3f at epoch %2.f" % (np.max(val_acc), np.
 ↪argmax(val_acc)+1))
```



```
Best validation accuracy was 0.831 at epoch 186
```

The best validation accuracy was 0.831 at epoch 186, which was less than the validation accuracy of the first model architecture (0.873 at epoch 164) but greater than the validation accuracy of the second model architecture (0.780 at epoch 114). The accuracies began high, most likely due to chance in the mini-batches, and then decreased within the first 5 epochs. Afterwards, the accuracies began to increase.The validation accuracy and training accuracy appear to be close together. More training time could potentially be done as the accuracies somewhat seem to have potential to continue increasing.

```
[ ]: # Loss over epochs
     plt.plot(epochs, train_loss, color='blue', label='Training Loss')
     plt.plot(epochs, val_loss, color='red', label='Validation Loss')
     plt.title("Loss over epochs", fontsize=14)
     plt.xlabel('Epochs')
     plt.legend(loc='upper right')
     plt.show()
```



The validation loss was consistently below the training loss. The loss in the validation seems to be around 0.40 by the end of the training, which matches that of the training loss. There could be potential for more training if there were more epochs.

7 Final Model Evaluation

The best model architecture appeared to be the third model architecture. This model had the second greatest validation accuracy (0.831) as compared to the other model architectures (0.873 and

0.780, respectively). The first model architecture observed overfitting, as the validation accuracy begin to deviate from the training accuracy at around epoch 70, then the validation accuracy plateaud afterwards. The second architecture had the slight potential to train more as it was slightly underfitting, where the losses were still trending downwards. The third architecture similar accuracy and loss between the training and testing dataset, and had a lower validation loss than the second model. I believe that the third model is the best model as the first architecture had much overfitting, and the second model architecture had slight underfitting, whereas the third model improved accuracy from the second model while also retaining close accuracy and loss between the training and validation set.

7.1 Obtain Best Model

[ ]:
```
# Get weights of models from epoch with best val accuracy
model.load_weights("model1.ckpt")
model2.load_weights("model2.ckpt")
model3.load_weights("model3.ckpt")

# Save models to local drive in case Google Colab crashes
!mkdir -p saved_model
model3.save('saved_model/model3')
model2.save('saved_model/model1')
model.save('saved_model/model2')
```

7.2 Accuracy

[ ]:
```
# Get accuracy on testing set
loss, accuracy = model3.evaluate(test_x, test_y)
print('Accuracy on test dataset: %5.3f' % (accuracy))
```

```
4/4 [==============================] - 0s 9ms/step - loss: 0.4281 - accuracy:
0.8136
Accuracy on test dataset: 0.814
```

7.3 Confusion Matrix

[ ]:
```
# Get predictions
test_pred = model3.predict(test_x)
```

```
4/4 [==============================] - 0s 3ms/step
```

[ ]:
```
# Check predictions
test_pred[0:5]
```

```
[ ]: array([[0.1500526 ],
            [0.18358165],
            [0.03791126],
            [0.14376739],
            [0.8128861 ]], dtype=float32)
```

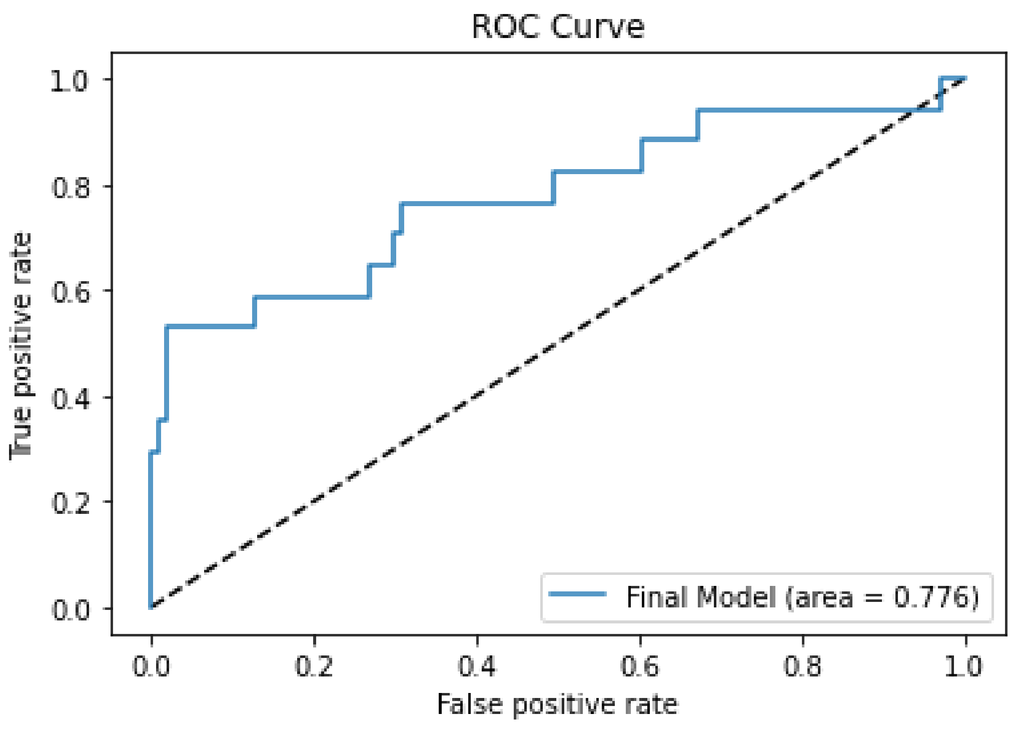
```
[ ]: # Get confusion matrix
     conf_matrix = tf.math.confusion_matrix(labels=test_y, predictions=np.
      ↪rint(test_pred))
     conf_matrix
```

```
[ ]: <tf.Tensor: shape=(2, 2), dtype=int32, numpy=
     array([[86, 15],
            [ 7, 10]], dtype=int32)>
```

7.4 ROC

```
[ ]: # Get ROC curve variables
     fpr, tpr, thresh = roc_curve(test_y, test_pred)
     model_auc = auc(fpr, tpr)
```

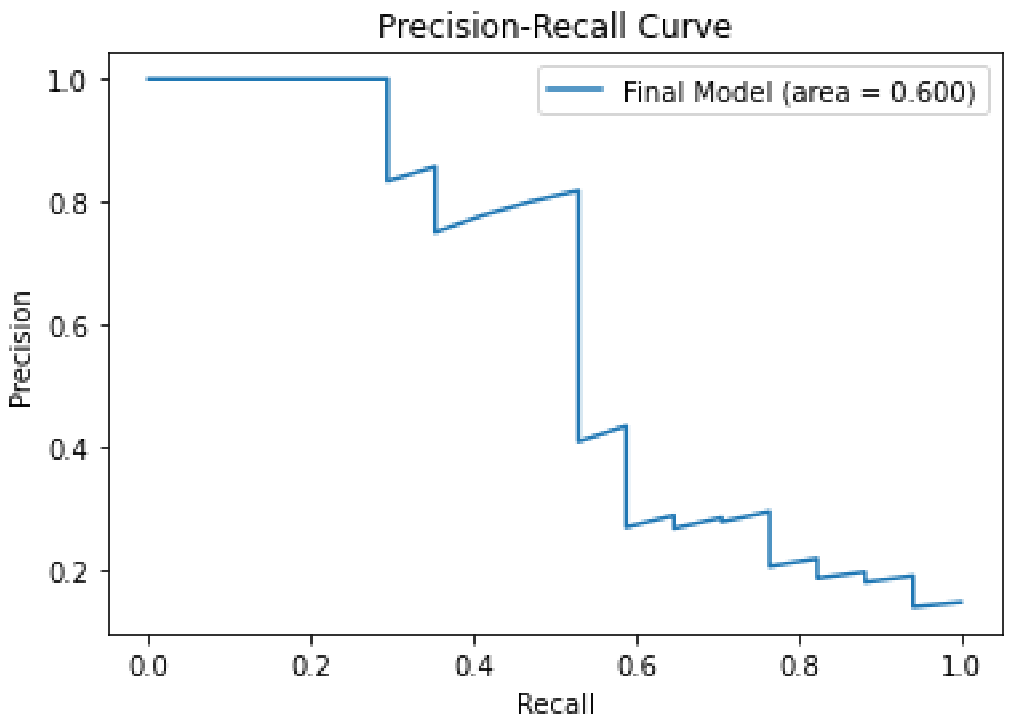
```
[ ]: # Plot ROC curve
     plt.plot([0, 1], [0, 1], 'k--')
     plt.plot(fpr, tpr, label='Final Model (area = {:.3f})'.format(model_auc))
     plt.xlabel('False positive rate')
     plt.ylabel('True positive rate')
     plt.legend(loc='lower right')
     plt.title('ROC Curve')
     plt.show()
```



7.5 Precision-Recall Curve

```
[ ]: # Get precision-recall variables
     precision, recall, thresholds = precision_recall_curve(test_y, test_pred)
     model_auprc = auc(recall, precision)
```

```
[ ]: # Plot precision-recall curve
     plt.plot(recall, precision, label='Final Model (area = {:.3f})'.
      ↪format(model_auprc))
     plt.xlabel('Recall')
     plt.ylabel('Precision')
     plt.legend(loc='upper right')
     plt.title('Precision-Recall Curve')
     plt.show()
```



7.6 F1-Score

```
[ ]: # Get F1 score
     f1 = f1_score(test_y, np.rint(test_pred))
     print("The F1-score was %5.3f" % (f1))
```

```
The F1-score was 0.476
```