Report Mini-project: Regression Model

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1 Introduction

The aim was to find the best regression model to predict the perceived pleasantness of an odor.

2 Results

2.1 Exploration

We were given a set of 4780 predictors for 708 observations. To have a better overview of the pleasantness, we plotted a histogram which seems to respect a Gaussian distribution. However, there is an unexpected proportion of people at the low grades-end of the distribution. Afterwards, we deleted the variables with zero variance and plotted a sample of the data to observe the eventual linear dependencies between the predictors.

2.2 Linear models

We started with a simple regression model using the $lm()$ method as a baseline. As expected, the MSE under those conditions was very bad (1.8 mio) and the predictions far exceeded the allowed range (i.e. 0 to 100). We then tried a sub-model selection, but the linear dependencies in the predictors prevented us from setting appropriately the parameters for an optimal research. We quickly turned to Lasso (L1) regression, which happened to be the most appropriate regularization method for the linear model, which gave us a reasonable MSE of 476 when using the best λ found by cross-validation. We experimented further with Lasso to see how the data behaved, but found no better linear model than that one.

2.3 Non-linear models

We observed that linear models did not fit our data well. Therefore, we hoped that non-linear models would show better results. We tried boosting and neural networks.

Boosting was interesting for us because it uses only three hyper-parameters and is applicable to large data sets (we have more than 3000 predictors for about 700 observations), it does not depend on initial condition and selects feature importance.

Neural networks had a chance to weight out the predictors in a more complex manner than linear regression could, and is widely applicable to large data sets.

2.3.1 Tree, boosting

First, we tried to fit a simple tree because the method is easy to implement and to interpret. We obtained a tree with 24 nodes and a mean squared error (MSE) of 560. This method selects automatically some predictors, and it works better than linear regression without selection. This was the baseline. To improve it, we did cross-validation using the $cv.tree()$ function, and selected the size of the tree with the smallest deviation. The size was 2, and we plotted the pruned tree with this previous size. The MSE was better, but by plotting the prediction in comparison with the data, we observed an underfit.

We decided to analyze the data with boosting, which should give more accurate results as long as we avoid under- or overfitting by tuning hyper-parameters properly. At first, we computed different

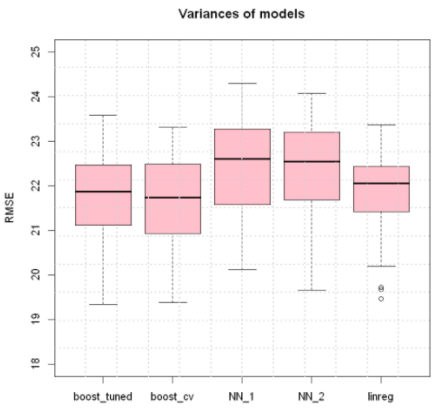
λ from $10^{-3.5}$ to $10^{-0.2}$, and we fixed the number of trees at 1000 and the maximal tree size at 3. With this procedure, we found the best model with an optimal shrinkage $\lambda \approx 0.003162$ and a $MSE \approx 404$. The function $xgb.importance()$ shows the most important predictors: the first one is $Mor24m$ and also appears at first position for the following models, but is not much more significant than the following ones. To evaluate more hyper-parameters, we computed another test, by making a hyper-grid containing different values of λ, maximal size d, and we performed cross-validation using $xgb.cv()$ with up to $5000 nrounds$. This code has unfortunately computational cost and takes a lot of time because it tries several compositions. It returned the best model for each one. The first model was boosting with $d = 1$, $\lambda = 0.1$, and $nrouds = 203$ with the validation $RMSE \approx 21.46$. Finally, we also compared to bagging and random forest with 1000 trees without particular tuning to have a glimpse. The results were in the same range.

2.3.2 Neural Networks

We tried to fit a Neural network to the scaled data (0,1), which improves the weights' convergence. After a few trials, we found that overfitting occurred rather quickly whatever the model, and used from there on validation sets combined with early stopping not to overfit the data. We found two main sources of variability of the model around a unique parameter combination: most of it came from the split between training and test sets, and in a lesser measure from the validation split taken for the early stopping. To tune hyper-parameters, we performed cross-validation over different training/test sets, and a compromise between lower mean MSE and lower variance was made. We tested both 1 and 2 hidden layers, but neither gave a significantly better conformation. We also observed the behavior of the predictions on a same training set, but with different validation splits, which was found to be a potential source of bias for the choice of the model. We went with the following optimal tuning: 2 hidden layers with shape 600 and 100 respectively, *relu* activation, and *linear* activation for the output layer, with reasonable variance and MSE. This model with 2 hidden layers predicts generally more spread responses than linear regression, with better MSE for some splits between training and test sets, but also worse for others. We could not find a way to reduce the variability to such an extent that the model would always be better than linear.

2.4 Variance of models

After tuning all our models to their best performance, we ran them on fifty different splits of the data set and plotted boxplots to compare their variance. As expected, non-linear models are often better, boosting in particular having a significantly lower mean MSE than the neural network. In addition, our Kaggle-submissions ranked in the same order as these observations would predict.



3 Conclusion

Using non-linear models, we could most of the time predict better responses than for linear regression, especially with boosting (ahead of neural network). However, the error drop is not very significant, and we could never get under a solid threshold of $MSE = 400$, with still highly variable results given the splits between training and test sets. In addition, the predictions stay pretty close to the mean, and the values at the extremes, under 15 and above 80, are never predicted within a reasonable range whatever the method and parameters when keeping the MSE low at the same time. We believe that important predictors are missing or that at the very least these predictors are not significant enough, making the predictions gather around the most probable answers of the training set rather than relying on heavy evidence given by the parameters.