Predicting Antibiotic Resistance Genes | Proof Of Concept

The situation is a simple binary classification on sequence data. The Dataset was original gathered from kaggle, but the author privated the dataset soon after I downloaded (not kidding).

Results:

all models consistantly get above 90% accuracy with little optimization

- MLP = 94%
- GRU = 97%
- CNN = 98%

In summary, resistance is easily identified through genes, predicting based off Pan / meta genomes will be less simple. Many improvements could have been made in light of future models.

```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt

import tensorflow as tf
from tensorflow import keras
from keras import layers

from functools import partial
from sklearn.metrics import ConfusionMatrixDisplay, accuracy_score
```

Setup

```
from google.colab import drive
drive.mount('/content/drive')
!cd /content/drive/MyDrive/
!ls
```

```
Drive already mounted at /content/drive; to attempt to forcibly remount, call drive.mou
drive  sample_data
```

```
np_data = np.load('/content/drive/MyDrive/datasets/dataset.npy', allow_pickle=True)
np_data
```

```
array({'resistant': array([False, False, False, ...,  True,  True, False]), 'genes':
array(['ATGCACTACCGTATGATCCCCCTTCACTGGATGATGGAAATTGACTGCAATGGCTGCGCTAATAATACTTTGTCTCGTC
'ATGCACTACCGTATGATTCACTGGATGATGGAAATTGACTGCAATGGCTGCGCTAATAATACTTTGTCTCGTCGTTGGAATTACGA

'ATGCACTACCGTATGATTCACTGGATCGTGATGGAAATTGACTGCAATGGCTGCGCTAATAATACTTTGTCTCGTCGTTGGAATTA
       ...,

'ATGCACTACCGTATGATTCACTGGATGATGGAAACTGCAATGGCTGCGCTAATAATACTTTGTCTCGTCGTTGGAATTACGACTTC

'ATGCACTACCGTATGATTCACTGGATGATGGAAATTGACTTGCAATGGCTGCGCTAATAATACTTTGTCTCGTCGTTGGAATTACG

'ATGCACTACCGTATGATTCACTGGATGATGGAAATTGACTGCAATGGCTGCGCTAATAATACTTTGTCTCGTCGTTGGAATTACGA
      dtype=object)}, dtype=object)
```

```
# thanks to Alexander Scarlat .MD for the pandas dataframe convertion
Datadict = np_data[()]
df = pd.DataFrame.from_dict(Datadict)
print(df.shape)
df
```

```
(100000, 2)
```

	resistant	ge
0	False	ATGCACTACCGTATGATCCCCCTTCACTGGATGATGGAAATTGA
1	False	ATGCACTACCGTATGATTCACTGGATGATGGAAATTGACTGCAA
2	False	ATGCACTACCGTATGATTCACTGGATCGTGATGGAAATTGACTG
3	False	ATGCACTACCGTATGATTCACTGGGTGATGGAAATTGACTGCAA
4	False	ATGCACGACCGTATCATTCACTGGATGATGGAAATTGACTGCAA
...	...	
99995	False	ATGCACTACCGTATGATTCACTGGATGATGGAAACTCTCTTTGA
99996	False	ATGCACTACCGTATGATTCACTGGATGATGGAAATTGACTGCAA
99997	True	ATGCACTACCGTATGATTCACTGGATGATGGAAACTGCAATGGC
99998	True	ATGCACTACCGTATGATTCACTGGATGATGGAAATTGACTTGCA

```
# gene
X = df['genes'].iloc[0]
print(len(X), X)
```

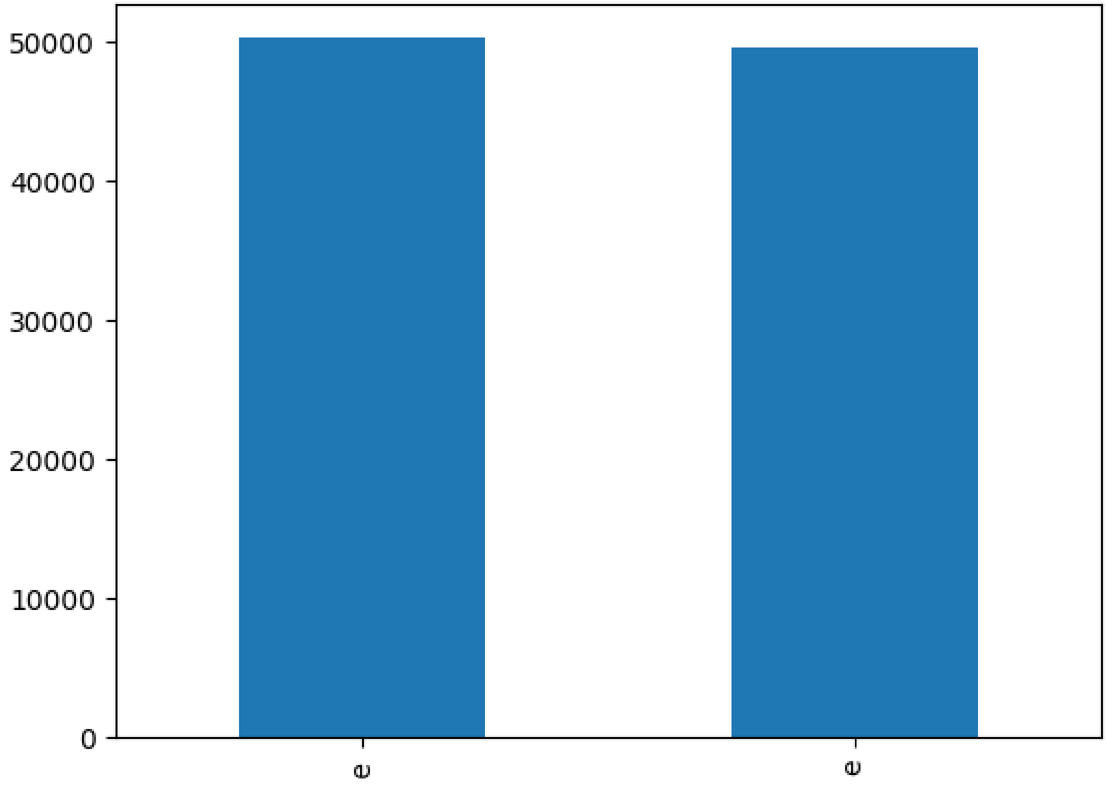
```
156 ATGCACTACCGTATGATCCCCCTTCACTGGATGATGGAAATTGACTGCAATGGCTGCGCTAATAATACTTTGTCTCGTCGTTG
```

```
df.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 100000 entries, 0 to 99999
Data columns (total 2 columns):
 #   Column     Non-Null Count   Dtype 
---  ------     --------------   ----- 
 0   resistant  100000 non-null  bool  
 1   genes      100000 non-null  object
dtypes: bool(1), object(1)
memory usage: 879.0+ KB
```

```
val_counts = df["resistant"].value_counts()
print(val_counts)
val_counts.plot(kind="bar")
```

```
False    50297
True     49703
Name: resistant, dtype: int64
<Axes: >
```



```
from keras.utils import pad_sequences

vocab = ['A', 'C', 'G', 'T']
char2idx = {
  char: (idx+1) for idx, char in enumerate(vocab)
}
```

```
# tokenize (convert to ATGC to 1-4)
def tokenize(sequence):
  return [char2idx[char] for char in sequence]

# one hot encode (convert to sparse vector)
def encode(tokens):
  tensor = tf.constant(tokens)
  one_hot = np.asarray(tf.one_hot(tensor, len(vocab)))
  return one_hot.astype("int32")

df['genes_tokenized'] = df['genes'].apply(tokenize)

# pad right with 0's for the tokenized column
X_token = pad_sequences(df['genes_tokenized'], maxlen=160, padding='post', truncating='post',

X_enc = np.array([encode(tokens) for tokens in X_token])

print(df.head(3))
print("OHE:\n ", X_enc[0][0][:5], "\n .... ")
```

```
      resistant                                             genes  \
   0      False  ATGCACTACCGTATGATCCCCCTTCACTGGATGATGGAAATTGACT...
   1      False  ATGCACTACCGTATGATTCACTGGATGATGGAAATTGACTGCAATG...
   2      False  ATGCACTACCGTATGATTCACTGGATCGTGATGGAAATTGACTGCA...

                                        genes_tokenized
   0  [1, 4, 3, 2, 1, 2, 4, 1, 2, 2, 3, 4, 1, 4, 3, ...
   1  [1, 4, 3, 2, 1, 2, 4, 1, 2, 2, 3, 4, 1, 4, 3, ...
   2  [1, 4, 3, 2, 1, 2, 4, 1, 2, 2, 3, 4, 1, 4, 3, ...
   OHE:
     [0 1 0 0]
    ....
```

```
y = np.array(df['resistant']).astype('int32')

def split(X, ratio=0.8):
  # take out test set (top 20%)
  test_split = int(len(X) * ratio)
  full_train, test = X[:test_split], X[test_split:]

  # hold out top 20% of training for per epoch validation
  validation_split = int(len(full_train) * ratio)
  train, validation = full_train[:validation_split], full_train[validation_split:]

  return train, validation, test

y_train, y_valid, y_test = split(y)
X_enc_train, X_enc_valid, X_enc_test = split(X_enc)
X_token_train, X_token_valid, X_token_test = split(X_token)
```

SVM

```
''' from sklearn.metrics import ConfusionMatrixDisplay, accuracy_score
from sklearn.svm import SVC

svm = SVC(kernel='linear')
svm.fit(X_token_train, y_train)

y_pred = svm.predict(X_token_test)

accuracy = accuracy_score(y_test, y_pred)
print("Accuracy: ", accuracy)

ConfusionMatrixDisplay.from_predictions(y_test, y_pred) '''

# colab dies -> to much data for non parametric
```

```
' from sklearn.metrics import ConfusionMatrixDisplay, accuracy_score\nfro
m sklearn.svm import SVC\n\nsvm = SVC(kernel=\'linear\')\nsvm.fit(X_token
_train, y_train)\n\ny_pred = svm.predict(X_token_test)\n\naccuracy = accu
```

MLP

```
DefaultDense = partial(
  layers.Dense,
  activation='relu',
  kernel_initializer="he_uniform",
  kernel_regularizer= keras.regularizers.l2(0.01)
)
mlp_model = keras.Sequential([
    keras.Input(160),
    DefaultDense(20), # technically not a MLP cos 2 hidden layers but who cares
    DefaultDense(10),
    layers.Dense(1, activation='sigmoid')
])
mlp_model.compile(
  loss='binary_crossentropy',
  optimizer='adam',
  metrics=['accuracy']
)
mlp_model.summary()
```

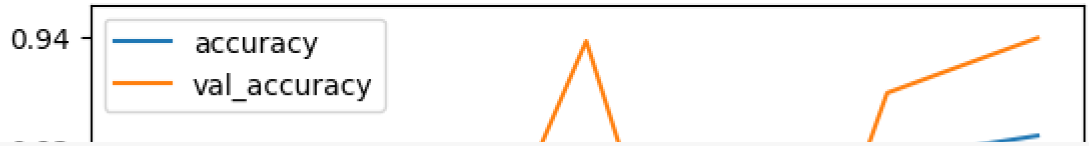
```
Model: "sequential_5"
_________________________________________________________________
 Layer (type)                Output Shape              Param #
=================================================================
 dense_5 (Dense)             (None, 20)                3220
 dense_6 (Dense)             (None, 10)                210       
                                                                 
 dense_7 (Dense)             (None, 1)                 11        
                                                                 
=================================================================
Total params: 3,441
Trainable params: 3,441
Non-trainable params: 0
_________________________________________________________________
```

```
early_stopping_cb = keras.callbacks.EarlyStopping(patience=3) # stop training if overfits
mlp_history = mlp_model.fit(X_token_train, y_train, epochs=7, batch_size=32,
                    validation_data=(X_token_valid, y_valid),
                    callbacks=[early_stopping_cb])
```

```
Epoch 1/7
2000/2000 [==============================] - 11s 4ms/step - loss: 0.5642 - accuracy: 0.
Epoch 2/7
2000/2000 [==============================] - 7s 4ms/step - loss: 0.3807 - accuracy: 0.8
Epoch 3/7
2000/2000 [==============================] - 7s 4ms/step - loss: 0.3240 - accuracy: 0.8
Epoch 4/7
2000/2000 [==============================] - 8s 4ms/step - loss: 0.2894 - accuracy: 0.9
Epoch 5/7
2000/2000 [==============================] - 7s 4ms/step - loss: 0.2677 - accuracy: 0.9
Epoch 6/7
2000/2000 [==============================] - 8s 4ms/step - loss: 0.2536 - accuracy: 0.9
Epoch 7/7
2000/2000 [==============================] - 7s 3ms/step - loss: 0.2382 - accuracy: 0.9
```

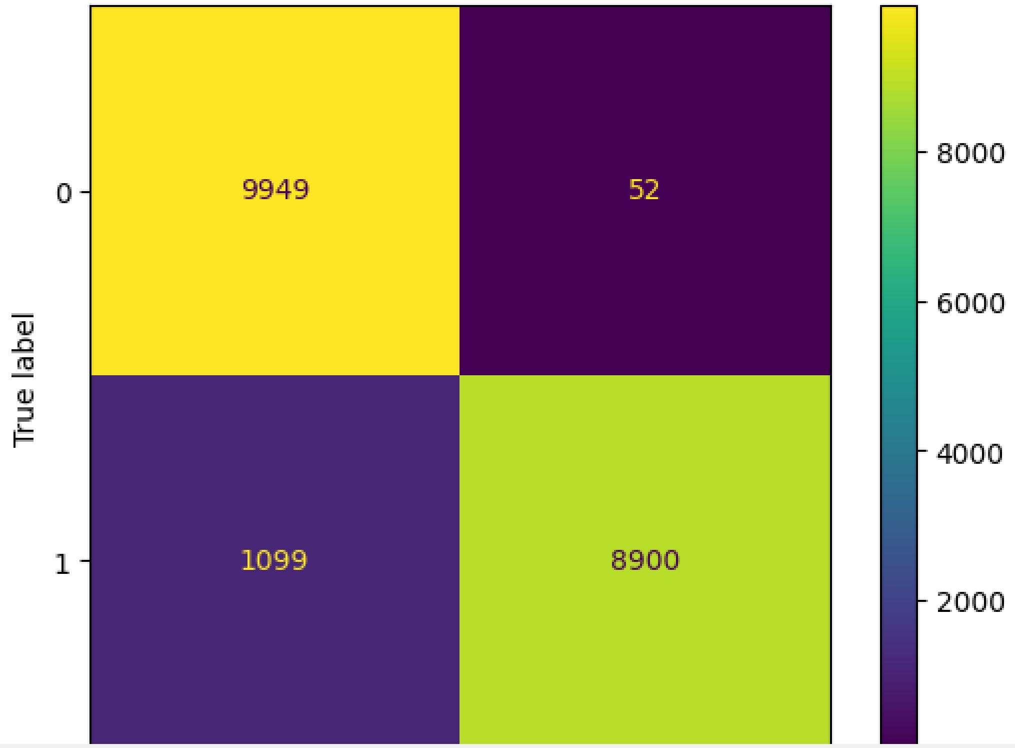
```
pd.DataFrame(mlp_history.history)[['accuracy', 'val_accuracy']].plot()
```

```
<Axes: >
```



```
y_pred = mlp_model.predict(X_token_test)
y_pred = (y_pred > 0.5).astype("int32")
mlp_accuracy = accuracy_score(y_test, y_pred)

print("Accuracy: ", mlp_accuracy)
print(ConfusionMatrixDisplay.from_predictions(y_test, y_pred))
```

```
625/625 [==============================] - 3s 4ms/step
Accuracy:  0.94245
<sklearn.metrics._plot.confusion_matrix.ConfusionMatrixDisplay object at 0
```



GRU

```
gru_model = keras.Sequential([
    layers.Bidirectional(
        # bidirection wrapper converts LSTM to GRU
        layers.LSTM(100, kernel_initializer='he_normal',
                    # kernel_regularizer='l2',
                    # dropout=0.3,
                    activation='tanh'),
        input_shape=(160, 4)
    ),
    # add another dense?
    layers.Dense(1, activation='sigmoid')
])
gru_model.compile(optimizer='adam', loss='binary_crossentropy', metrics=['accuracy'])
gru_model.summary()
```

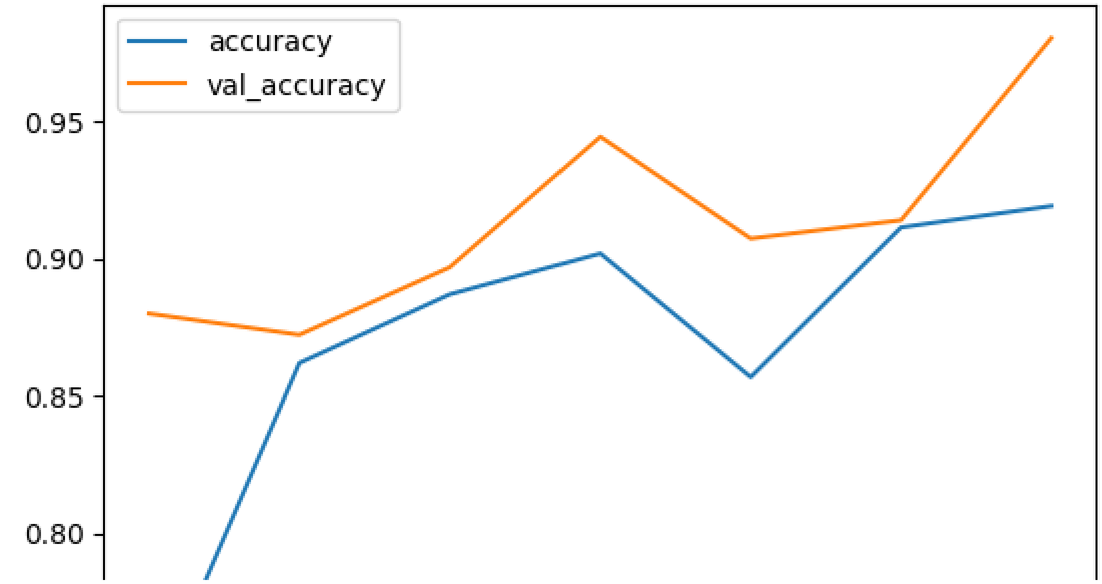
```
Model: "sequential_4"
_________________________________________________________________
 Layer (type)                Output Shape              Param #   
=================================================================
 bidirectional_5 (Bidirectio  (None, 200)              84000     
 nal)                                                            
                                                                 
 dense_4 (Dense)             (None, 1)                 201       
                                                                 
=================================================================
Total params: 84,201
Trainable params: 84,201
Non-trainable params: 0
_________________________________________________________________
```

```
early_stopping_cb = keras.callbacks.EarlyStopping(patience=3)
gru_history = gru_model.fit(X_enc_train, y_train, epochs=7, batch_size=32,
                    validation_data=(X_enc_valid, y_valid),
                    callbacks=[early_stopping_cb])
```

```
Epoch 1/7
2000/2000 [==============================] - 39s 18ms/step - loss: 0.4432 - accuracy: 0
Epoch 2/7
2000/2000 [==============================] - 36s 18ms/step - loss: 0.2597 - accuracy: 0
Epoch 3/7
2000/2000 [==============================] - 35s 17ms/step - loss: 0.2255 - accuracy: 0
Epoch 4/7
2000/2000 [==============================] - 34s 17ms/step - loss: 0.1987 - accuracy: 0
Epoch 5/7
2000/2000 [==============================] - 38s 19ms/step - loss: 0.3001 - accuracy: 0
Epoch 6/7
2000/2000 [==============================] - 31s 15ms/step - loss: 0.1954 - accuracy: 0
Epoch 7/7
2000/2000 [==============================] - 30s 15ms/step - loss: 0.1679 - accuracy: 0
```

```
pd.DataFrame(gru_history.history)[['accuracy', 'val_accuracy']].plot()
```

```
<Axes: >
```



overfits; should re-add dropout/regularization

```
y_pred = gru_model.predict(X_enc_test)
y_pred = (y_pred > 0.5).astype("int32")
gru_accuracy = accuracy_score(y_test, y_pred)

print("Accuracy: ", gru_accuracy)
print(ConfusionMatrixDisplay.from_predictions(y_test, y_pred))
```

```
625/625 [==============================] - 5s 6ms/step
Accuracy:  0.9799
```

CNN

```
DefaultConv = partial(layers.Conv1D, kernel_size=3, strides=1, use_bias=False,
                        padding='same', kernel_initializer='he_normal')

cnn_model = keras.Sequential([

  DefaultConv(32, strides=1, input_shape=(160, 4)),

  layers.Dropout(0.4),

  layers.MaxPooling1D(3, strides=2),

  DefaultConv(64),

  layers.MaxPooling1D(2, strides=2),

  layers.Flatten(),

  layers.Dropout(0.4),

  layers.Dense(64, activation="relu"),

  layers.Dense(1, activation="sigmoid")

])

cnn_model.compile(optimizer='adam', loss='binary_crossentropy', metrics=['accuracy'])
cnn_model.summary()
```

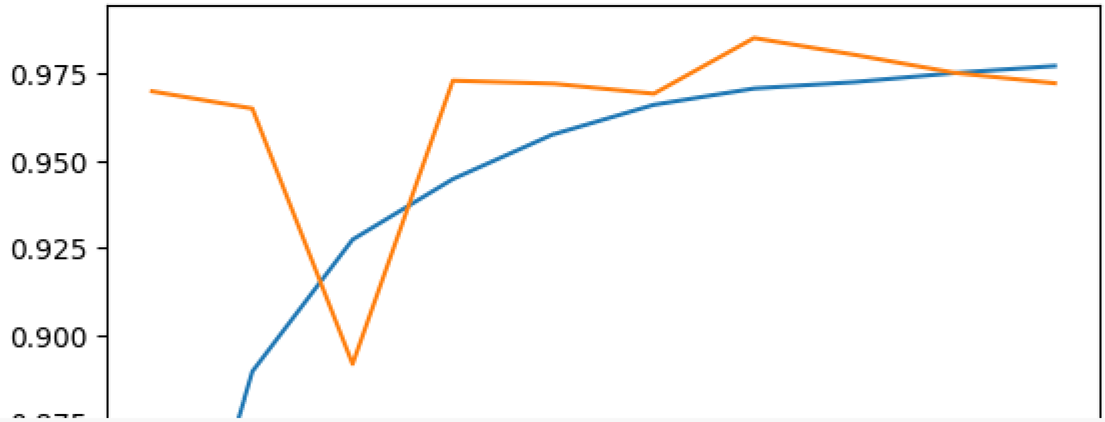
```
Model: "sequential_7"
_________________________________________________________________
 Layer (type)                Output Shape              Param #   
=================================================================
 conv1d_6 (Conv1D)           (None, 160, 32)           384       
                                                                 
 dropout_6 (Dropout)         (None, 160, 32)           0         
                                                                 
 max_pooling1d_2 (MaxPooling  (None, 79, 32)           0         
 1D)                                                             
                                                                 
 conv1d_7 (Conv1D)           (None, 79, 64)            6144      
                                                                 
 max_pooling1d_3 (MaxPooling  (None, 39, 64)           0         
 1D)                                                             
                                                                 
 flatten_4 (Flatten)         (None, 2496)              0         
 dropout_7 (Dropout)         (None, 2496)              0

 dense_11 (Dense)            (None, 64)                159808

 dense_12 (Dense)            (None, 1)                 65

=================================================================
Total params: 166,401
Trainable params: 166,401
Non-trainable params: 0
_________________________________________________________________
```

```
early_stopping_cb = keras.callbacks.EarlyStopping(patience=3)
cnn_history = cnn_model.fit(X_enc_train, y_train, epochs=15, batch_size=32,
                    validation_data=(X_enc_valid, y_valid),
                    callbacks=[early_stopping_cb])
```

```
Epoch 1/15
2000/2000 [==============================] - 10s 4ms/step - loss: 0.3479 - accuracy: 0.
Epoch 2/15
2000/2000 [==============================] - 9s 4ms/step - loss: 0.2311 - accuracy: 0.8
Epoch 3/15
2000/2000 [==============================] - 8s 4ms/step - loss: 0.1686 - accuracy: 0.9
Epoch 4/15
2000/2000 [==============================] - 8s 4ms/step - loss: 0.1372 - accuracy: 0.9
Epoch 5/15
2000/2000 [==============================] - 9s 5ms/step - loss: 0.1126 - accuracy: 0.9
Epoch 6/15
2000/2000 [==============================] - 8s 4ms/step - loss: 0.0960 - accuracy: 0.9
Epoch 7/15
2000/2000 [==============================] - 9s 4ms/step - loss: 0.0875 - accuracy: 0.9
Epoch 8/15
2000/2000 [==============================] - 8s 4ms/step - loss: 0.0834 - accuracy: 0.9
Epoch 9/15
2000/2000 [==============================] - 8s 4ms/step - loss: 0.0774 - accuracy: 0.9
Epoch 10/15
2000/2000 [==============================] - 9s 4ms/step - loss: 0.0732 - accuracy: 0.9
```

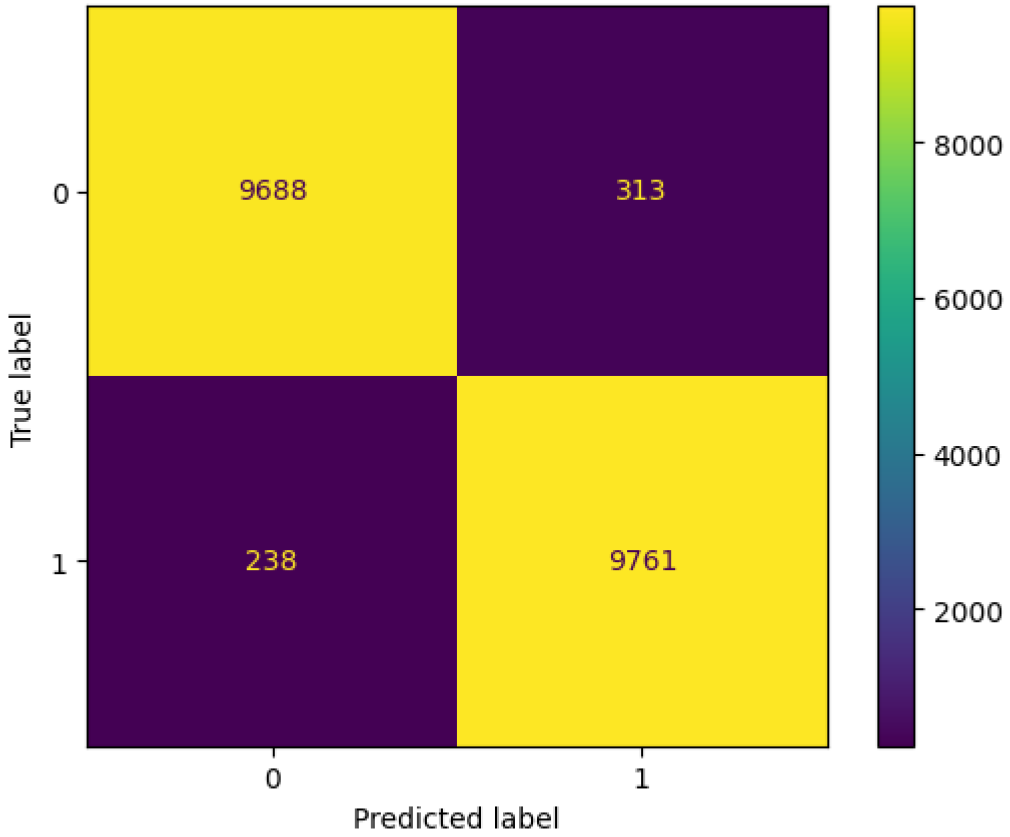
```
pd.DataFrame(cnn_history.history)[['accuracy', 'val_accuracy']].plot()
```

```
<Axes: >
```



```
y_pred = cnn_model.predict(X_enc_test)
y_pred = (y_pred > 0.5).astype("int32")
cnn_accuracy = accuracy_score(y_test, y_pred)

print("Accuracy: ", cnn_accuracy)
print(ConfusionMatrixDisplay.from_predictions(y_test, y_pred))
```

```
625/625 [==============================] - 1s 2ms/step
Accuracy:  0.97245
<sklearn.metrics._plot.confusion_matrix.ConfusionMatrixDisplay object at 0x7f7a9c16f340
```



Improvements that could have been made

- padding sequences is lazy and not sutable for GRU; real scenario would make use of variable length sequences
- Hyper params werent optimized
- didnt use codons