1 Introduction

- **Group members:** Enrico Borba, Claire Goeckner-Wald

- **Team name:** Papa Mart's Mini Gary (for 2008), Papa Mart's Giant Gary (for 2012).

- **Division of labour:** **Enrico Borba:** programming, tweaking numbers; **Claire Goeckner-Wald:** model suggestion & research of models, compilation of report.

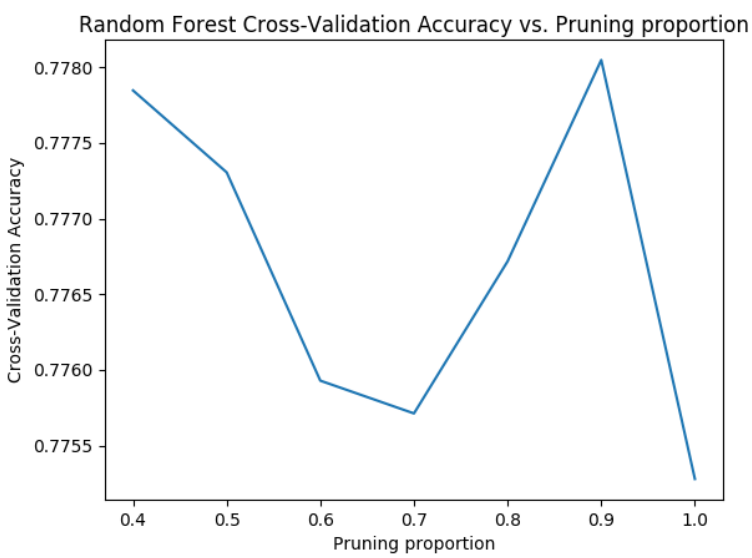
2 Overview

- **Models and techniques tried**
  - **Neural networks:** Attempted one-hot encoding across all features, attempted different optimizers. Determined ineffective at categorical data.
  - **Decision trees:** Attempted different kinds of trees. Extremely random trees, random trees.
  - **Ensembles:** Mostly focused on ensembles of extremely random trees. The most effective of which was 500 trees with a min_samples_split of 11.
    Ensembles of different models were also attempted, specifically, Linear SVM + Neural network + Extremely random tree with little success.
  - **SVMs:** Tried two different kernels, rbf and linear. RBF kernel was deemed unusable from the beginning due to its more than quadratic runtime complexity for training (with respect to the number of data points).
  - **Cross-validation:** Main method for determining the strength of a model.
  - **Removing unecessary columns:** Columns that had more than 95% BLANK responses (-1), were removed entirely from the input data before training and before predicting.
  - **Data normalization:** Normalizing data before training and prediction.
- **Work timeline**
  - **Week 1:** Discussing models, setting up data inputs
  - **Week 2:** Github repo, Cross-validation of models to determine which was best, determining which data columns were unnecessary, researching other models, and final submissions

3 Approach

- **Data processing and manipulation**
  - **Feature Pruning:** When inspecting the input data, we quickly see that there are several BLANK (-1) entries. So, we were willing to try to prune some features, depending on the proportion of BLANK responses in that specific feature.

    Here is a graph representing this behavior, and the extent of pruning.



    The model being trained is a random forest with min_samples_split=4 (a detailed explanation given on page 4). The x-axis is the tolerance of pruning. That is, if x = 0.9, then features for which the proportion of BLANK responses is greater than 0.9 are pruned. The y-axis is the mean validation accuracy in 3-fold cross validation. The data is not shuffled, so the same sets of inputs are used for each model being trained.

  - **Data Normalization:** We determined normalization was not extremely useful in increasing classification accuracy when using decision trees. For an Extremely random forest of 100 trees, we had cross validation accuracy with normalization: 0.757032214087 and without: 0.772078501506.

- **Details of models and techniques**
  - **Neural networks:** Neural networks did not immediately seem useful, as we felt that we would have to one-hot encode every feature, and we believed it would be surpassed by decision trees in classification.

    We wanted to test the strength of a neural network. We generated 100 random neural networks of the form:

Layer (type)	Output Shape	Number of Parameters
Dense	d_1	p_1
Activation	d_1	0
Dropout	d_1	0
Dense	d_2	p_2
$\vdots$	$\vdots$	$\vdots$
Dense	3	p_n

    The number of hidden layers ranged from 10 to 20 and the number of neurons in each layer ranged from 300 to 600. We normalized and one-hot-encoded all features and outputs. The activation layers were randomly selected to all be either tanh, sigmoid, or ReLU. Furthermore, the dropout was one of 0.1, 0.2, . . . , 0.5.

    The strongest neural network had a cross-validation error of 0.737165.

    We quickly noticed that the neural network was merely learning to always output ones. The 2008 training dataset contained 0.745% ones, in the PES1 column. Thus, the best neural network was doing worse than simply outputting ones.

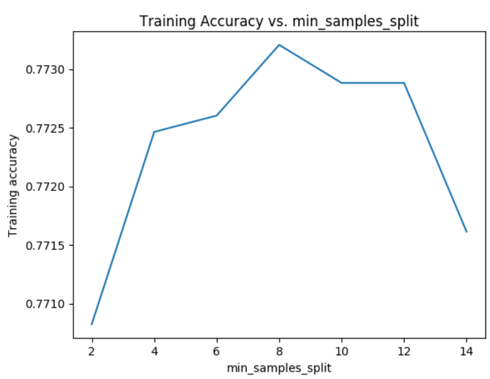
- **Decision Trees/Ensembles:** We had two tree classifiers in mind: RandomForestClassifier and ExtraTreesClassifier. Both were provided by sklearn.Both of these classifiers are ensembles of decision trees.

  ExtraTreesClassifier fits a number of randomized decision trees (a.k.a. extra-trees) on various sub-samples of the dataset and use averaging to improve the predictive accuracy and control over-fitting.

  RandomForestClassifier fits a number of decision tree classifiers on various sub-samples of the dataset and use averaging to improve the predictive accuracy and control over-fitting.

  * **ExtraTreesClassifier:** We first wanted to test the proper regularization parameter for ExtraTreesClassifier. We tested different values for the minimum number of samples required to split an internal node. We had min_samples_split range from 2 to 14, and the y-axis is the cross-validation error of 3 folds.

    We also wanted to test the min_samples_leaf, the minimum number of samples required to be at a leaf node. Again, the Training accuracy is a cross-validation error of 3 folds.

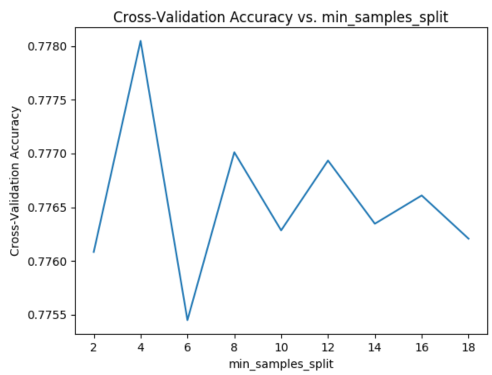
    

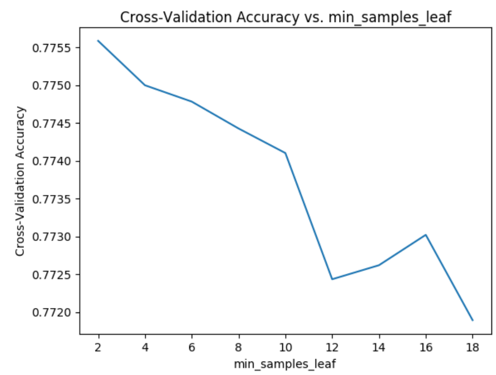
    

    We see the strength of the model is maximized when min_samples_split is 8, and when min_-samples leaf is 3.

    The combination of the two with an 100 tree ensemble yields a cross-validation accuracy of approximately 0.77342, a clear improvement over the neural network. With 500 trees, the cross-validation accuracy increases to 0.77389. A small but still clear improvement.

  * **RandomForestClassifier:** We attempted the same experiment with the RandomForestClassifier, with interesting results.

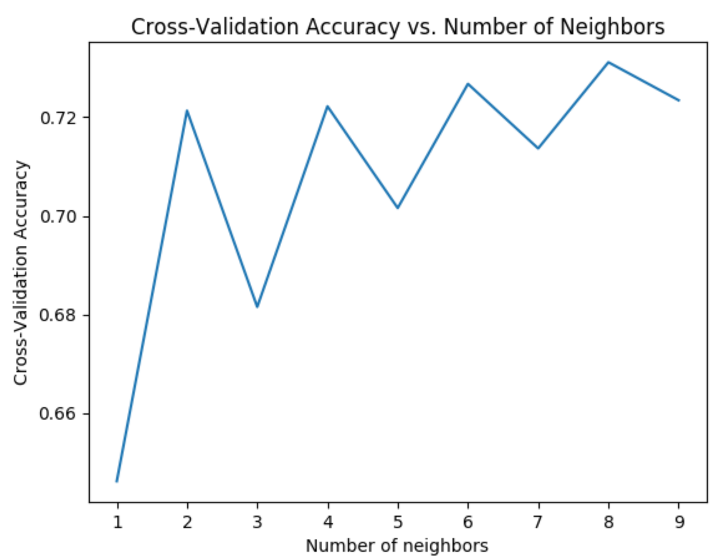




    It seems that regularization should be very small when using the RandomForestClassifier.

    Using min_samples_split = 4 and min_samples_leaf = 2, with 500 trees we achieve a cross validation accuracy of 0.77704, noticeably higher than that of the extremely random tree.

- **K-Nearest Neighbors:** We also shortly investigated KNeighborsClassifier from sklearn, to see if the data had similar points in clusters. This ended up being very much not the case, as we can see in this graph here.



We see that the strongest k-nearest neighbor classifier had a validation accuracy of 0.74449, far from that of the extremely random tree ensemble.

- **SVMs:**
  - **RBF Kernel:** We were interested in training the rbf kernel support vector machine, specifically sklearn's svm.SVC(). However, the computational complexity of training is greater than

    $$O(n_{\text{features}} \times n^4_{\text{observations}})$$

    Therefore, we could not train on more than 10000 points. Because of this, we were already sure that we would not use the rbf kernel svm, since it could not train on the entire dataset, however, we still wished to determine its strength.

    Training on a random 10000 points in the dataset and using the rest as a validation set yielded 0.75350 as the test error. Unfortunately, not much better than the neural network, and definitely worse than the extra random tree classifier.

  - **Linear Kernel:** We also tried a linear kernel. Since it's training computational complexity is linear in the number of observations, it could be evaluated on the entire dataset. The linear kernel has a cross-validation error of 0.52452, implying the data is far from linearly seperable. Fitting the linear kernel was worse than guessing one always. This seems very counter intuitive, as the hyperplane with the least error should be one that is simply entirely outside of the whole dataset.

4 Model Selection

- **Scoring**

  We selected from the models described above. The metrics the models were scored on varied from metric to metric (specifically, the loss functions differed in each model). For Neural Networks, the Nesterov Adam (Adam optimizer with momentum), was the optimizer that fared best. We used categorical_crossentropy as the loss parameter when training the neural networks.

  For the decision trees, (both the extra random and the regular random forests) used Gini index as a metric for impurity.

  The k-nearest neighbors classifier used sklearn's BallTree algorithm for training.

  For the support vector classifiers we attempted both a linear and the radial-basis function kernels, with little success.

  It was clear that the Random Forest was the most promising classifier.

- **Validation and Test**
  Cross validation (3 fold) was used to determine the strength and selection of all models. For the Extremely Random Tree and Random Forest Classifiers, we refined the measurement and used 10 fold validation. We came to the same result that the RandomForest was slightly stronger.

5 Conclusion

- **Discoveries**
  We discovered the intuitive fact that some columns contain worthless information, and will only hinder learning. Removing these columns carefully has a visible positive effect on the strength of the model.

  Neural networks are not extremely powerful classification problems which have discrete inputs, unless each feature is one-hot encoded. Decision trees are much more effective at these kinds of problems.

- **Challenges**
  We had a lot of challenge improving the model moderately after achieving a classification of about 0.778%. We also had difficuly in implementing boosting.

- **Concluding Remarks**
  If given more time, boosting would have been properly implemented with a random forest as the model being boosted. This would have also had a strong positive impact in the strength of the final model.

  The final model chosen was a Random Forest with min_samples_split=4 of 1000 trees.