Week 5 Progress Report

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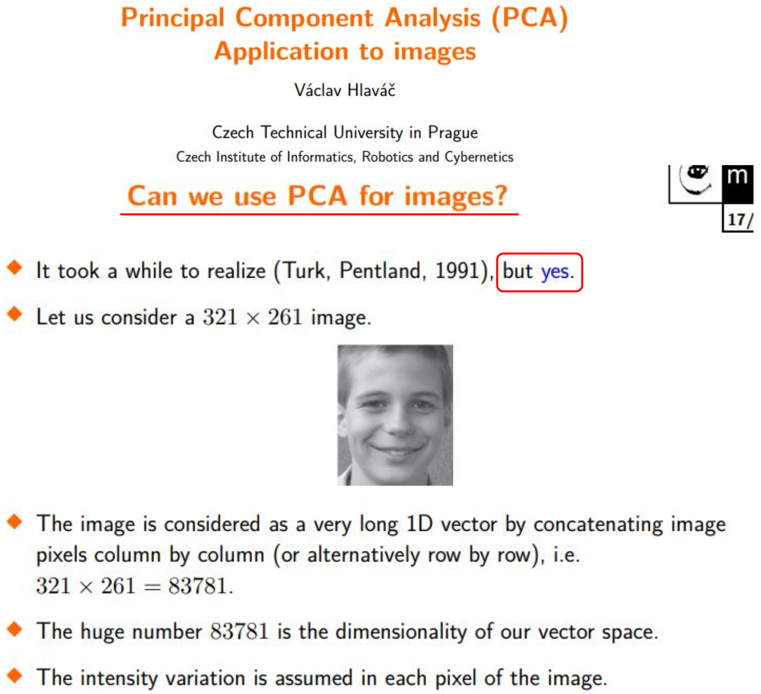
Initial Research and Understanding of PCA

- For high dimensional data, PCA is a method used to reduce the number of variables in data by extracting the important features from a large pool.
- PCA combines variables that are highly correlated together and form groups called ‘principal components’ that accounts for most variance in data
- Helps avoid overfitting by focusing on principal components instead of learning from non-important features
    - ‘Denoising’
- In our dataset, find features (areas or pixels) that are most important in determining if it the melt pool will result in a good or bad part

Using PCA on Images



Principal Component Analysis (PCA)
Application to images

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Can we use PCA for images?

17/

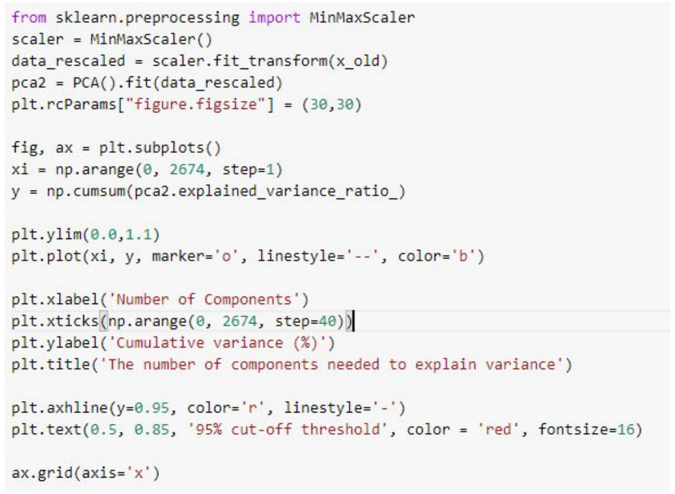
- It took a while to realize (Turk, Pentland, 1991), but yes.
- Let us consider a 321×261 image.

- The image is considered as a very long 1D vector by concatenating image pixels column by column (or alternatively row by row), i.e. $321 \times 261 = 83781$.
- The huge number 83781 is the dimensionality of our vector space.
- The intensity variation is assumed in each pixel of the image.

- First, to know that it is valid to use PCA on images, I read PCA Application to images by Dr. Hlavac from Czech Technical University in Prague
- Asserts that images can be used in PCA, as they can be converted to a one-dimensional vector by row-by-row or column-by-column concatenation
- Like our dataset, a grayscale image is a matrix of values with pixels corresponding to a value (the image on the slide represents intensity in the photo, our dataset a pixel represents a corresponding temperature)

Achieving a Desirable Variance

Code for Graph on Next Slide



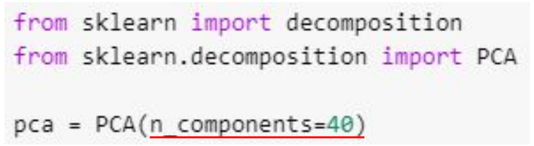
```python
from sklearn.preprocessing import MinMaxScaler
scaler = MinMaxScaler()
data_rescaled = scaler.fit_transform(x_old)
pca2 = PCA().fit(data_rescaled)
plt.rcParams["figure.figsize"] = (30,30)

fig, ax = plt.subplots()
xi = np.arange(0, 2674, step=1)
y = np.cumsum(pca2.explained_variance_ratio_)

plt.ylim(0.0,1.1)
plt.plot(xi, y, marker='o', linestyle='--', color='b')

plt.xlabel('Number of Components')
plt.xticks(np.arange(0, 2674, step=40))
plt.ylabel('Cumulative variance (%)')
plt.title('The number of components needed to explain variance')

plt.axhline(y=0.95, color='r', linestyle='-')
plt.text(0.5, 0.85, '95% cut-off threshold', color = 'red', fontsize=16)

ax.grid(axis='x')
```

- PCA wants to account for the most variability possible in the dataset so that you can get unique features of the dataset
    - Choosing a number of components is important for PCA because it can yield a certain of variance
    - 95% variance seems to be a common for PCA models
- Instead of manually picking components, we can use visualization to figure out how many components to pick

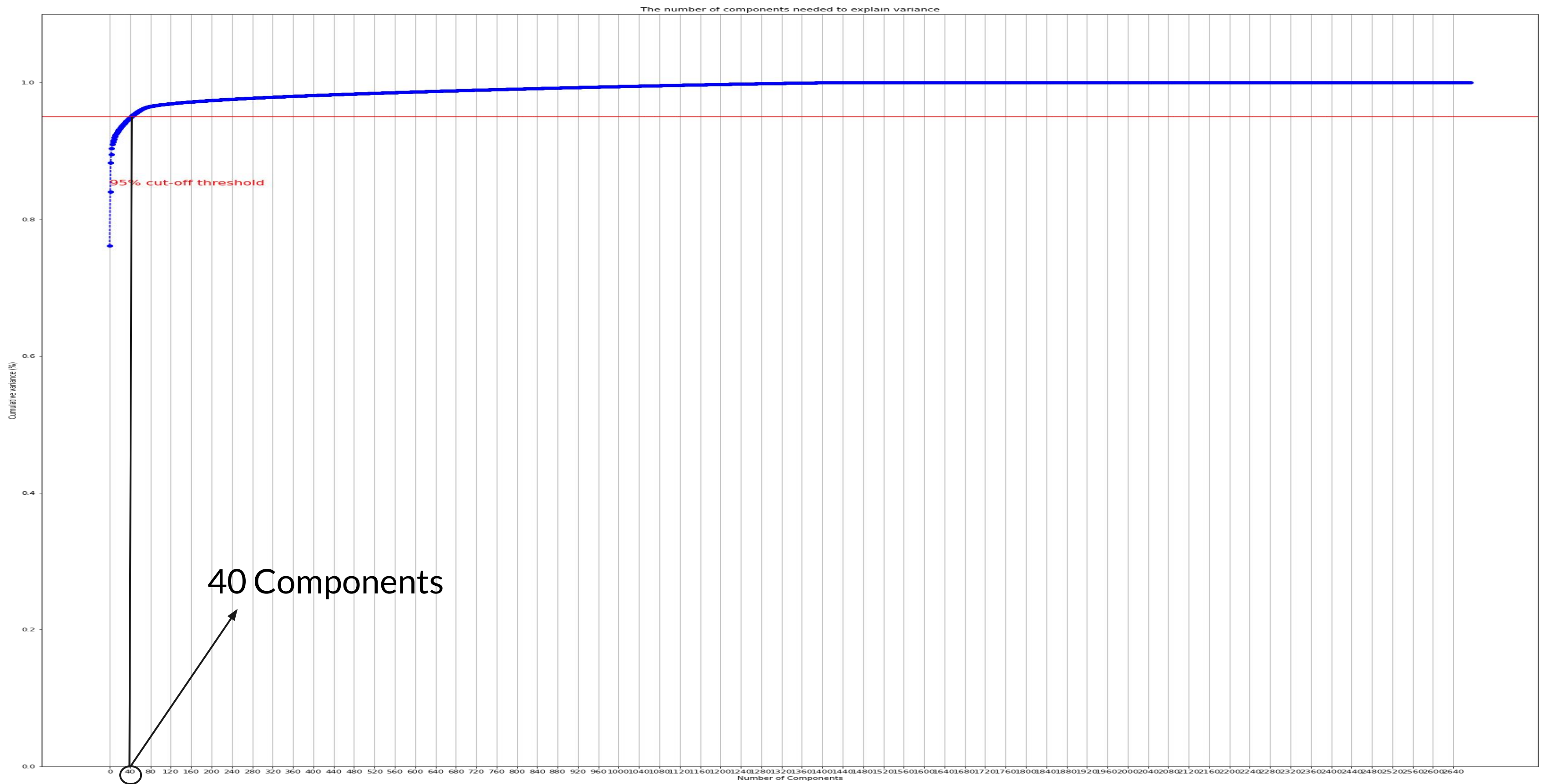
Variance Formula

$$S^2 = \frac{\sum (x_i - \bar{x})^2}{n - 1}$$

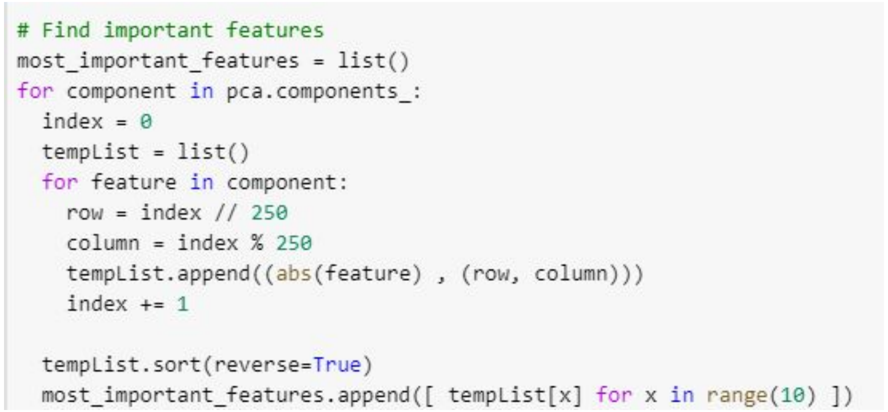
Choosing Components



```python
from sklearn import decomposition
from sklearn.decomposition import PCA

pca = PCA(n_components=40)
```


The number of components needed to explain variance
95% cut-off threshold
40 Components
Cumulative variance (%)
Number of Components

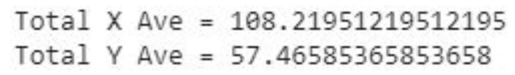
Finding Important Features



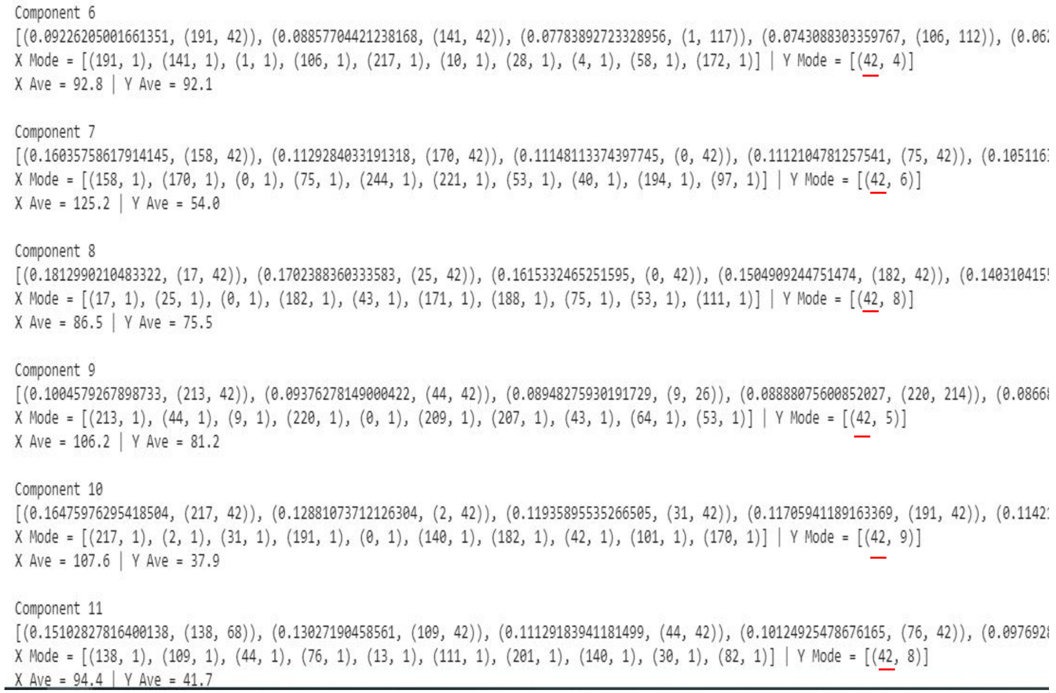
```
# Find important features
most_important_features = list()
for component in pca.components_:
  index = 0
  tempList = list()
  for feature in component:
    row = index // 250
    column = index % 250
    tempList.append((abs(feature) , (row, column)))
    index += 1

  tempList.sort(reverse=True)
  most_important_features.append([ tempList[x] for x in range(10) ])
```

- For each component, every feature has a magnitude of its corresponding values of its eigenvector
  - Bigger the magnitude, the more important it is
- To find these important components
  - Take the absolute value to get a magnitude
  - Sort by largest to smallest
  - Resulting in most important features being at top of list
- Added a (row, column) to see side-by-side how important each pixel is
- Took the top 10 most influential pixels for each component

Summary of PCA Results



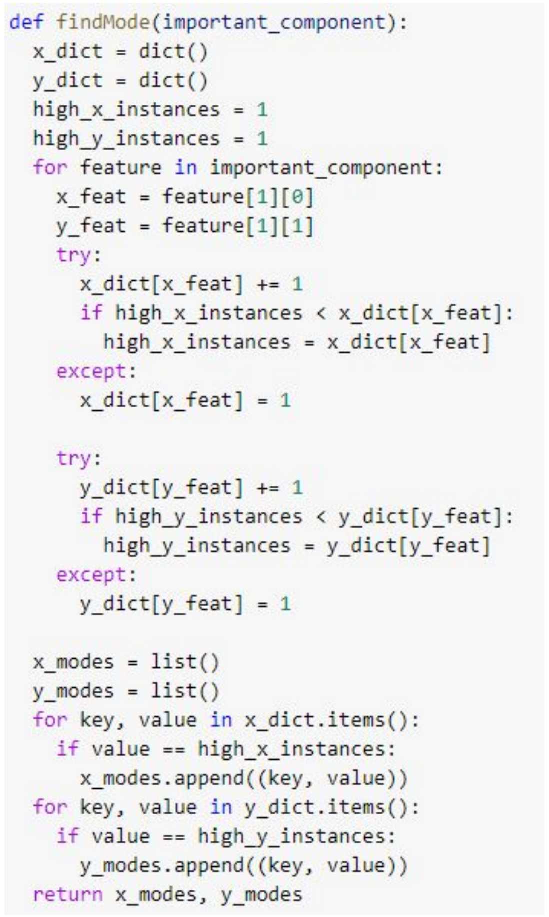
```
Total X Ave = 108.21951219512195
Total Y Ave = 57.46585365853658
```



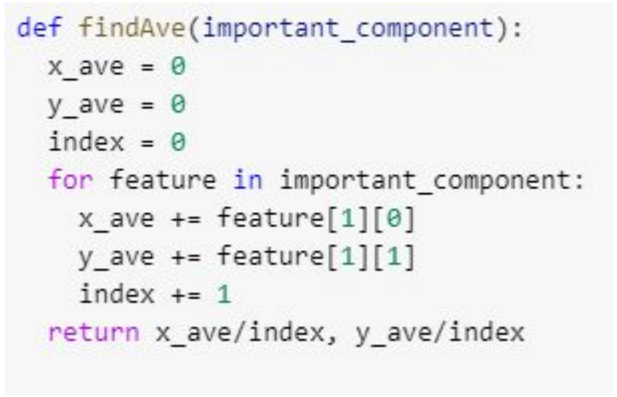
```
Component 6
[(0.09226205001661351, (191, 42)), (0.08857704421238168, (141, 42)), (0.07783892723328956, (1, 117)), (0.0743088303359767, (106, 112)), (0.06
X Mode = [(191, 1), (141, 1), (1, 1), (106, 1), (217, 1), (10, 1), (28, 1), (4, 1), (58, 1), (172, 1)] | Y Mode = [(42, 4)]
X Ave = 92.8 | Y Ave = 92.1

Component 7
[(0.16035758617914145, (158, 42)), (0.1129284033191318, (170, 42)), (0.11148113374397745, (0, 42)), (0.1112104781257541, (75, 42)), (0.105116
X Mode = [(158, 1), (170, 1), (0, 1), (75, 1), (244, 1), (221, 1), (53, 1), (40, 1), (194, 1), (97, 1)] | Y Mode = [(42, 6)]
X Ave = 125.2 | Y Ave = 54.0

Component 8
[(0.1812990210483322, (17, 42)), (0.1702388360333583, (25, 42)), (0.1615332465251595, (0, 42)), (0.1504909244751474, (182, 42)), (0.140310415
X Mode = [(17, 1), (25, 1), (0, 1), (182, 1), (43, 1), (171, 1), (188, 1), (75, 1), (53, 1), (111, 1)] | Y Mode = [(42, 8)]
X Ave = 86.5 | Y Ave = 75.5

Component 9
[(0.1004579267898733, (213, 42)), (0.09376278149000422, (44, 42)), (0.08948275930191729, (9, 26)), (0.08888075600852027, (220, 214)), (0.0866
X Mode = [(213, 1), (44, 1), (9, 1), (220, 1), (0, 1), (209, 1), (207, 1), (43, 1), (64, 1), (53, 1)] | Y Mode = [(42, 5)]
X Ave = 106.2 | Y Ave = 81.2

Component 10
[(0.16475976295418504, (217, 42)), (0.12881073712126304, (2, 42)), (0.11935895535266505, (31, 42)), (0.11705941189163369, (191, 42)), (0.1142
X Mode = [(217, 1), (2, 1), (31, 1), (191, 1), (0, 1), (140, 1), (182, 1), (42, 1), (101, 1), (170, 1)] | Y Mode = [(42, 9)]
X Ave = 107.6 | Y Ave = 37.9

Component 11
[(0.1510282781640138, (138, 68)), (0.13027190458561, (109, 42)), (0.11129183941181499, (44, 42)), (0.10124925478676165, (76, 42)), (0.097692
X Mode = [(138, 1), (109, 1), (44, 1), (76, 1), (13, 1), (111, 1), (201, 1), (140, 1), (30, 1), (82, 1)] | Y Mode = [(42, 8)]
X Ave = 94.4 | Y Ave = 41.7
```

- For Modes (position, instances)
  - Position is either its x or y position
  - Instances is how many time that position occurred
- Can see the magnitude of an eigenvector (importance) next to its row, column coordinates
- Took x and y averages of top 10 most important features
- Took averages of the 40 componentes x and y averages
- y = 42, showed up a lot as a mode

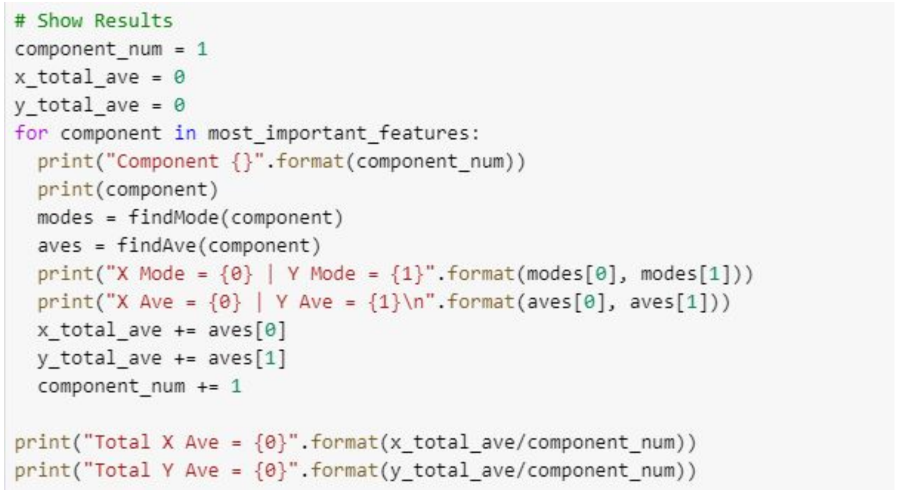
Code for Summary of PCA Results



```python
def findMode(important_component):
  x_dict = dict()
  y_dict = dict()
  high_x_instances = 1
  high_y_instances = 1
  for feature in important_component:
    x_feat = feature[1][0]
    y_feat = feature[1][1]
    try:
      x_dict[x_feat] += 1
      if high_x_instances < x_dict[x_feat]:
        high_x_instances = x_dict[x_feat]
    except:
      x_dict[x_feat] = 1

    try:
      y_dict[y_feat] += 1
      if high_y_instances < y_dict[y_feat]:
        high_y_instances = y_dict[y_feat]
    except:
      y_dict[y_feat] = 1

  x_modes = list()
  y_modes = list()
  for key, value in x_dict.items():
    if value == high_x_instances:
      x_modes.append((key, value))
  for key, value in y_dict.items():
    if value == high_y_instances:
      y_modes.append((key, value))
  return x_modes, y_modes
```



```python
def findAve(important_component):
  x_ave = 0
  y_ave = 0
  index = 0
  for feature in important_component:
    x_ave += feature[1][0]
    y_ave += feature[1][1]
    index += 1
  return x_ave/index, y_ave/index
```



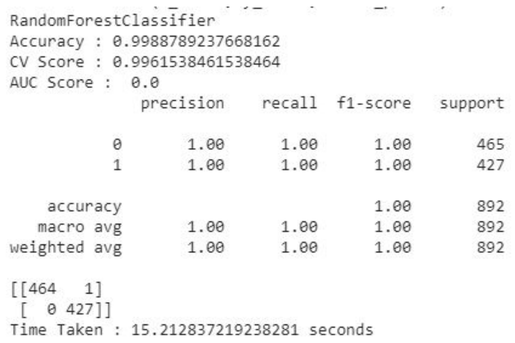
```python
# Show Results
component_num = 1
x_total_ave = 0
y_total_ave = 0
for component in most_important_features:
  print("Component {}".format(component_num))
  print(component)
  modes = findMode(component)
  aves = findAve(component)
  print("X Mode = {0} | Y Mode = {1}".format(modes[0], modes[1]))
  print("X Ave = {0} | Y Ave = {1}\n".format(aves[0], aves[1]))
  x_total_ave += aves[0]
  y_total_ave += aves[1]
  component_num += 1

print("Total X Ave = {0}".format(x_total_ave/component_num))
print("Total Y Ave = {0}".format(y_total_ave/component_num))
```

Random Forest Exploration

1. Why further explore Random Forest Classifier
2. Understanding of Vectorizing a Matrix
3. More testing and results of Random Forest for various parameters

Why further explore Random Forest Classifier?

- Had very high accuracy (above 99% accuracy in classifying)
- Had very fast time compared to other ensemble methods
- Test to see if it can if the first trial was dumb luck or if it can be repeated
- Address whether vectorizing a matrix would lose relationships from the data

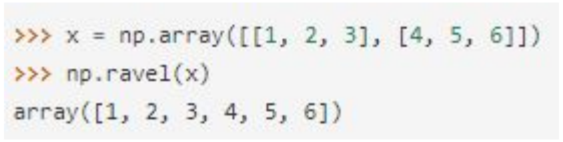


```
RandomForestClassifier
Accuracy : 0.9988789237668162
CV Score : 0.9961538461538464
AUC Score :  0.0
              precision    recall  f1-score   support

           0       1.00      1.00      1.00       465
           1       1.00      1.00      1.00       427

    accuracy                           1.00       892
   macro avg       1.00      1.00      1.00       892
weighted avg       1.00      1.00      1.00       892

[[464   1]
 [  0 427]]
Time Taken : 15.212837219238281 seconds
```

Vectorizing a Matrix Keeps Order and Relationship

$$data = \begin{bmatrix} (0,0) & \ldots & (0,249) \\ \vdots & \ddots & \\ (249,0) & & (249,249) \end{bmatrix} \xrightarrow{\text{Flatten}} vector = [\underset{\substack{\uparrow \\ (0,0)}}{0} \quad \ldots \quad \underset{\substack{\uparrow \\ (0,249)}}{249} \quad \ldots \quad \underset{\substack{\uparrow \\ (249,0)}}{62250} \quad \ldots \quad \underset{\substack{\uparrow \\ (249,249)}}{62499}]$$

Example Python Code



```
>>> x = np.array([[1, 2, 3], [4, 5, 6]])
>>> np.ravel(x)
array([1, 2, 3, 4, 5, 6])
```

Conversion Formulas

From Vector to Matrix

- Row = Vector_i / 250
- Column = Vector_i % 250
- In Matrix: (Row, Column) Order

From Matrix to Vector

- Vector_i = Row * 250 + Column

Testing Random Forest Classifier

Procedure

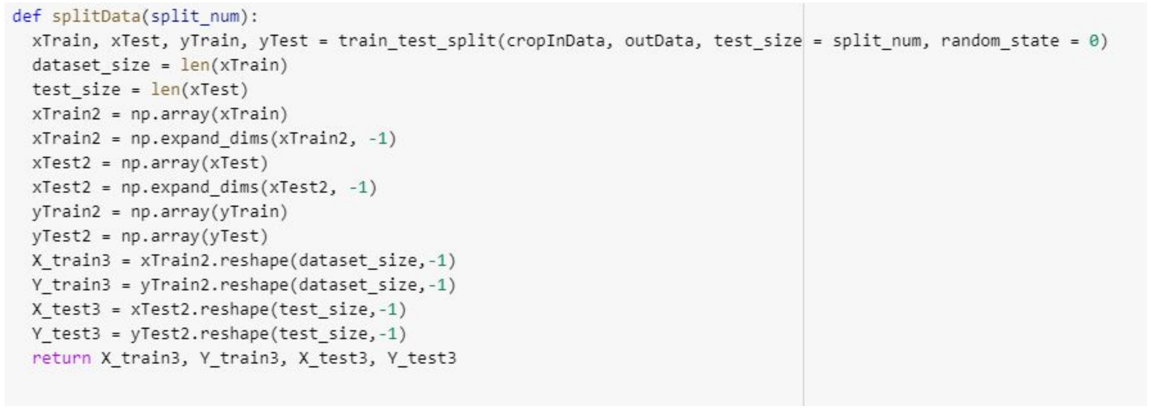
- 100 Total Trials
- 25 Trials each for
  - 50/50 Train/Test Split
  - 60/40 Train/Test Split
  - 70/30 Train/Test Split
  - 80/20 Train/Test Split
- Every trial a new data split will be calculated to ensure random splits

Outcomes

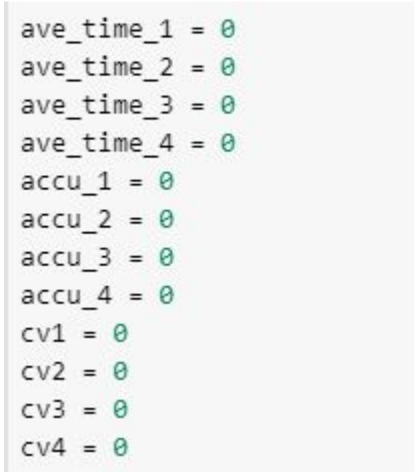
For each type of train/test split over 25 trials:

1. Average Accuracy Score
2. Average Cross Validation Score
3. Average Time Taken per Trial

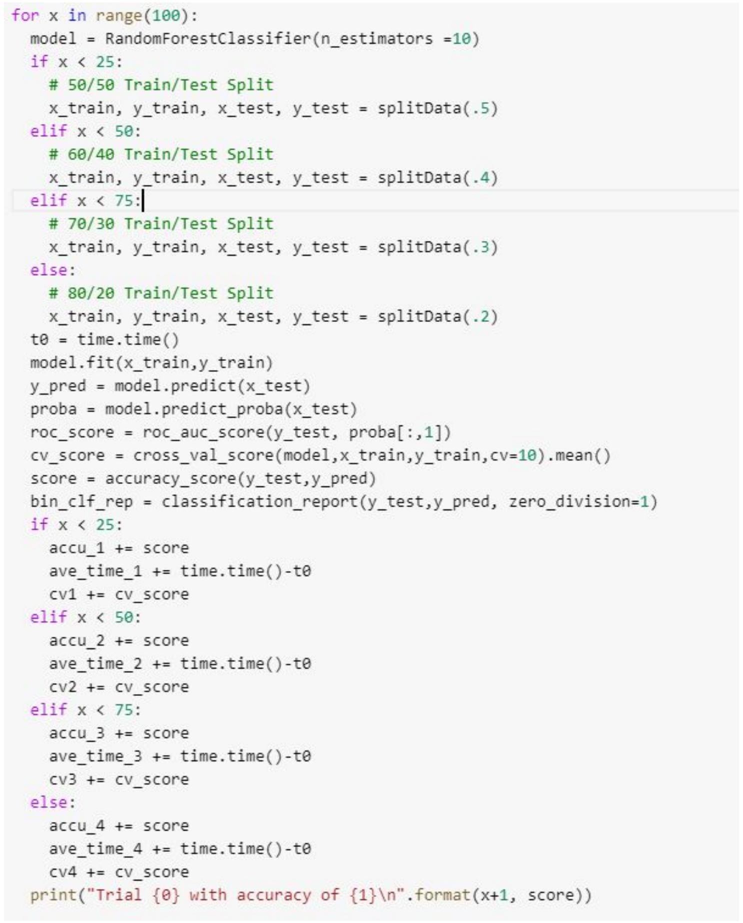
Code for Testing Random Forest Classifier



```
def splitData(split_num):
  xTrain, xTest, yTrain, yTest = train_test_split(cropInData, outData, test_size = split_num, random_state = 0)
  dataset_size = len(xTrain)
  test_size = len(xTest)
  xTrain2 = np.array(xTrain)
  xTrain2 = np.expand_dims(xTrain2, -1)
  xTest2 = np.array(xTest)
  xTest2 = np.expand_dims(xTest2, -1)
  yTrain2 = np.array(yTrain)
  yTest2 = np.array(yTest)
  X_train3 = xTrain2.reshape(dataset_size,-1)
  Y_train3 = yTrain2.reshape(dataset_size,-1)
  X_test3 = xTest2.reshape(test_size,-1)
  Y_test3 = yTest2.reshape(test_size,-1)
  return X_train3, Y_train3, X_test3, Y_test3
```

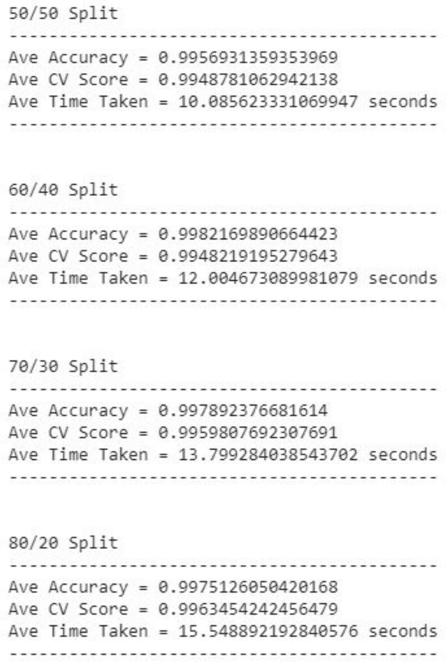


```
ave_time_1 = 0
ave_time_2 = 0
ave_time_3 = 0
ave_time_4 = 0
accu_1 = 0
accu_2 = 0
accu_3 = 0
accu_4 = 0
cv1 = 0
cv2 = 0
cv3 = 0
cv4 = 0
```



```
for x in range(100):
  model = RandomForestClassifier(n_estimators =10)
  if x < 25:
    # 50/50 Train/Test Split
    x_train, y_train, x_test, y_test = splitData(.5)
  elif x < 50:
    # 60/40 Train/Test Split
    x_train, y_train, x_test, y_test = splitData(.4)
  elif x < 75:
    # 70/30 Train/Test Split
    x_train, y_train, x_test, y_test = splitData(.3)
  else:
    # 80/20 Train/Test Split
    x_train, y_train, x_test, y_test = splitData(.2)
  t0 = time.time()
  model.fit(x_train,y_train)
  y_pred = model.predict(x_test)
  proba = model.predict_proba(x_test)
  roc_score = roc_auc_score(y_test, proba[:,1])
  cv_score = cross_val_score(model,x_train,y_train,cv=10).mean()
  score = accuracy_score(y_test,y_pred)
  bin_clf_rep = classification_report(y_test,y_pred, zero_division=1)
  if x < 25:
    accu_1 += score
    ave_time_1 += time.time()-t0
    cv1 += cv_score
  elif x < 50:
    accu_2 += score
    ave_time_2 += time.time()-t0
    cv2 += cv_score
  elif x < 75:
    accu_3 += score
    ave_time_3 += time.time()-t0
    cv3 += cv_score
  else:
    accu_4 += score
    ave_time_4 += time.time()-t0
    cv4 += cv_score
  print("Trial {0} with accuracy of {1}\n".format(x+1, score))
```

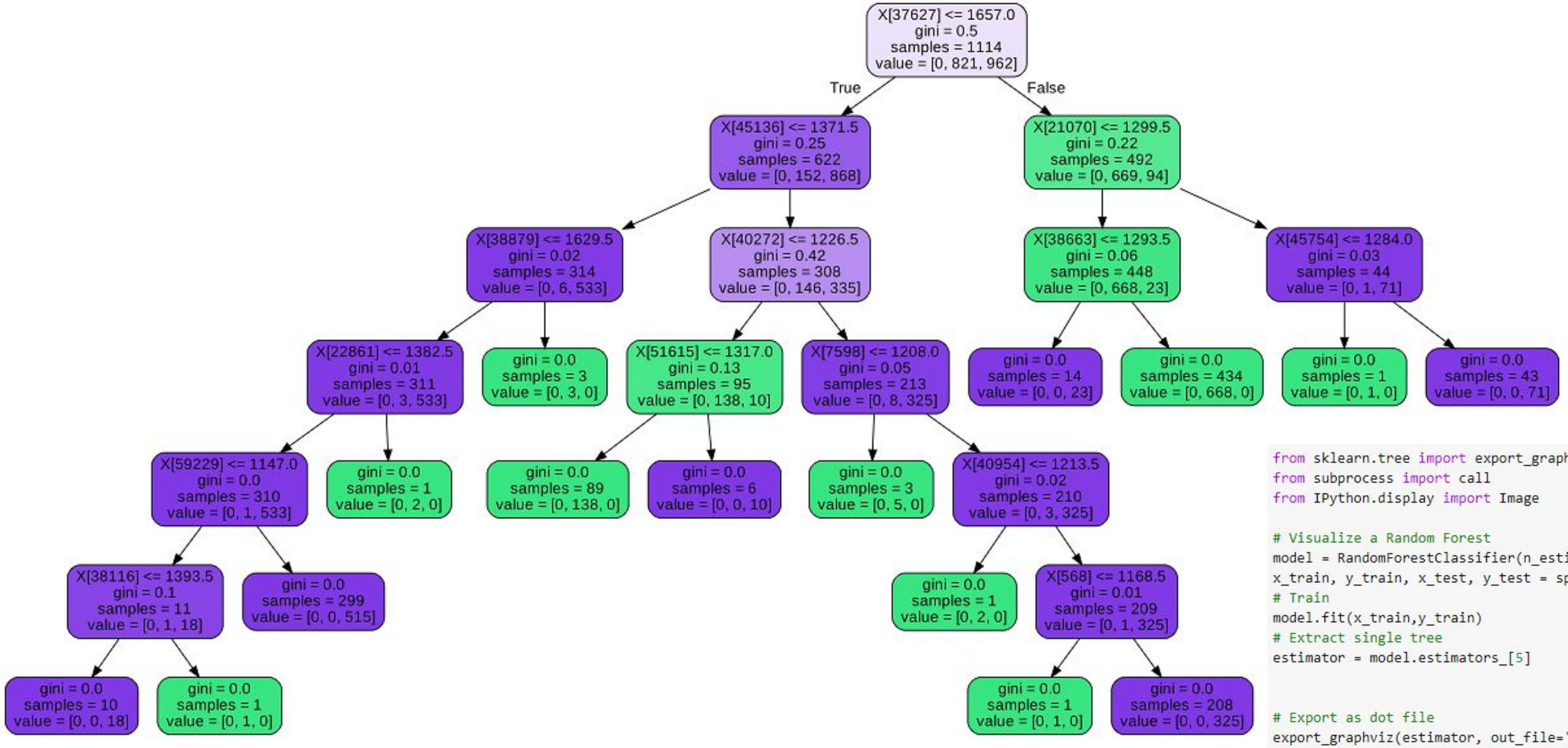
Results for Testing Random Forest

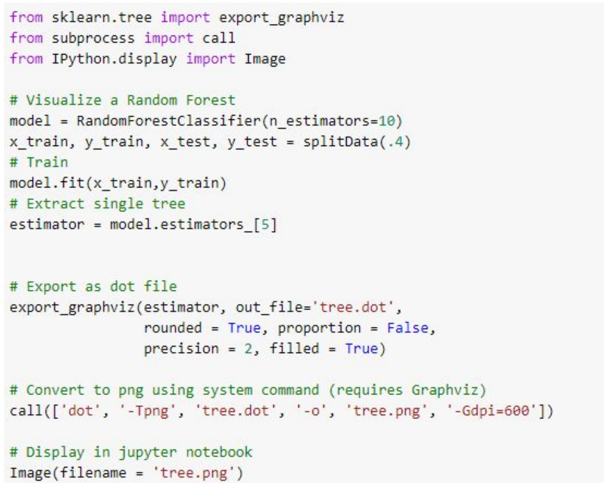


```
50/50 Split
-------------------------------------------
Ave Accuracy = 0.9956931359353969
Ave CV Score = 0.9948781062942138
Ave Time Taken = 10.085623331069947 seconds
-------------------------------------------


60/40 Split
-------------------------------------------
Ave Accuracy = 0.9982169890664423
Ave CV Score = 0.9948219195279643
Ave Time Taken = 12.004673089981079 seconds
-------------------------------------------


70/30 Split
-------------------------------------------
Ave Accuracy = 0.997892376681614
Ave CV Score = 0.9959807692307691
Ave Time Taken = 13.799284038543702 seconds
-------------------------------------------


80/20 Split
-------------------------------------------
Ave Accuracy = 0.9975126050420168
Ave CV Score = 0.9963454242456479
Ave Time Taken = 15.548892192840576 seconds
-------------------------------------------
```

- Highest average accuracy was 60/40 Train/Test split
  - Accuracy of 99.821...%
- Lowest average accuracy was 50/50 Train/Test split
  - Accuracy of 99.569...%
- Time went up with the greater the split towards training
  - Logically, this makes sense as the model has more to data values to train on, the longer it will take

Visualizing a Decision Tree in a Random Forest Classifier





```
from sklearn.tree import export_graphviz
from subprocess import call
from IPython.display import Image

# Visualize a Random Forest
model = RandomForestClassifier(n_estimators=10)
x_train, y_train, x_test, y_test = splitData(.4)
# Train
model.fit(x_train,y_train)
# Extract single tree
estimator = model.estimators_[5]


# Export as dot file
export_graphviz(estimator, out_file='tree.dot',
                rounded = True, proportion = False,
                precision = 2, filled = True)

# Convert to png using system command (requires Graphviz)
call(['dot', '-Tpng', 'tree.dot', '-o', 'tree.png', '-Gdpi=600'])

# Display in jupyter notebook
Image(filename = 'tree.png')
```

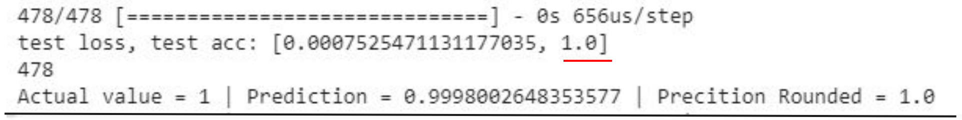
Trying More Neural Networks

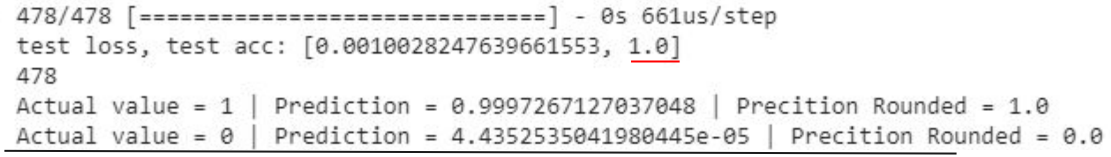
1. Overview of what parameters and architectures I was using
2. Overview of code and results of a currently successful model
3. Need for more testing

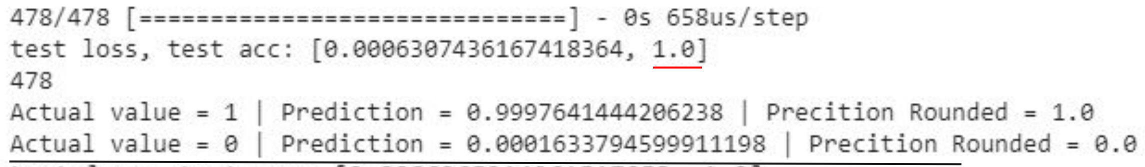
Trying different Models Tried

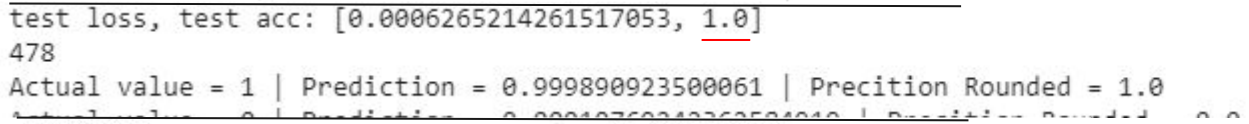
- A lot of time was spent editing different parameters from last weeks neural network (ave 79% test accuracy over 10 trials)
- Different parameters included:
  - Epochs
  - Batch Size
  - Learning Rate
  - Optimizers
  - Activation Functions
  - Many Hidden Layers
  - Few Hidden Layers
  - Different Types of Layer
  - Batch Normalization
  - Dropout Rates

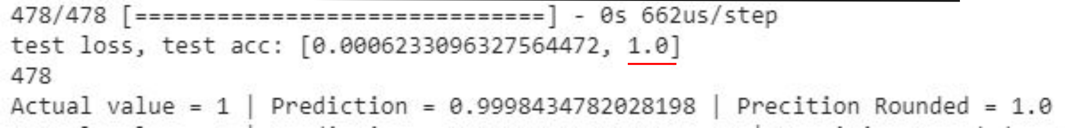
A Promising Result

1.

```
478/478 [==============================] - 0s 656us/step
test loss, test acc: [0.0007525471131177035, 1.0]
478
Actual value = 1 | Prediction = 0.9998002648353577 | Precition Rounded = 1.0
```

2.

```
478/478 [==============================] - 0s 661us/step
test loss, test acc: [0.0010028247639661553, 1.0]
478
Actual value = 1 | Prediction = 0.9997267127037048 | Precition Rounded = 1.0
Actual value = 0 | Prediction = 4.4352535041980445e-05 | Precition Rounded = 0.0
```

3.

```
478/478 [==============================] - 0s 658us/step
test loss, test acc: [0.0006307436167418364, 1.0]
478
Actual value = 1 | Prediction = 0.9997641444206238 | Precition Rounded = 1.0
Actual value = 0 | Prediction = 0.00016337945999111198 | Precition Rounded = 0.0
```

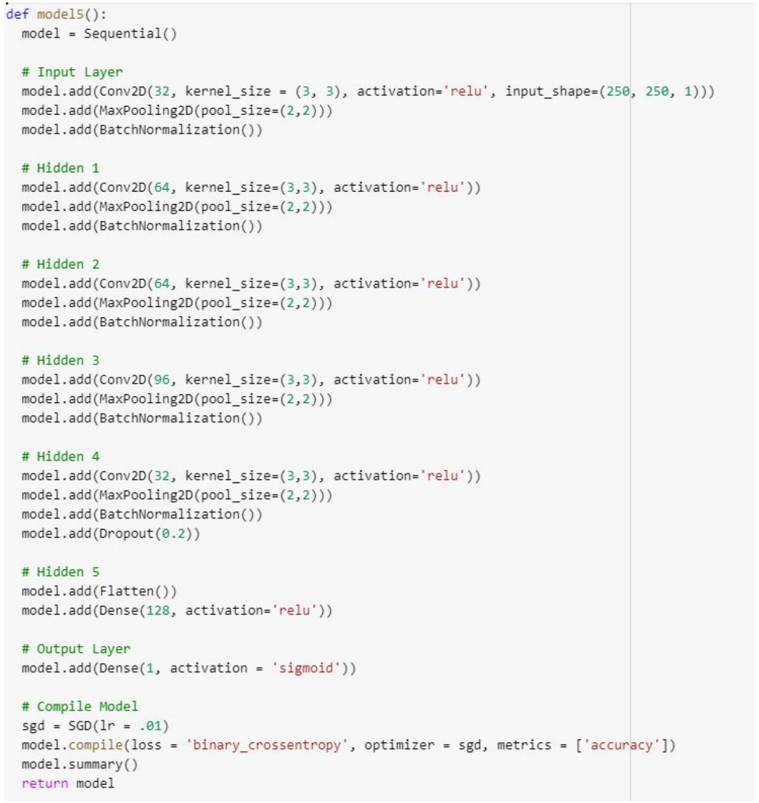
4.

```
test loss, test acc: [0.0006265214261517053, 1.0]
478
Actual value = 1 | Prediction = 0.999890923500061 | Precition Rounded = 1.0
[illegible]
```

5.

```
478/478 [==============================] - 0s 662us/step
test loss, test acc: [0.0006233096327564472, 1.0]
478
Actual value = 1 | Prediction = 0.9998434782028198 | Precition Rounded = 1.0
[illegible]
```

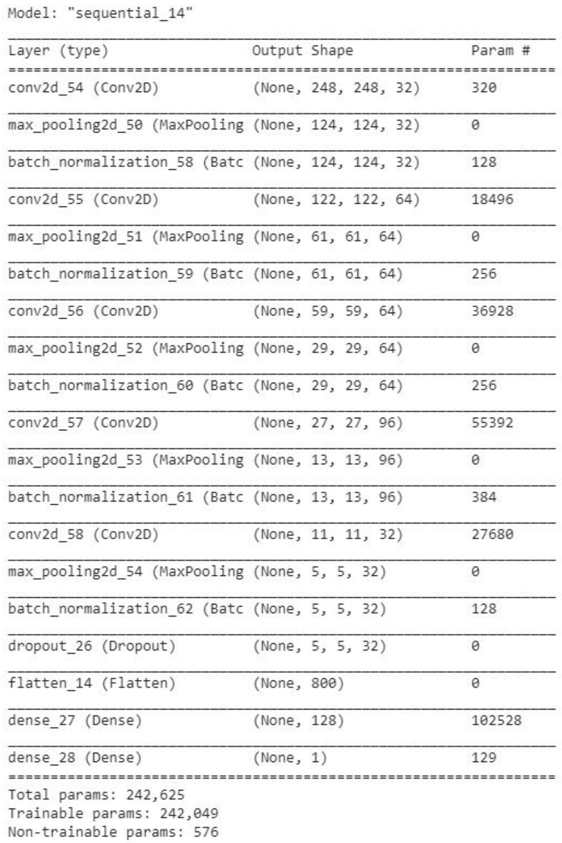
5 Trials of

- 70/30 Train/Test Split
  - Every trial had a different split
- Every trail had a test accuracy of 100%
- 20 Epochs
- Batch Size of 32

The Model’s Architecture / Code



```
def model5():
  model = Sequential()

  # Input Layer
  model.add(Conv2D(32, kernel_size = (3, 3), activation='relu', input_shape=(250, 250, 1)))
  model.add(MaxPooling2D(pool_size=(2,2)))
  model.add(BatchNormalization())

  # Hidden 1
  model.add(Conv2D(64, kernel_size=(3,3), activation='relu'))
  model.add(MaxPooling2D(pool_size=(2,2)))
  model.add(BatchNormalization())

  # Hidden 2
  model.add(Conv2D(64, kernel_size=(3,3), activation='relu'))
  model.add(MaxPooling2D(pool_size=(2,2)))
  model.add(BatchNormalization())

  # Hidden 3
  model.add(Conv2D(96, kernel_size=(3,3), activation='relu'))
  model.add(MaxPooling2D(pool_size=(2,2)))
  model.add(BatchNormalization())

  # Hidden 4
  model.add(Conv2D(32, kernel_size=(3,3), activation='relu'))
  model.add(MaxPooling2D(pool_size=(2,2)))
  model.add(BatchNormalization())
  model.add(Dropout(0.2))

  # Hidden 5
  model.add(Flatten())
  model.add(Dense(128, activation='relu'))

  # Output Layer
  model.add(Dense(1, activation = 'sigmoid'))

  # Compile Model
  sgd = SGD(lr = .01)
  model.compile(loss = 'binary_crossentropy', optimizer = sgd, metrics = ['accuracy'])
  model.summary()
  return model
```



```
Model: "sequential_14"
_________________________________________________________________
Layer (type)                 Output Shape              Param #
=================================================================
conv2d_54 (Conv2D)           (None, 248, 248, 32)      320
_________________________________________________________________
max_pooling2d_50 (MaxPooling (None, 124, 124, 32)      0
_________________________________________________________________
batch_normalization_58 (Batc (None, 124, 124, 32)      128
_________________________________________________________________
conv2d_55 (Conv2D)           (None, 122, 122, 64)      18496
_________________________________________________________________
max_pooling2d_51 (MaxPooling (None, 61, 61, 64)        0
_________________________________________________________________
batch_normalization_59 (Batc (None, 61, 61, 64)        256
_________________________________________________________________
conv2d_56 (Conv2D)           (None, 59, 59, 64)        36928
_________________________________________________________________
max_pooling2d_52 (MaxPooling (None, 29, 29, 64)        0
_________________________________________________________________
batch_normalization_60 (Batc (None, 29, 29, 64)        256
_________________________________________________________________
conv2d_57 (Conv2D)           (None, 27, 27, 96)        55392
_________________________________________________________________
max_pooling2d_53 (MaxPooling (None, 13, 13, 96)        0
_________________________________________________________________
batch_normalization_61 (Batc (None, 13, 13, 96)        384
_________________________________________________________________
conv2d_58 (Conv2D)           (None, 11, 11, 32)        27680
_________________________________________________________________
max_pooling2d_54 (MaxPooling (None, 5, 5, 32)          0
_________________________________________________________________
batch_normalization_62 (Batc (None, 5, 5, 32)          128
_________________________________________________________________
dropout_26 (Dropout)         (None, 5, 5, 32)          0
_________________________________________________________________
flatten_14 (Flatten)         (None, 800)               0
_________________________________________________________________
dense_27 (Dense)             (None, 128)               102528
_________________________________________________________________
dense_28 (Dense)             (None, 1)                 129
=================================================================
Total params: 242,625
Trainable params: 242,049
Non-trainable params: 576
```

- Uses ‘blocks’ of Conv2D, MaxPooling2D, and Batch Normalization
- Finally flattens to a dense layer
- Uses SGD optimizer
- Every layer but the final layer uses relu
- Final layer uses sigmoid

Need to Further Test This Model

- Got first promising results for this model yesterday (6/24)
- Need to test:
  - Different train/test split ratios
  - More Epoch Sizes
    - Originally tested 5 epochs, that had lower accuracy scores
    - 20 Epochs was the text value tested, which yielded very good accuracy scores
  - Batch Size
- Essentially, test this model more thoroughly like the Random Forest Classifier

Future Steps and Goals

Also Google Colab has Corgi Mode, it's great =)

- Test the new neural network model more thorough and give results
- What to do with PCA data / results?
- Suffering from Black Box Testing when construction Neural Networks
  - Advice?
- Ultimate Goal of Project Clarification
  - Should the final model be a neural network, or whatever ascertains a high classification accuracy?
- Any obvious next steps?