Case Study 6: Particle Detection

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1 Introduction

The goal of this study is to develop a dense neural network that maximizes accuracy when detecting the particle.

2 Methods

2.1 Data Examination

An initial examination of the data revealed 7,000,000 observations and 29 features, including label, the response variable, $f\theta - f26$, and mass. There is no missing data, and the response variable is almost exactly weighted between the two classes (Table 1).

Class	Count
1.0	3,500,879
0.0	3,499,121

Table 1: Response Variable Count

The only work that was done prior to building the model was to convert the response variable, label, to an integer.

2.2 Model Preparation & Execution

The data was split into test and training data sets using a 90/10 split with a stratified shuffle and a MinMaxScaler was applied. To set a baseline for the neural network's performance, I first ran a model using logistic regression to determine how it performed on the data. That model produced an accuracy score of 83.7%.

Two neural networks were built for this project in order to explore how different parameters affected the final accuracy performance. The first network was comprised of an input layer, two dense layers with rectified linear unit (relu) activation functions, and a final dense layer with a 'sigmoid' activation (Figure 1).

Model: "sequential"

Layer (type)	Output Shape	Param #
dense (Dense)	(None, 100)	2900
dense_1 (Dense)	(None, 100)	10100
dense_2 (Dense)	(None, 1)	101
Total params: 13,101 Trainable params: 13,101 Non-trainable params: 0		

Figure 1: Model 1 Summary

Finally, the model was compiled using a binary cross-entropy loss function with an 'adam' optimizer. This network was fit using batch sizes of 10,000 and 1,000 epochs.

The second neural network alternated dense and dropout layers in an effort to prevent overfitting and ran with batch sizes of 1,000 and 100 epochs.

Model: "sequential_1"

Layer (type)	Output Shape	Param #			
flatten (Flatten)	(None, 28)	0			
dense_3 (Dense)	(None, 128)	3712			
dropout (Dropout)	(None, 128)	0			
dense_4 (Dense)	(None, 128)	16512			
dropout_1 (Dropout)	(None, 128)	0			
dense_5 (Dense)	(None, 1)	129			
		.=========			
Total params: 20,353 Trainable params: 20,353 Non-trainable params: 0					

3 Results

3.1 Model 1

In plotting the loss of the training and testing data, I noticed a relatively smooth decrease in the training loss (Figure 2). The testing loss follows a similar slope, but there was much more variation among the epochs.

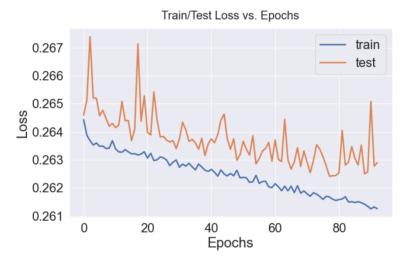


Figure 2: Loss Over Epochs

The classification report for the first neural network shows the model performed with an accuracy of 88%. This result was similar to other variations of batch size and epochs (Figure 3).

	precision	recall	f1-score	support
0	0.89	0.87	0.88	349912
1	0.87	0.89	0.88	350088
accuracy			0.88	700000
macro avg	0.88	0.88	0.88	700000
weighted avg	0.88	0.88	0.88	700000

Figure 3: Model 1 Classification Report

The confusion matrix shows where misclassifications occurred. There were almost 37,000 false positives and 46,000 false negatives (Figure 4).

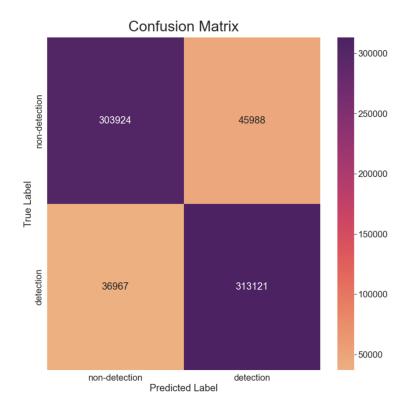


Figure 4: Model 1 Confusion Matrix

3.2 Model 2

The classification report for the second neural network shows the model performed with an accuracy of 83% (Figure 5). In this case the use of the dropout layers decreased the model's performance.

	precision	recall	f1-score	support
0	0.80	0.87	0.83	349912
1	0.85	0.78	0.82	350088
accuracy			0.82	700000
macro avg	0.83	0.82	0.82	700000
weighted avg	0.83	0.82	0.82	700000

Figure 5: Model 2 Classification Report

The confusion matrix shows where misclassifications occurred. The greatest change from the first model is the significant increase in false positives—almost 77,000—an increase of almost 40,000 (Figure 6).

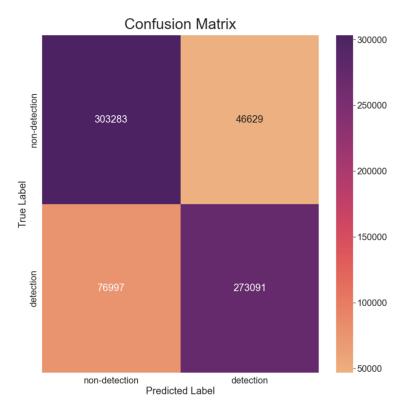


Figure 6: Model 2 Confusion Matrix

4 Conclusion

In conclusion, the first neural network, with its' relatively simple structure performed the best in terms of accuracy. That said, the second neural network ran much more quickly, albeit with a notable drop in accuracy. If I were to redo the second neural network in the future, I'd explore the parameters of the dropout layers to see if an increase in accuracy could be achieved while keeping the model's speed performance.

Appendix

Code

Code begins on the following page.

Case Study 6

Description

Build a dense neural network to accurately detect the particle. The goal is to maximize your accuracy. Include a discussion of how you know your model has finished training as well as what design decisions you made while building the network.

Submit your assignment to the Assignments section of the online campus. For more information regarding case studies, see the syllabus.

```
In [1]: # Import general libraries
        import graphviz
        import joblib
        import numpy as np
        import pandas as pd
        import pickle
        # Import plotting libraries
        import matplotlib as mpl
        import matplotlib.pyplot as plt
        import pydot
        import seaborn as sns
        # Import sklearn libraries
        from sklearn.compose import ColumnTransformer
        from sklearn.linear model import LogisticRegression
        from sklearn.metrics import classification report, confusion matrix
        from sklearn.model selection import GridSearchCV
        from sklearn.model selection import KFold
        from sklearn.model selection import train test split
        from sklearn.pipeline import Pipeline
        from sklearn.preprocessing import MinMaxScaler
        # Set up OS-level processes
        import os
        cwd = os.getcwd()
        d = os.path.dirname(cwd)
        os.environ['TF_CPP_MIN_LOG_LEVEL'] = '2'
        # Import tensorflow libraries
        import tensorflow as tf
        from tensorflow import keras
        from tensorflow.keras.models import Sequential
        from tensorflow.keras.layers import InputLayer, Dense, Activation, Dropout
        from tensorflow.keras.callbacks import EarlyStopping
        # Set pandas display options
        pd.options.display.max_rows = 99999
        pd.options.display.max_columns = 99999
In [2]: # %%time
        # # Read in data and save it as a pickle file
        # data = pd.read csv('all train.csv')
        # data.to_pickle("data.pkl")
In [3]: # Load pickle file
        df = pd.read pickle("data.pkl")
```

Exploratory Data Analysis

```
In [4]: df.shape
```

Out[4]: (7000000, 29) In [5]: df.head() Out[5]: f1 f2 f3 f6 f0 f4 f5 label 1.0 -0.346368 0.416306 0.475342 0.427493 -0.005984 0.3 0 0.999236 1.989833 1.0 -0.871906 -0.005984 -0.001047 -1.C 1.708236 -0.319394 -1.241873 -0.887231 2 -0.360693 -0.472273 -0.292344 -1.054221 -1.150495 0.0 1.794174 0.264738 1.4 1.0 -0.377914 -0.103932 -0.649434 -2.125015 -1.643797 -0.005984 1.011112 -1.0 0.0 -0.067436 -0.636762 -0.620166 -0.062551 1.588715 -0.005984 -0.595304 -1.2 In [6]: df.tail() Out[6]: # f0 f1 f2 f3 f4 f5 f label 6999995 0.0 1.617264 -0.537084 -1.275867 0.650799 -1.511621 0.850488 0.59639 6999996 0.0 -0.511357 0.270927 0.085989 -0.243802 -1.035668 -0.005984 -0.12721 6999997 0.062408 -0.987203 0.570667 1.517195 0.639548 -1.054221 1.11523 1.0 6999998 1.0 1.659131 1.096223 0.562821 1.627193 0.767236 -1.054221 1.07999 6999999 1.0 0.002034 0.744152 -0.908839 -0.770454 1.008405 -1.054221 -0.37015

In [7]: df.info()

```
RangeIndex: 7000000 entries, 0 to 6999999
Data columns (total 29 columns):
 #
     Column
              Dtype
 0
     # label float64
     f0
 1
              float64
 2
     f1
              float64
 3
     f2
              float64
 4
     f3
              float64
 5
     f4
              float64
 6
     f5
              float64
 7
     f6
              float64
     f7
              float64
 8
 9
     f8
              float64
 10
     f9
              float64
 11
     f10
              float64
 12
     f11
              float64
 13
     f12
              float64
 14
     f13
              float64
 15
     f14
              float64
 16
    f15
              float64
 17
     f16
              float64
 18
     f17
              float64
 19
    f18
              float64
 20
     f19
              float64
 21
    f20
              float64
 22
    f21
              float64
 23
    f22
              float64
 24
    f23
              float64
 25
    f24
              float64
 26
     f25
              float64
 27
     f26
              float64
              float64
 28 mass
dtypes: float64(29)
```

<class 'pandas.core.frame.DataFrame'>

```
In [8]: df.describe()
```

memory usage: 1.5 GB

Out[8]:		# label	fO	f1	f2	f3	
	count	7.000000e+06	7.000000e+06	7.000000e+06	7.000000e+06	7.000000e+06	7.00000
	mean	5.001256e-01	1.612528e-02	4.770022e-04	2.686578e-05	1.056081e-02	-1.05(
	std	5.000000e-01	1.004417e+00	9.974864e-01	1.000080e+00	9.956003e-01	9.9986
	min	0.000000e+00	-1.960549e+00	-2.365355e+00	-1.732165e+00	-9.980274e+00	-1.73213
	25%	0.000000e+00	-7.288206e-01	-7.332548e-01	-8.656704e- 01	-6.092291e-01	-8.658
	50%	1.000000e+00	-3.930319e-02	8.523957e-04	3.199154e-04	1.963316e-02	-5.07010
	75%	1.000000e+00	6.900799e-01	7.347832e-01	8.659464e-01	6.798818e-01	8.65764
	max	1.000000e+00	4.378282e+00	2.365287e+00	1.732370e+00	4.148023e+00	1.73197
In [9]:		sing values?					
Out[9]:	# labe f0 f1 f2 f3 f4 f5 f6 f7 f8 f9 f10 f11 f12 f13	el 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0					

f14

f15

f16

f17

f18

f19 f20 f21 f22

f23

f24 f25 f26 mass

dtype: int64

0

0

0

0

0

0

0

```
In [10]: # Number of unique values per feature
          df.nunique()
         # label
Out[10]:
                     1142885
          f1
                     2311224
          f2
                     1849439
          f3
                     1359060
          f4
                     1849442
          f5
                           10
          f6
                     1129730
                     2383592
          f7
          f8
                     1850813
          f9
                     1063674
          f10
                     2358787
          f11
                     1850048
          f12
          f13
                      979658
          f14
          f15
                     2320116
          f16
                     1851285
          f17
                            2
          f18
                      882518
          f19
                     2263637
          f20
                     1850152
          f21
          f22
                     1142839
          f23
                      568614
          f24
                      393987
          f25
                      862612
          f26
                      931270
          mass
                            5
          dtype: int64
In [11]:
         df['# label'].value_counts()
          1.0
                 3500879
Out[11]:
          0.0
                 3499121
          Name: # label, dtype: int64
In [12]: # Convert label to an integer
          df['# label'] = df['# label'].astype(int)
          # Verify conversion
          df['# label'].value_counts()
               3500879
Out[12]:
               3499121
          Name: # label, dtype: int64
```

Helper Functions

```
In [13]: def get confusion matrix(y, yhat, mat title = "Confusion Matrix"):
             plt.figure(figsize = (15,15))
             sns.set(font scale = 2)
             x_axis_labels = ['non-detection','detection']
             y axis labels = ['non-detection','detection']
             cm_n = confusion_matrix(y, yhat)
             ax = sns.heatmap(cm n,
                               cmap = 'flare',
                               annot = True,
                               fmt = '2d',
                               xticklabels = x_axis_labels,
                               yticklabels = y_axis_labels)
             ax.set(xlabel = 'Predicted Label',
                    ylabel = 'True Label')
             ax.set title(mat title,
                           fontdict = {'fontsize':36},
                           pad = 15)
         def get classification report(x train, y train, x test, y test, pred, model)
             print("Classification Report:")
             print(classification_report(y_test,pred))
             get confusion matrix(y test,pred)
```

Set up Train/Test Data

Baseline Model with Logistic Regression

```
In [15]: lr = LogisticRegression(solver = 'lbfgs', max_iter = 1000)
    lr.fit(X_train, y_train)
    print(lr.score(X_test, y_test))
```

0.8369685714285714

Build Initial Neural Network

```
In [16]: # Build a sequential NN model using Tensorflow and Keras
     model = Sequential()
     model.add(InputLayer(input shape = (28,)))
     model.add(Dense(units = 100, activation = 'relu'))
     model.add(Dense(units = 100, activation = 'relu'))
     model.add(Dense(units = 1, activation = 'sigmoid'))
     model.compile(loss = 'binary_crossentropy', optimizer = 'adam')
In [26]: %%time
     model.fit(x = X train,
           y = y train,
           batch size = 10000,
           epochs = 100,
           validation_data = (X_test, y_test),
           verbose = 1,
           callbacks = [EarlyStopping(monitor = 'val loss',
                           mode = 'min',
                           verbose = 1,
                           patience = 15)]
           )
     Epoch 1/100
     loss: 0.2646
     Epoch 2/100
     loss: 0.2651
     Epoch 3/100
     630/630 [============= ] - 9s 14ms/step - loss: 0.2637 - val
     loss: 0.2674
     Epoch 4/100
     630/630 [=============] - 9s 15ms/step - loss: 0.2635 - val
     loss: 0.2652
     Epoch 5/100
     loss: 0.2652
     Epoch 6/100
     loss: 0.2646
     Epoch 7/100
     loss: 0.2648
     Epoch 8/100
     loss: 0.2645
     Epoch 9/100
     loss: 0.2642
     Epoch 10/100
     loss: 0.2643
     Epoch 11/100
     loss: 0.2641
     Epoch 12/100
```

```
loss: 0.2642
Epoch 13/100
loss: 0.2651
Epoch 14/100
loss: 0.2644
Epoch 15/100
1 loss: 0.2644
Epoch 16/100
1 loss: 0.2637
Epoch 17/100
l loss: 0.2641
Epoch 18/100
l loss: 0.2671
Epoch 19/100
1 loss: 0.2644
Epoch 20/100
1 loss: 0.2653
Epoch 21/100
loss: 0.2640
Epoch 22/100
1 loss: 0.2639
Epoch 23/100
1 loss: 0.2654
Epoch 24/100
630/630 [============ ] - 10s 16ms/step - loss: 0.2630 - va
1 loss: 0.2644
Epoch 25/100
630/630 [============ ] - 10s 16ms/step - loss: 0.2631 - va
1 loss: 0.2638
Epoch 26/100
1 loss: 0.2638
Epoch 27/100
loss: 0.2637
Epoch 28/100
1_loss: 0.2636
Epoch 29/100
loss: 0.2637
Epoch 30/100
loss: 0.2634
Epoch 31/100
```

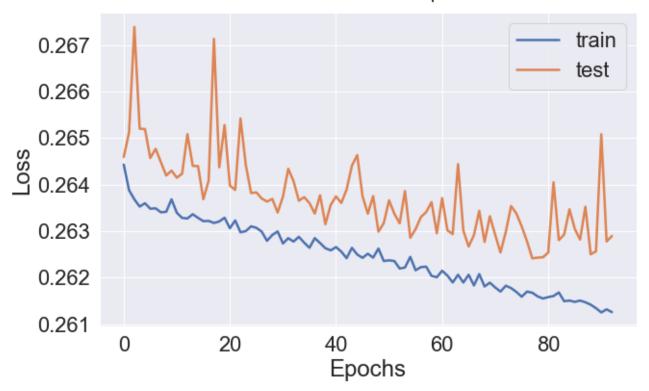
```
630/630 [============ ] - 10s 15ms/step - loss: 0.2627 - va
1 loss: 0.2637
Epoch 32/100
630/630 [============== ] - 10s 16ms/step - loss: 0.2628 - va
1 loss: 0.2643
Epoch 33/100
l loss: 0.2641
Epoch 34/100
loss: 0.2637
Epoch 35/100
1 loss: 0.2637
Epoch 36/100
1 loss: 0.2636
Epoch 37/100
1 loss: 0.2634
Epoch 38/100
1 loss: 0.2638
Epoch 39/100
l loss: 0.2631
Epoch 40/100
1 loss: 0.2636
Epoch 41/100
1 loss: 0.2637
Epoch 42/100
1 loss: 0.2636
Epoch 43/100
630/630 [============ ] - 10s 15ms/step - loss: 0.2624 - va
1 loss: 0.2639
Epoch 44/100
630/630 [============ ] - 10s 15ms/step - loss: 0.2626 - va
1 loss: 0.2644
Epoch 45/100
1 loss: 0.2646
Epoch 46/100
1 loss: 0.2637
Epoch 47/100
1_loss: 0.2634
Epoch 48/100
630/630 [============ ] - 10s 16ms/step - loss: 0.2624 - va
1 loss: 0.2638
Epoch 49/100
1 loss: 0.2630
Epoch 50/100
```

```
630/630 [============ ] - 10s 16ms/step - loss: 0.2624 - va
1 loss: 0.2632
Epoch 51/100
1 loss: 0.2637
Epoch 52/100
1 loss: 0.2634
Epoch 53/100
1 loss: 0.2632
Epoch 54/100
1 loss: 0.2639
Epoch 55/100
1 loss: 0.2629
Epoch 56/100
1 loss: 0.2630
Epoch 57/100
1 loss: 0.2633
Epoch 58/100
1 loss: 0.2634
Epoch 59/100
1 loss: 0.2636
Epoch 60/100
1 loss: 0.2630
Epoch 61/100
1 loss: 0.2637
Epoch 62/100
630/630 [============ ] - 10s 15ms/step - loss: 0.2620 - va
1 loss: 0.2630
Epoch 63/100
630/630 [============= ] - 9s 15ms/step - loss: 0.2619 - val
loss: 0.2629
Epoch 64/100
1 loss: 0.2644
Epoch 65/100
1 loss: 0.2630
Epoch 66/100
1_loss: 0.2627
Epoch 67/100
630/630 [============ ] - 10s 15ms/step - loss: 0.2618 - va
1 loss: 0.2629
Epoch 68/100
1 loss: 0.2634
Epoch 69/100
```

```
630/630 [============ ] - 10s 15ms/step - loss: 0.2618 - va
1 loss: 0.2628
Epoch 70/100
1 loss: 0.2633
Epoch 71/100
1 loss: 0.2629
Epoch 72/100
loss: 0.2625
Epoch 73/100
1 loss: 0.2630
Epoch 74/100
1 loss: 0.2635
Epoch 75/100
1 loss: 0.2634
Epoch 76/100
l loss: 0.2631
Epoch 77/100
1 loss: 0.2628
Epoch 78/100
1 loss: 0.2624
Epoch 79/100
1 loss: 0.2624
Epoch 80/100
1 loss: 0.2624
Epoch 81/100
630/630 [============] - 9s 14ms/step - loss: 0.2616 - val
loss: 0.2625
Epoch 82/100
630/630 [============= ] - 9s 15ms/step - loss: 0.2616 - val
loss: 0.2640
Epoch 83/100
loss: 0.2628
Epoch 84/100
1 loss: 0.2629
Epoch 85/100
_loss: 0.2635
Epoch 86/100
1 loss: 0.2630
Epoch 87/100
1 loss: 0.2628
Epoch 88/100
```

```
loss: 0.2635
      Epoch 89/100
      1 loss: 0.2625
      Epoch 90/100
      1 loss: 0.2626
      Epoch 91/100
      loss: 0.2651
      Epoch 92/100
      loss: 0.2628
      Epoch 93/100
      loss: 0.2629
      Epoch 93: early stopping
      CPU times: user 42min 15s, sys: 15min 4s, total: 57min 19s
      Wall time: 14min 52s
      <keras.callbacks.History at 0x1423068f0>
Out[26]:
In [27]: # Visualize model summary
      model.summary()
      Model: "sequential"
       Layer (type)
                         Output Shape
                                           Param #
      ______
       dense (Dense)
                          (None, 100)
                                           2900
       dense_1 (Dense)
                          (None, 100)
                                           10100
       dense_2 (Dense)
                          (None, 1)
                                           101
      ______
      Total params: 13,101
      Trainable params: 13,101
      Non-trainable params: 0
In [28]: model loss = pd.DataFrame(model.history.history)
In [29]: def plot_early_stop_rounds(model_loss):
         plt.subplots(figsize = (10, 6))
         plt.plot(model_loss['loss'], lw = 2.5, label = 'train')
         plt.plot(model_loss['val_loss'], lw = 2.5, label = 'test')
         plt.title('Train/Test Loss vs. Epochs', fontdict = {'fontsize':20}, pad =
         plt.ylabel('Loss')
         plt.xlabel('Epochs')
         plt.legend()
         plt.show()
In [30]: plot early stop rounds(model loss)
```

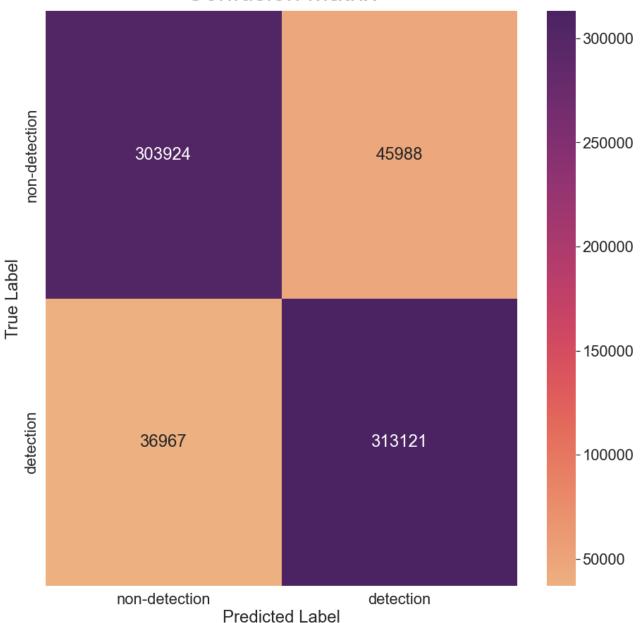
Train/Test Loss vs. Epochs



```
In [31]:
          # Save the train/test loss history
          file_name_model_history = "train_test_history.sav"
          joblib.dump(model_loss, file_name_model_history)
         ['train_test_history.sav']
Out[31]:
In [32]:
         # Load the loss history
          model_loss = joblib.load(file_name_model_history)
In [33]: predictions = (model.predict(X_test) > 0.5).astype("int32")
          get_classification_report(X_train,
                                    y_train,
                                    X_test,
                                    y_test,
                                    predictions,
                                    model)
```

	Precision	recarr	11-50016	auppor c
0	0.89	0.87	0.88	349912
1	0.87	0.89	0.88	350088
accuracy			0.88	700000
macro avg	0.88	0.88	0.88	700000
weighted avg	0.88	0.88	0.88	700000

Confusion Matrix



```
In [34]: # Define path to keras model
  path = cwd + "/keras_model"

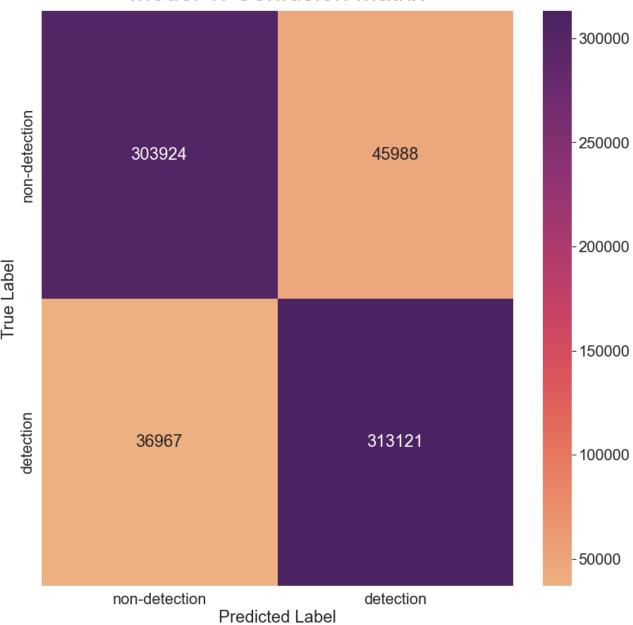
# Save model
  model.save(path)
```

INFO:tensorflow:Assets written to: /Users/matt/Documents/GitHub/7333-qtw/Cas
e Study 6/keras_model/assets

```
In [35]: # Load model
  model = keras.models.load_model(path)

In [36]: get_confusion_matrix(y_test, predictions, mat_title = 'Model 1: Confusion Ma
```

Model 1: Confusion Matrix



Define 2nd Model

```
In [39]: # Define early stopping
      early stop = EarlyStopping(monitor = 'val loss', patience = 3)
In [41]: # Fit the model
      history = model.fit(X train,
                    y_train,
                    epochs = 10,
                    validation_data = (X_test, y_test),
                    callbacks = [early_stop],
                    batch size = 1000)
      Epoch 1/10
      ccuracy: 0.7887 - val_loss: 0.3736 - val_accuracy: 0.8305
      Epoch 2/10
      ccuracy: 0.8081 - val_loss: 0.3622 - val_accuracy: 0.8330
      Epoch 3/10
      6300/6300 [============= ] - 27s 4ms/step - loss: 0.4301 - a
      ccuracy: 0.8049 - val_loss: 0.3860 - val_accuracy: 0.8245
      ccuracy: 0.8110 - val loss: 0.3689 - val accuracy: 0.8370
      ccuracy: 0.8119 - val loss: 0.4331 - val accuracy: 0.8234
In [42]: model.summary()
      Model: "sequential 1"
       Layer (type)
                          Output Shape
                                             Param #
      ______
       flatten (Flatten)
                          (None, 28)
       dense_3 (Dense)
                          (None, 128)
                                             3712
       dropout (Dropout)
                          (None, 128)
       dense 4 (Dense)
                          (None, 128)
                                            16512
       dropout 1 (Dropout)
                          (None, 128)
       dense 5 (Dense)
                                             129
                          (None, 1)
      ______
      Total params: 20,353
      Trainable params: 20,353
      Non-trainable params: 0
```

0.87

0.78

0.82

0.82

0.83

0.82

0.82

0.82

0.82

349912

350088

700000

700000

700000

0

1

accuracy macro avg

weighted avg

0.80

0.85

0.83

0.83

Confusion Matrix

