Capstone Project

Machine Learning Engineer Nanodegree

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DEFINITION

PROJECT OVERVIEW

About 12% of women living in America will develop some form of invasive breast cancer. It is estimated that 41,760 of women in the US will die from breast cancer in 2019. Breast cancer remains among the most commonly diagnosed types of cancer in older women especially, and a leading cause of death compared to most other types of cancer [1]. In this project we will use the Breast Cancer Wisconsin (Diagnostic) Data Set to build a model that can predict the presence of a malignant cancer based on the given features in the dataset. We will also determine which features are more significant in the detection of malignant breast cancer. The dataset is derived from digitized images of a fine needle aspirate (FNA) biopsy of breast mass samples. The features describe characteristics of the cell nuclei present in the image [^2]. Machine learning techniques have already been used in the diagnosis of breast cancer from Fine Needle Aspirates [3][4]. Early detection of breast cancer can be life-saving and Machine Learning is increasingly being relied upon in early detection methods. It is the real life-saving results using machine learning that draws me to the subject.

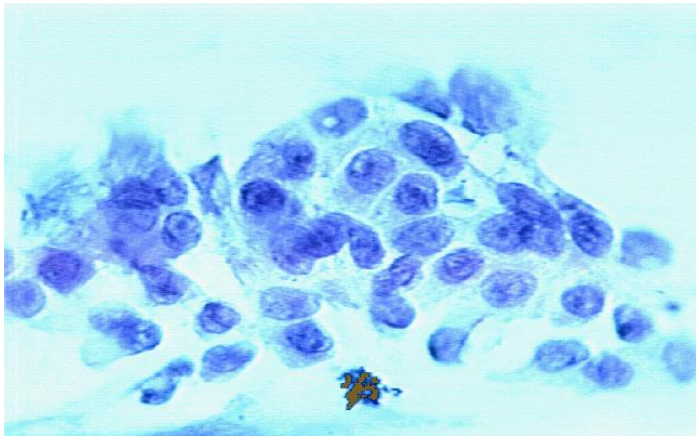


Figure 1. A sample image of an FNA biopsy.

PROBLEM STATEMENT

There are 30 feature measurements contained in the dataset with each sample labeled as either (M) Malignant or (B) Benign. The goal is to determine which features are most important and to build and compare an AdaBoost model and a DNN model that will be able to predict the malignancy of the FNA sample based on the given features. The 2 models will be compared using standard evaluation metrics.

The first model will be an AdaBoost ensemble model and will be used as the benchmark model. The second model will be a Deep Neural Network (DNN) model built with the Keras modules for neural network architecture. AdaBoost and neural network algorithms are popular algorithms in machine learning and have been compared in a number of studies before [5][6]. The 2 competing models will be compared by their evaluation metrics as described below. We will also identify the most important features in the feature set.

METRICS

To compare the AdaBoost and DNN models, we will be using an accuracy score, recall and processing time. Precision and F1 score will also be calculated, but not considered as important for our comparison. Accuracy will give us a measure of how well the model is able to predict the correct outcome. Recall is important because we want to be able to minimize the False Negatives since this is a test for the presence of cancer in a breast mass. Processing time is only relevant if the deployment of the solution has limited resources. It is always good to see how the 2 models compare in time. For processing time, we will use the python time modules to calculate time difference between the training start and stop of each of the 2 models. The formulae for the accuracy, precision, recall, F1 Score and processing time evaluation metrics are shown below.

Accuracy = True Positives + True Negatives / Total number of Samples
Precision = True Positives / (True Positives + False Positives)
Recall = True Positives / (False Negatives + True Positives)
*F1 = 2 * (precision * recall) / (precision + recall)*
Processing Time = Time elapsed between (Training start, Prediction end)

ANALYSIS

DATA EXPLORATION

The Breast Cancer Wisconsin (Diagnostic) Data Set was acquired from the Kaggle website at https://www.kaggle.com/uciml/breast-cancer-wisconsin-data. It is also available from the UCI Website Archive at https://archive.ics.uci.edu/ml/datasets/Breast+Cancer+Wisconsin+%28Diagnostic%29. And from the ftp server at ftp://ftp.cs.wisc.edu/math-prog/cpo-dataset/machine-learn/cancer/. The data consists of a single file of interest of 32 columns and 569 sample instances. Creators of the data set are listed below:

- Dr. William H. Wolberg, General Surgery Dept., University of Wisconsin, Clinical Sciences Center, Madison, WI 53792, wolberg@eagle.surgery.wisc.edu
- W. Nick Street, Computer Sciences Dept., University of Wisconsin, 1210 West Dayton St., Madison, WI 53706,street@cs.wisc.edu 608-262-6619
- Olvi L. Mangasarian, Computer Sciences Dept., University of Wisconsin, 1210 West Dayton St., Madison, WI 53706 olvi@cs.wisc.edu

The data consists of an ID column, a labeled target column that shows (M) for malignant or (B) for Benign and the following 10 features.

1. radius (mean of distances from center to points on the perimeter)
2. texture (standard deviation of gray-scale values)
3. perimeter
4. area
5. smoothness (local variation in radius lengths)
6. compactness (perimeter^2 / area - 1.0)
7. concavity (severity of concave portions of the contour)
8. concave points (number of concave portions of the contour)
9. symmetry
10. fractal dimension ("coastline approximation" - 1)

Each of these 10 features have a mean, standard error and worst or largest (mean of the three largest values) value which makes the total feature set 3 x 10 = 30 features in total. Feature values have been recorded with 4 significant digits.

A sample of the raw data is shown in the Table below.

	id	diagnosis	radius_mean	texture_mean	perimeter_mean	area_mean	smoothness_mean	compactness_mean	concavity_mean	concave points_mean	...
0	842302	M	17.99	10.38	122.80	1001.0	0.11840	0.27760	0.3001	0.14710	...
1	842517	M	20.57	17.77	132.90	1326.0	0.08474	0.07864	0.0869	0.07017	...
2	84300903	M	19.69	21.25	130.00	1203.0	0.10960	0.15990	0.1974	0.12790	...
3	84348301	M	11.42	20.38	77.58	386.1	0.14250	0.28390	0.2414	0.10520	...
4	84358402	M	20.29	14.34	135.10	1297.0	0.10030	0.13280	0.1980	0.10430	...

5 rows × 33 columns

Table 1. A sample of the raw data taken FNA biopsy images.

There are 2 columns in the raw data, viz. **id** and **Unnamed: 32** that were dropped since they carry no significant information for our task. We encoded the diagnosis column with **1** and **0** representing Malignant and Benign respectively. After the 2 columns were dropped, there were no missing or problematic feature values left in the data set. The counts of Malignant and Benign samples in the data is shown below.

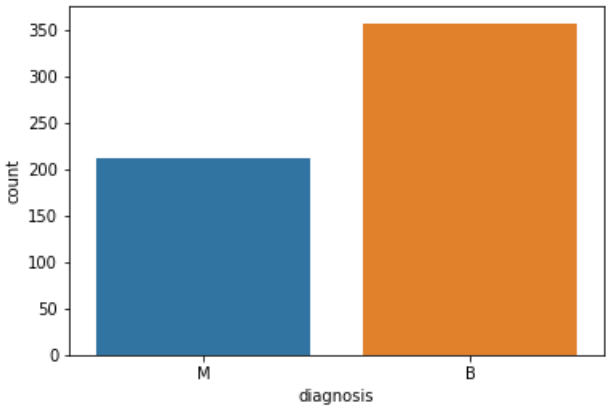


Figure 2. Count of Malignant and Benign diagnoses in the data.

A sample of a table with the statistics of the data is shown below.

	radius_mean	texture_mean	perimeter_mean	area_mean	smoothness_mean	compactness_mean	concavity_mean	concave points_mean	symmetry_mean	fract
count	569.000000	569.000000	569.000000	569.000000	569.000000	569.000000	569.000000	569.000000	569.000000	
mean	14.127292	19.289649	91.969033	654.889104	0.096360	0.104341	0.088799	0.048919	0.181162	
std	3.524049	4.301036	24.298981	351.914129	0.014064	0.052813	0.079720	0.038803	0.027414	
min	6.981000	9.710000	43.790000	143.500000	0.052630	0.019380	0.000000	0.000000	0.106000	
25%	11.700000	16.170000	75.170000	420.300000	0.086370	0.064920	0.029560	0.020310	0.161900	
50%	13.370000	18.840000	86.240000	551.100000	0.095870	0.092630	0.061540	0.033500	0.179200	
75%	15.780000	21.800000	104.100000	782.700000	0.105300	0.130400	0.130700	0.074000	0.195700	
max	28.110000	39.280000	188.500000	2501.000000	0.163400	0.345400	0.426800	0.201200	0.304000	

8 rows × 30 columns

Table 2. Description of basic statistics in the feature set.

We notice that the feature ranges and means are significantly different which we will have to normalize later for a Deep Neural Network model. Also, since we have the mean values, standard error (se) and the mean of the top 3 worst values for each significant feature, we expect that the feature set may be reduced by removing some features that are highly correlated or not as important.

EXPLORATORY VISUALIZATION

Since the feature set consist of 30 columns, we are particularly interested to see if there are highly correlated features that we can use to reduce the input size for the models that we will use. The pair-plot below is a graphical representation of how each of the features are related to every other feature in the feature set.

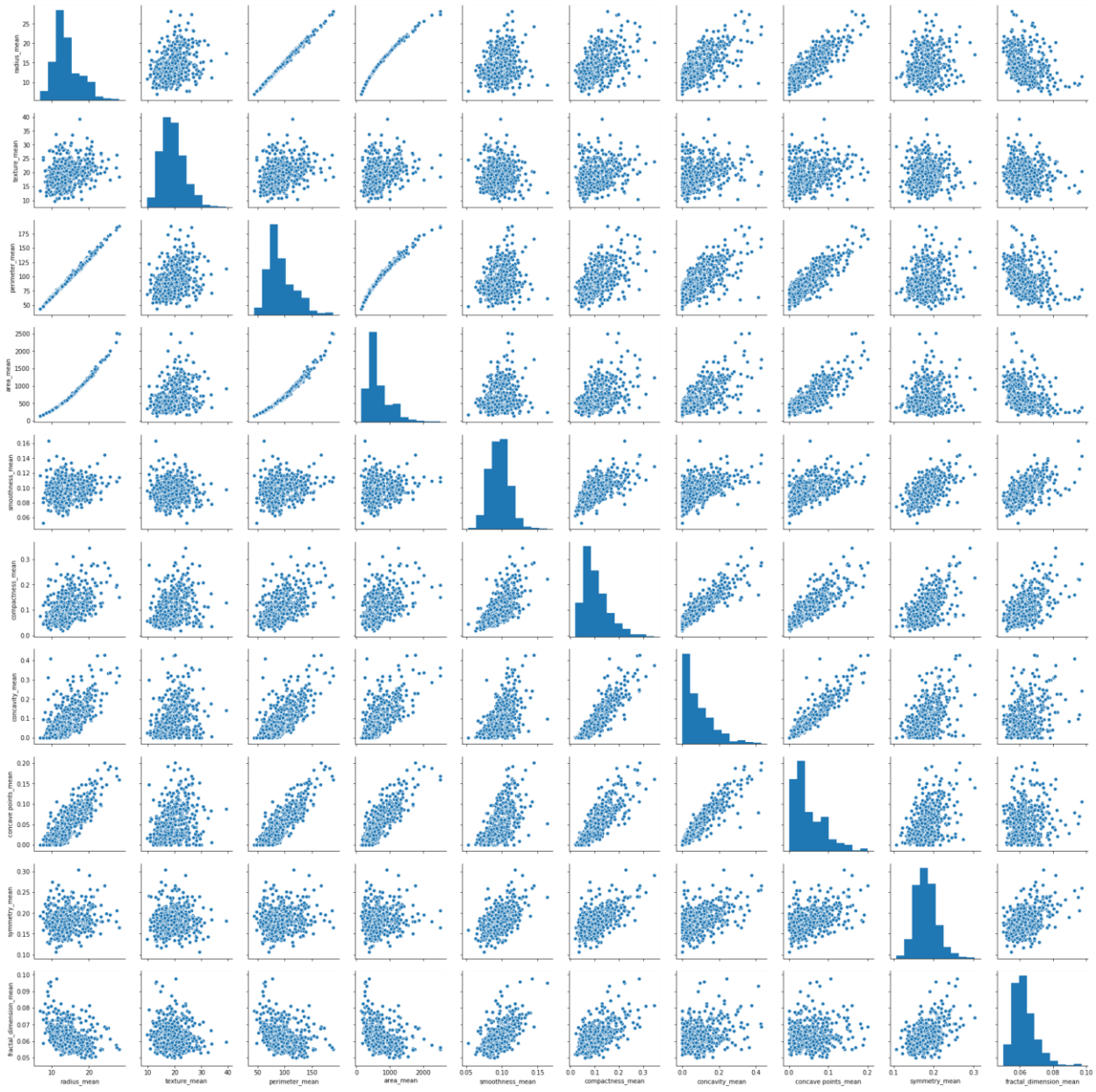


Figure 3: Pair-plot of features showing the pair-wise relationship between features.

We notice that the radius_ features are highly correlated with the area_ and perimeter_ features. This is to be expected given the clearly defined relationship between radius, area and perimeter (or circumference). We also notice that the concavity_ features are correlated to the concavity_points features. This relationship is confirmed by looking at the Pearson's correlation matrix below.

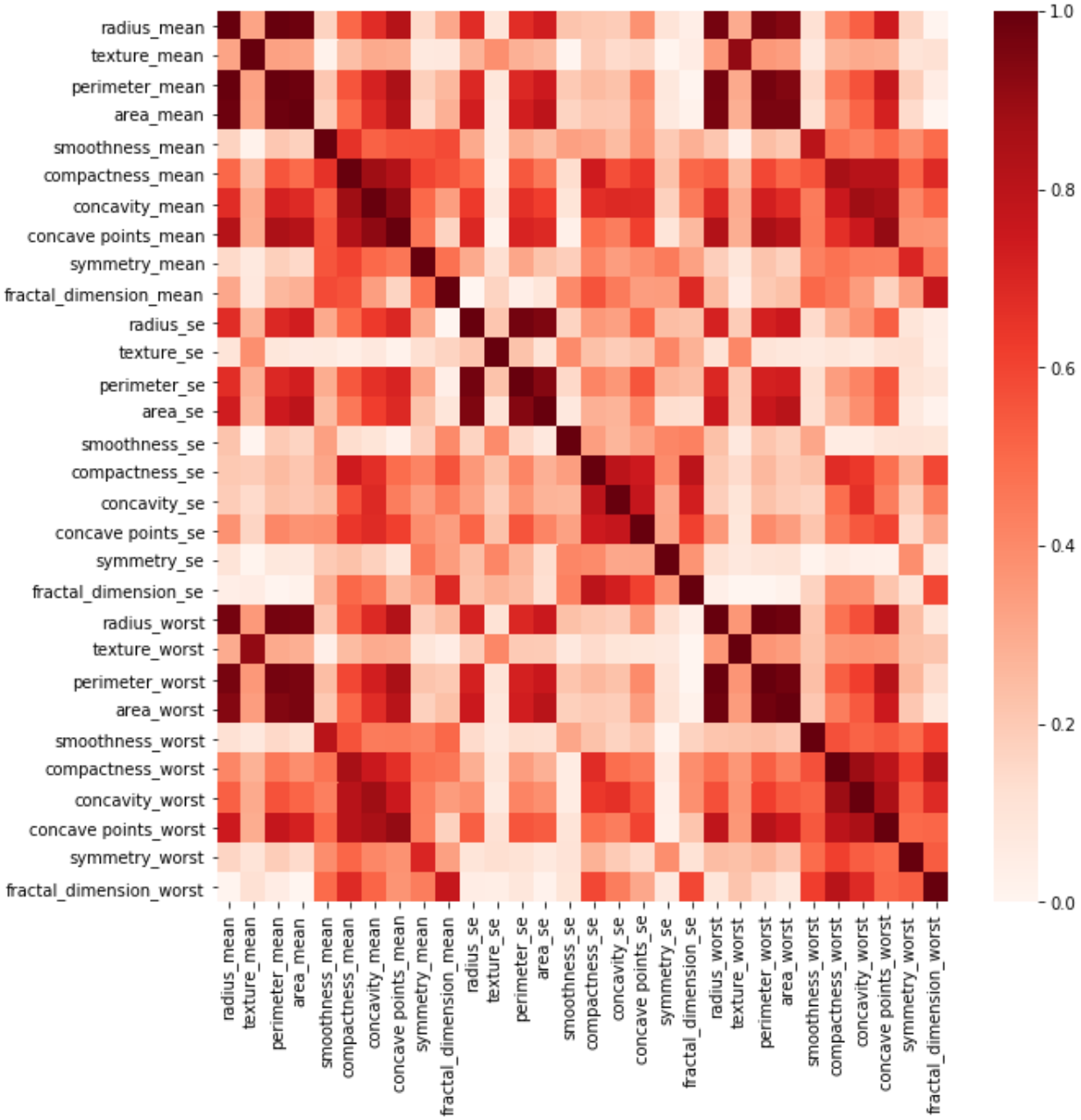


Figure 4: Pearson's Correlation Matrix

We used joint-plots to have a closer look at the relationship between radius, area and perimeter means, as well as concavity_mean and concavepoints_mean.

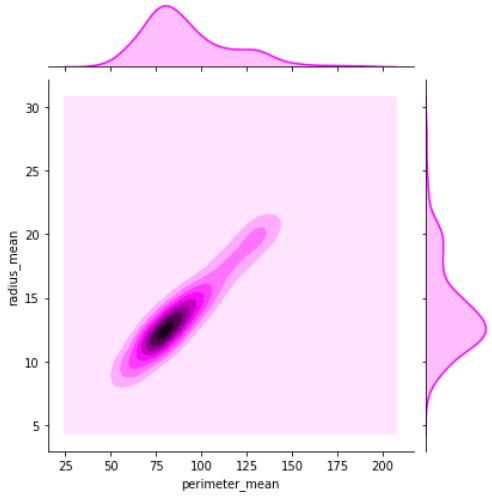


Figure 5: Joint plot of radius_mean and perimeter mean features.

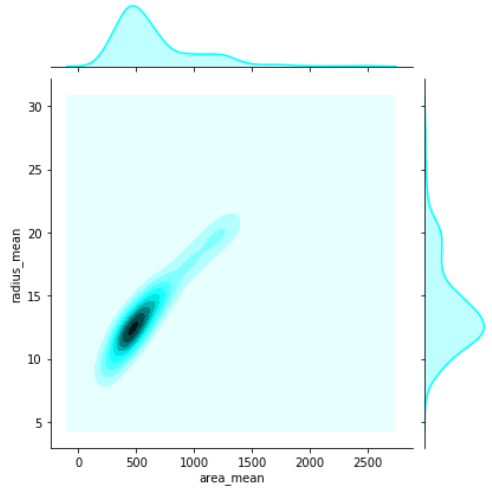


Figure 6: Joint plot of radius_mean and area_mean features.

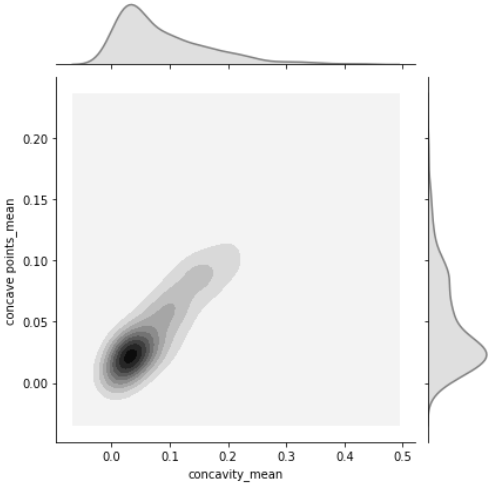


Figure 7: Joint plot of concavity_mean and concavity points_mean features.

From this we conclude that it is not necessary to include the radius_, area_ and perimeter_ features and instead we will only include the radius_ values. For the concavity_ and concave points_ features, we will retain only the concavity_ features.

Another interesting characteristic of the feature set is the distribution of points in each feature category. We used boxed plots to illustrate how the feature distributions compare to each other. The features were separated according to their aggregation categories (mean, se, worst) and then illustrated in a box-plot.

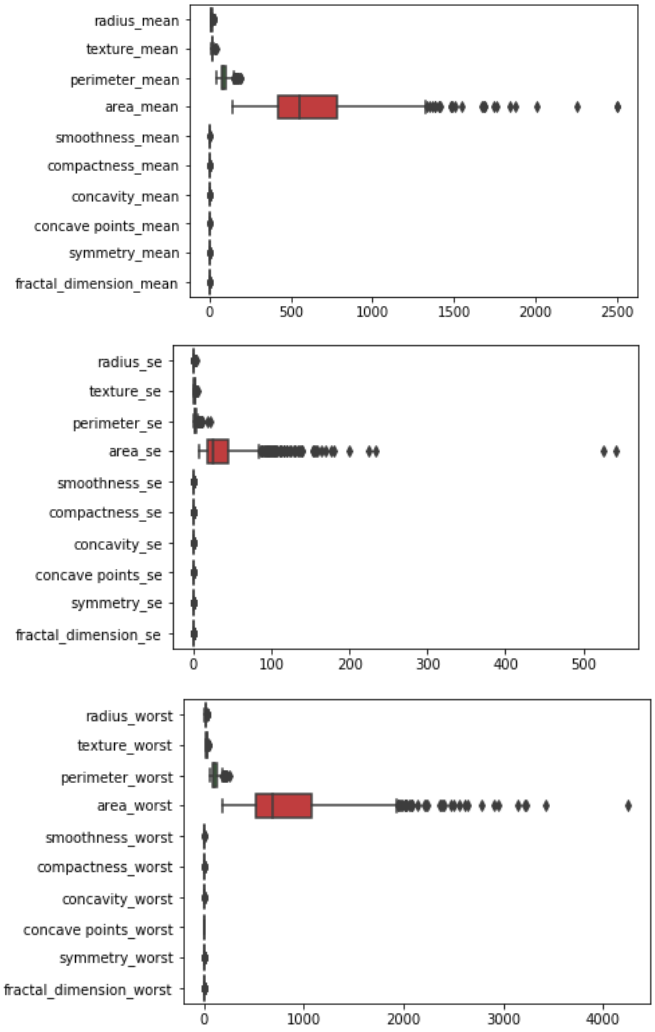


Figure 8: Distributions of Features per Aggregation Category

ALGORITHMS AND TECHNIQUES

After filtering and preprocessing the data, we will employ 2 classification models, the first using AdaBoost and the second a Deep Neural network. AdaBoost and neural network algorithms are popular algorithms in machine learning and have been compared in a number of studies before [5][6]. Both these models have hyper-parameters that can be tweaked to refine the model to achieve the highest possible evaluation metric scores. Each of the models and their hyper-parameters are described below.

AdaBoost

We used an AdaBoost Model as our benchmark model. Boosting is an ensemble method that creates a strong classifier from many weak classifiers such as small decision trees. The output of the weak learners is combined in a weighted sum to produce the boosted classifier output. You can think of a weak learner as a learner that is not very accurate, say just slightly better than 50% right most of the time. Each of these weak learners are assigned weights based on how they have classified a sample. Weights are increased to punish incorrectly classified points of each weak learner. Based on these weights, each learner will vote based on the weights assigned. The sum of these weights are minimized in an error function iteratively improving the error as weak learners are combined.

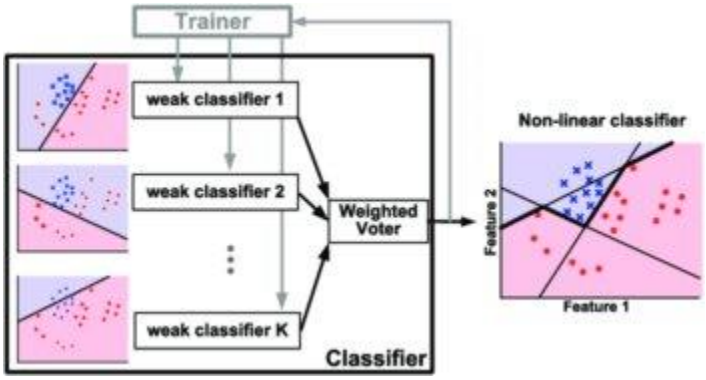


Figure 9. Illustration of AdaBoost Model.

Deep Neural Network Model

The competing model will be a Deep Neural Network. Neural networks are modeled after the human brain that recognizes patterns based on features perceived in the real world. In the human brain we have a complex interconnected network of neurons that are trained through experience to help us recognize patterns. A Deep neural network models the brain function in that it has a set of inputs that are fed to several hidden layers of multiple nodes each that are combined in an output layer to produce the result. Each layer is responsible for some feature extraction. Each node is a computational point and weights are used between these nodes in each layer to modify the computational output of each node. The weights are summed and passed through an activation layer to produce a single output for output nodes. A loss function is used to evaluate the effectiveness of the neural network prediction compared to the actual output values. A optimization method such as Gradient Descent is used to reduce the error by updating the weights in the neural network. Through an iterative process of updating the weights the neural network can be trained to predict more accurate results.

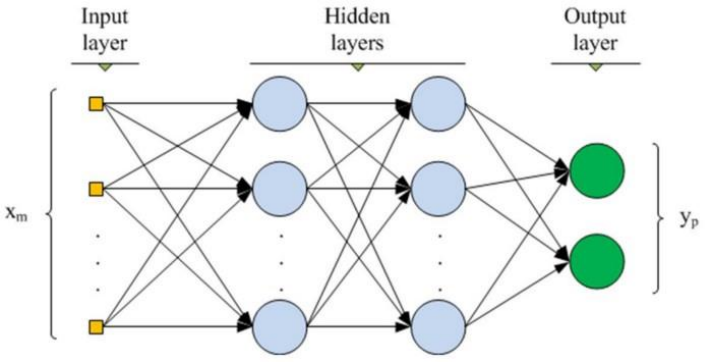


Figure 10. Illustration of DNN with 2 hidden layers.

BENCHMARK MODEL

In our case, since we compared 2 competing models, the AdaBoost model (already described above) was used as the benchmark model. The evaluation metrics of accuracy and recall, in particular, but also precision, F1 Score and processing time was used for comparison with our Deep neural network model. The model was also used to determine the most important features from the feature set. The learning rate was refined to produce the best evaluation metrics to be compared against. We also used a defined random_state to improve the possibility of getting improved results on successive attempts of running the model.

METHODOLOGY

Data Preprocessing

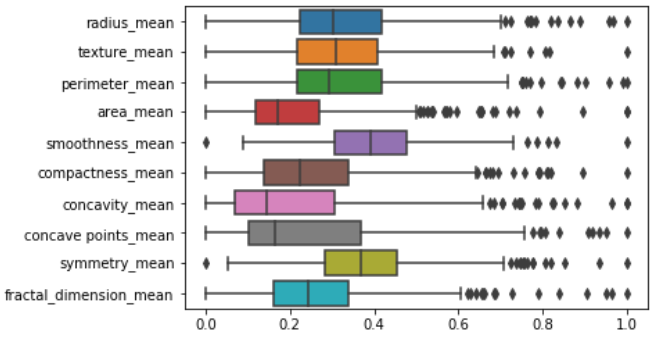
Since the original data file is in a compressed format, we decompressed the data file and then read it into a Pandas data frame, using the variable *X* for the features and *y* for the labels.

We explored the possibility of using the Low Variance method to reduce the number of features to be used for the AdaBoost and DNN models. We used a Low Variance threshold value of *0.9 x (1 - 0.9)*. However, since we used a normalized feature set for the DNN, but not for the AdaBoost model, this method of reducing the feature set was not suitable.

Based on the high correlation seen between radius_, area_ and perimeter_ feature values, as well as between concavity_ and concave points_ feature values, the following features were dropped, thus reducing the feature set from 30 features to only 23 features.

- area_mean
- perimeter_mean
- area_worst
- perimeter_worst
- area_se
- perimeter_se
- concave points_mean

Since it is clear from the box-plots that the ranges, means and variances differ considerably for the different features, with the numerical values of area being larger than the rest, we chose to normalize the feature set for the Deep Neural network model. Normalized distributions of this data are shown below.



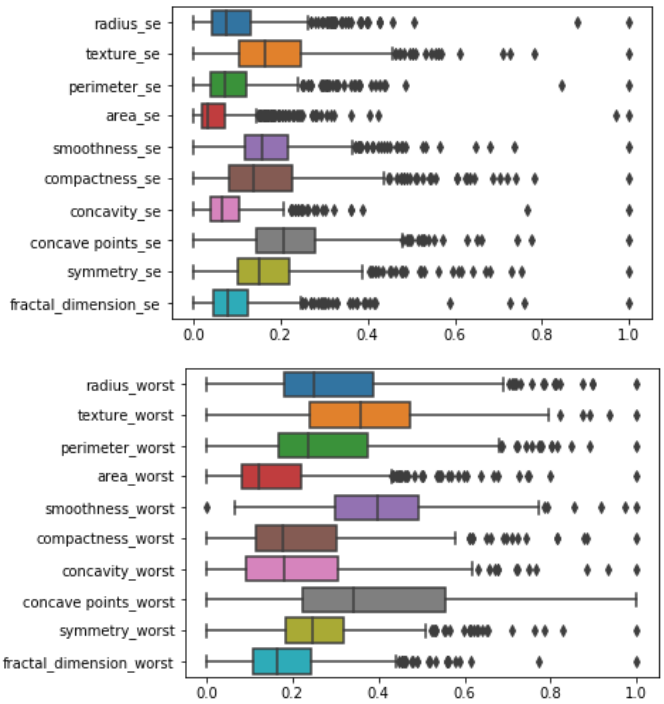


Figure 11: Normalized Features per Feature Aggregation Category.

Implementation

The following flowchart and discussion that follows describes the process followed for our model comparison.

Data Validation and Exploration

We completed some basic data exploration by checking for valid data, removing invalid on unnecessary data, generating some statistics on the features and plotting charts to show some of the characteristics of features. We used the `seaborn` Statistical Data Validation toolset for all visualizations.

Feature Selection and Normalization

We investigated the features, using the low variance method to see if there were any features with low variance that could be excluded. We used a Low Variance threshold value of *0.9 x (1 - 0.9)*. However, this method proved unsuitable for the model comparison since we used normalized features using the MinMaxScaler for the DNN only. We also used the pearson Correlation Matrix to identify highly correlated features which were removed as described before.

Split into Training and Test datasets

Using the *sklearn.model_selection.train_test_split()* module, we split the data into a training set and a testing set. This was done for both the feature set after filtering with and without normalization. We used 20% of the data for testing, 80% for training, with the `shuffle` parameter set to True to ensure a good mix of malignant and benign samples in both training and testing data sets.

Build the Benchmark Adaboost Model

We built an AdaBoost Model as our benchmark model. The following hyper-parameters were used as a baseline, but learning rate was later refined to 0.9 to produce the best evaluation metric results for the benchmark model.

1. base_estimator: DecisionTreeClassifier(max_depth=1)
2. n_estimators: 1000
3. learning_rate: 1.0 (changed to 0.9 on refinement)
4. algorithm: SAMME.R
5. random_state: 19

After fitting the model to the training set, we used it to predict the outcome on the test data set. Thereafter we calculated the following evaluation metrics:

Accuracy = True Positives + True Negatives / Total number of Samples
Recall = True Positives / (False Negatives + True Positives)
Processing Time = Time elapsed between (Training start, Prediction end)

Build the DNN Model

The competing model was a Deep Neural Network. We built this model with Keras. The model architecture consisted of the input layer, 2 hidden layers of 16 nodes each with *relu* activation functions and a dense layer for the output with *softmax* activation function. The DNN model used the *binary_crossentropy* loss function with the *rmsprop* optimizer against the `accuracy` metric. We trained the model using *batch_size* of 32 for 1000 epochs as a baseline model. Thereafter the batch size was changed to 16 and 64. Since the best result was found using batch_size of 64, we used that batch_size to further change the model by adding drop_out layers with a drop_out value tweaked to 0.4 for the best result.

Compare Evaluation Metrics

Once both models were trained and used to predict the outcomes on the test set, we compared the results of the evaluation metrics for each of the models. Finally we will drew some conclusions on the strengths and weaknesses of the competing models based on these results.

REFINEMENT

The AdaBoost model and Deep Neural Network model were both refined with multiple runs adjusting the hyperparameters. For the AdaBoost model the final Hyperparameter values selected are shown below:

1. base_estimator: DecisionTreeClassifier(max_depth=1)
2. n_estimators: 1000
3. learning_rate: 0.9
4. algorithm: SAMME.R
5. random_state: 19

The initial results with learning_rate set to 1 is shown below:

Accuracy score	0.947
Precision score	0.976
Recall score	0.889
F1 score	0.930
Elapsed Time	1.531

Table 3: Evaluation Metrics for First AdaBoost Model

Accuracy score	0.956
Precision score	1.000
Recall score	0.889
F1 score	0.941
Elapsed Time	1.547

Table 4: Evaluation Metrics for Final AdaBoost Model

In the final AdaBoost model, the Accuracy score, Precision score and F1 score is higher with the processing time being just slightly more than the previous model.For the DNN, the baseline model had 2 hidden layers of 16 nodes with relu activation functions, using a batch_size of 32 and no Dropout layers. Below are the results for the baseline DNN model.

Accuracy score	0.974
Precision score	0.957
Recall score	0.978
F1 score	0.967
Elapsed Time	47.938

Table 5: Evaluation Metrics for Baseline DNN Model

After refining the baseline model by changing the batch_size and experimenting with adding dropout layers, the model that produced the best results had batch_size of 64 with no dropout layers. The evaluation metrics for the best DNN model is shown below.

Accuracy score	0.982
Precision score	1.000
Recall score	0.956
F1 score	0.977
Elapsed Time	27.094

Table 6: Evaluation Metrics for Best DNN Model

RESULTS

There were 2 goals to this project viz. find the most important features in the data set and find the best of the 2 competing models between AdaBoost and a DNN. We used the results from the AdaBoost model to find the most important features. This is shown in the chart below:

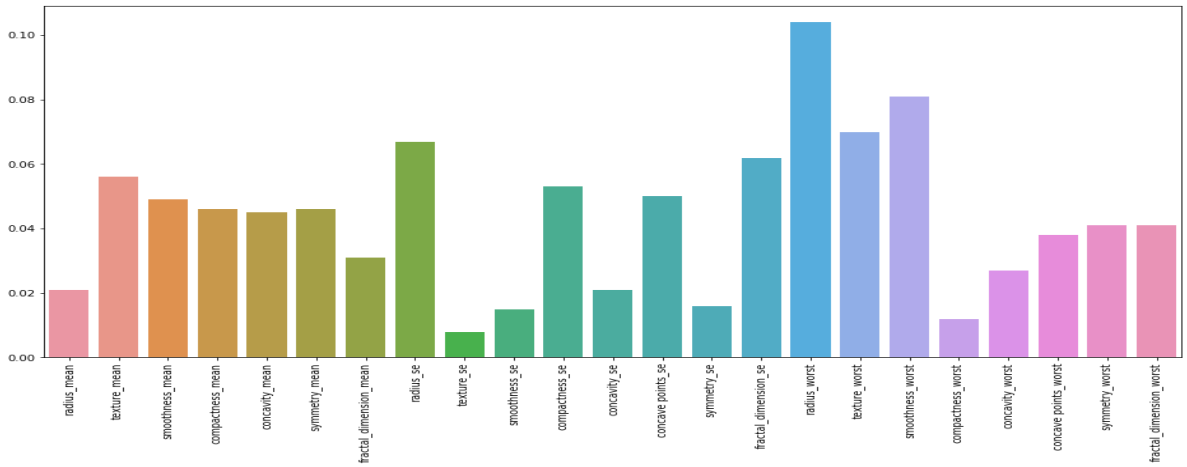


Figure 12: The Most Important Features

The table below shows the results of all the models built for each of the evaluation metrics.

Evaluation Metric	AdaBoost, lr=1.0	AdaBoost lr =0.9	DNN, bs=32, no Dropouts	DNN, bs=16, no Dropouts	DNN, bs=64, no Dropouts	DNN, bs=64, with Dropout=0.4
Accuracy score	0.947	0.956	0.974	0.974	**0.982**	0.965
Precision score	0.976	1.0	0.957	1.0	**1.0**	0.977
Recall score	0.889	0.889	0.9778	0.9334	**0.9556**	0.933
F1 score	0.930	0.941	0.967	0.966	**0.977**	0.955
Elapsed Time	1.531	1.547	47.938	90.734	**27.094**	37.797

Table 7: Evaluation Metrics of all AdaBoost and DNN models

MODEL EVALUATION AND VALIDATION

The final model selected from all the models tested is the Deep Neural Network with 2 hidden layers of 16 nodes each, with relu activation functions and a Dense output layer with sigmoid activation function. The DNN architecture does not have Dropout layers and the batch size = 64.

This model was selected based on the results shown in Table 7 above. This model has the highest accuracy, precision and F1 scores with the second highest recall score. Only the DNN with batch-size of 32 and not Dropouts had a recall score higher than this model. Even though recall is important to us for a Breast Cancer Malignancy test, it is a small trade-off for the gains on all other metrics.

Several runs of this model have shown it to be superior. The input has been varied by the shuffle=True setting in the splitting of the training and testing data sets. Dropout layers have not improved this model either.

JUSTIFICATION

I believe the final solution is the best solution of all the models tested. While the DNN takes significantly longer to train, it has produced higher evaluation metrics in every evaluation category. The table below shows the Benchmark AdaBoost model compared to the Final DNN Solution.

Evaluation Metric	Benchmark Model AdaBoost lr =0.9	Final Solution DNN, bs=64, no Dropouts
Accuracy score	0.956	**0.982**
Precision score	1.0	**1.0**
Recall score	0.889	**0.956**
F1 score	0.941	**0.977**
Elapsed Time	1.547	**27.094**

Table 8. Comparing the Final Solution to the Baseline Model

CONCLUSION

FREE FORM VISUALIZATION

One significant conclusion from this project is in regard to the features found to be most important. Based on the most important features shown in Figure 8 above, we notice that the radius_worst, smoothness_worst and texture_worst , in that order, are the most important features for this data set. This is also intuitively what we would expect, however, I was expecting the mean radius to be among the top 3 most important features as well.

What is even more interesting is that when we look at the relational plots of radius_worst with the smoothness_worst and texture_worst, we notice that malignant samples are very closely tied to the radius_worst feature. In fact, where the radius_worst is mostly above a value of 15 – 20, the malignancy outcome is very likely and above 25 virtually a certainty.

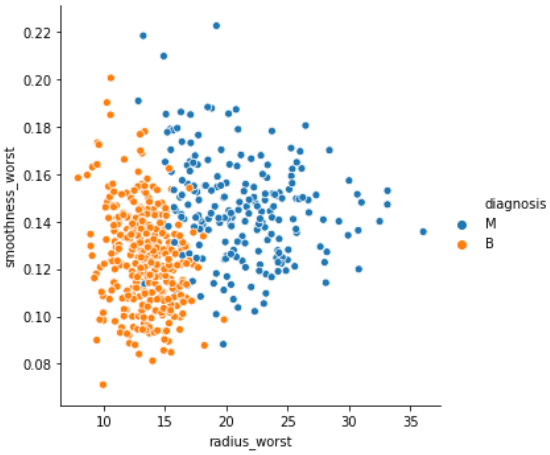


Figure 9: Relational plot of diagnosis for radius_worst vs smoothness_worst

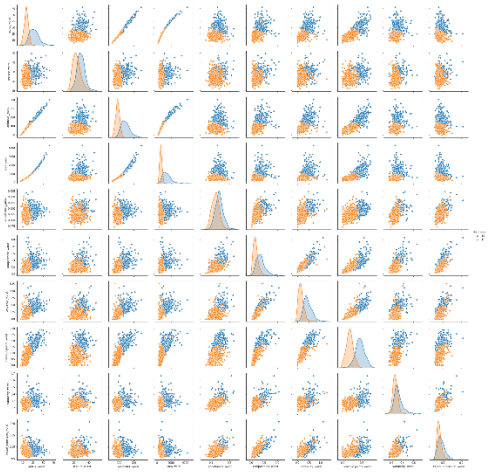


Figure 10: Pair-plot showing relationship between all worst features.

Looking at the pair-plot of all the worst features we notice distinct peaks a distance from each other in the distributions on the diagnonal for radius_worst and concave_points_worst. The relational plot of these 2 features show that they may be used wit a single line discriminator for the malignancy test.

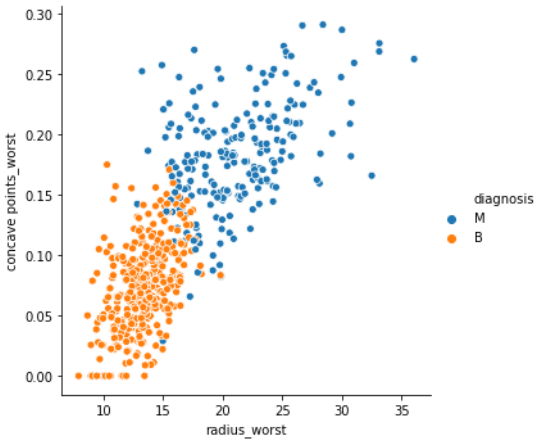


Figure 11: Relational plot of diagnosis for radius_worst vs concave points_worst

Another interesting conclusion drawn from the results is that, for this project, the Deep Neural Network results from the best tuned model repeatedly produced better results compared to the best tuned AdaBoost model. However, the DNN processing time was significantly larger than that required for the AdaBoost model. This could be a consideration where a trade-off between processing time and accuracy needs to be made for the deployed solution.

REFLECTION

This was a very interesting project to work on and I learnt a great deal about breast cancer and the machine learning algorithms we used for classification. Building the process from data exploration to feature selection to building and comparing the models gave me a good view of the process end-to-end. There were several challenges in working with the data and trying to find the best fit models for the solution.

One of the greatest challenges was in deciding on hyper-parameters for the 2 models. For the DNN, I had to research guidelines for selecting the number of hidden layers and the number of nodes per hidden layer. Then selecting the batch size and number of epochs also appears to be rather arbitrary at first and you really need to get a feel for what seems to work well. This appears to be more of an art rather than a science, but I was pleased with the results of the architecture and hyper-parameters I selected.

Feature selection seems to be key in fine-tuning the models to produce the best results. Initially I used the full feature set from the raw files and was not able to get as good results for either the AdaBoost or DNN models. I had a failed attempt in trying to reduce the feature set with the Low Variance Feature Selection method. Using the Pearson's Correlation Matrix was the best approach I found for this project. I believe the final solution using the DNN can be a practical solution for this classification problem.

Building insights into the most important features and how they relate to each other was really interesting for me. For future research, it would be interesting to see if we could get better or worse classification by using only the top 3-5 features or possibly even 2-3 features. Certainly, the radius_worst feature is a dominant feature for determining the malignancy of the breast mass. Having this knowledge alone could be very useful for future diagnoses.

IMPROVEMENT

Based on my analysis, it appears that the feature set can be further reduced. It may be possible to select anywhere from only 2 – 5 features to build a practical model without too much loss of accuracy. We could then

use a clustering algorithm like the k-means algorithm to draw conclusions from how these features are clustered. This is one area that can be further researched.

Also, for the DNN, it is possible to explore more hidden layers and/or a different number of nodes per hidden layer. I was unable to improve the model by including dropout layers, but I feel it can be improved and made more robust by adding dropout layers possibly in combination with adding one or more hidden layers. It's also possible that instead of 2 hidden layers of 16 nodes, perhaps making the second hidden layer 8 nodes could produce better results. All of these options can only be explored through trial and error or using a combination of a DNN and another learning algorithm to optimize its architecture and hyper-parameters. Some of these optimization techniques have already been discussed in other research papers [5][6].

It would also be interesting if other patient features could be added to the feature set. It is possible that there are other bio indicators that can be added to the data set to improve the classification models.

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