

STAT 652: Predicting Flight Delays Project

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1 Introduction

The goal of this project is to predict the response variable, departure delays, for a particular flight given the explanatory variables.

* Please note that you can click on a figure or table number to jump to that figure or table.

2 Data

The dataset consists of information about all the flights leaving from New York City in 2013. The dataset contains 43 variables in total. The dataset is an amalgamation of several datasets, including datasets containing information on weather, the airports, the flights, and the models of airplanes. The training dataset provided to us contains 200,000 observations. Please see table 2 to view a small sample of the data.

3 Methods

We will now outline the various methods used to clean and perform prediction on the data. We will discuss our techniques for data preprocessing and cross validation, and the different models that we tried.

3.1 Data Preprocessing

We performed data preprocessing on the nycflights13 dataset. Our data preprocessing steps included the following:

- Load the data from a csv.
- Set the random seed for reproducibility of results.
- Cast all the columns with the character data type into the factor data type.
- Convert the ‘sched_arr_time’ and ‘sched_dep_time’ columns into the POSIX time format, then take the difference between them to create the ‘sched_air_time’ (scheduled air time) column.
- Drop columns ‘dep_time’, ‘arr_time’, ‘air_time’, and ‘arr_delay’ which contain data from after the flights’ departures which might have leaked information about the response variable ‘dep_delay’.
- Drop column ‘year.x’ because all values were 2013.
- Drop column ‘tailnum’ because it produces too many dummy variable columns for one-hot encoding.
- Drop columns which consist of over 50% NAs, which includes the speed column
- Impute the missing values with the median or mode depending on the datatype of the column and created a flag column which indicates whether or not data was imputed for that variable and row.
- Normalize the data, to work well with methods like lasso regression.
- Exclude data which has a departure delay of more than 30 minutes late, which reduced the dataset from 200,000 rows to approximately 170,000.

3.2 Exploratory Analysis

3.2.1 Plots

We created some plots of ‘dep_delay’ versus the explanatory variables. Some plots such as Figure 3 show that there may be some non-linear relationship between variables like ‘dep_delay’ and ‘sched_dep_time_num_minute’. This suggests that using a model such as GBM that can capture non-linear relationships would be a good idea.

3.2.2 Correlations

First, we created a correlation plot for the numeric variables to see if there any correlations between the variables. We see that there is very little correlation between the response variable dep_delay and any of the other variables. Some of the strongest correlations include the correlation between distance and longitude and time zone and a smaller correlation between distance and latitude. This makes sense as most of the planes are inter US flights from west to east or vice versa, there is not as much distance flown in the north south direction. Please see figure 1 for the correlation plot. The lack of correlations between ‘dep_delay’

and the other variables suggest that a linear model will not work well. We should try a non-linear model or interaction terms.

3.3 Principal Component Analysis (PCA)

Next we performed Principal Component Analysis (PCA) on only the numeric variables as techniques to perform PCA on mixed datasets (numerical and categorical) were not covered in class. When looking at the contribution of each variable to the first principal component, we notice that the variables ‘lon’, ‘distance’, ‘tz’, ‘seats’, ‘alt’, ‘sched_air_time’ have the greatest absolute coefficients for the first principal component. The fact that the aforementioned variables have large coefficients in the first principal component suggests that they are highly correlated with each other. The fact that ‘dep_delay’ has a small coefficient in the first principal component suggests that ‘dep_delay’ is not highly correlated with any of the above variables.

As expected, it turns out that variables like ‘lon’, ‘distance’ and ‘tz’ are not important for predicting ‘dep_delay’ according to the GBM model. This maybe be because although variables like ‘lon’, ‘distance’ and ‘tz’ help explain most of the variance in the dataset, they have a weak relationship with ‘dep_delay’.

Please see table 3 for the proportion of variance explained by each principal component. Please see table 4 for the variable coefficients for each principal component ordered by the magnitude of the variable coefficient for the first principal component.

3.4 Validation

Initially, we used the most basic validation technique where we have a training dataset and a validation dataset. We reserved 2/3 of the original dataset’s observations for the training dataset and 1/3 of the observations for the validation dataset. There is additional data which was provided at a later date which we use as the holdout test set. 2/3 of the data gives enough data for the models to train on while 1/3 is enough data to get an accurate assessment of the error. After the data preprocessing steps, which included removing all rows where ‘dep_delay’ was greater than 30 minutes, we were left with 170,645 observations. Of these 170,645 observations, 113,763 were used as the training dataset and 56,882 were used as the validation set. The training dataset and the validation dataset do not have any common observations. k-folds cross validation was not used in order to save on compute time as GBM was already time intensive to train. k-folds cross validation would increase training time for the models by a factor of k. However, k-folds cross validation would lead to a lower variance estimate of holdout test set error.

3.5 Models

We first explored some basic models to establish baseline performance against which we compare our most sophisticated model, the Generalized Boosted Regression Model (GBM).

3.5.1 Basic Models

‘dep_delay’ is the number of minutes that the plane departs late. Negative numbers indicate early departures. First, to establish baseline performance, we used a basic model of simply predicting the ‘dep_delay’ to always be 0. This model had a root mean squared error (RMSE) of 8.30571. The model in which we always predict the mean had an RMSE of 8.29977.

3.5.2 Linear Regression

A linear regression model assumes a linear relationship between the explanatory variables and the response variable. Linear regression minimizes a squared loss function to obtain the coefficients of this linear relationship.

Table 1: benchmark on the validation set comparing all the models that we tried

model_description	rmse
predicting 0	8.30571
predicting the mean	8.29977
predicting the median	8.46926
linear regression	7.98999
GBM (tuned)	7.89071

Our linear regression model was better than predicting the mean, with an RMSE of 7.98999. This suggests that there is some linear relationship between the ‘dep_delay’ and the explanatory variables.

3.5.3 Generalized Boosted Regression Model (GBM)

3.5.3.1 Explanation of Model

GBMS work as follows: we iteratively build an ensemble of simple models starting with a baseline model, such as predicting the mean. Then at each iteration, we train a new base classifier (i.e. regressor tree) on the residuals multiplied by the shrinkage hyperparameter. Then this base classifier is added to the ensemble. A lower shrinkage effectively means a lower learning rate and therefore you need more iterations to reduce the train set residuals by the same amount. The benefit of a smaller shrinkage (with sufficient trees) is that you end up with a larger ensemble of trees that can reach a lower cross validation loss. This iterative prediction process is called boosting. In our case, our base classifiers are regressor trees. Each tree decides on its splitting criterion greedily by picking the split which results in the lowest mean squared error or some other splitting heuristic. We continue for n number of trees where n is specified by the user. Each iteration produces one tree, so the number of iterations is equal to the number of trees.

3.5.3.2 Tuning

The GBM with our best tuned hyperparameters had the lowest RMSE of 7.89071 on the validation set after it was tuned to have a shrinkage of 0.01 and 8,192 trees. Shrinkage is similar to a learning rate. 8,192 is the number of trees used in the model. According to the vignette provided by the ‘GBM’ package, the RMSE can always be improved by decreasing shrinkage, but this provides diminishing returns. A good strategy would be to pick a small shrinkage that balances performance and compute time. Then with this fixed shrinkage value, increase the number of trees until you get diminishing returns. We decided to follow the aforementioned strategy. See figure 2 for a summary of our tuning experiments.

4 Results

In regression and GBM, we found different features to be important.

Please see table 1 below for all the models and their root mean squared errors (RMSE) on the validation set.

4.1 GBM

4.1.1 Influence

For a GBM, the improvement in the splitting criterion (which is mean squared error for regression) for a given variable is calculated at each step. The relative influence for a given variable is the average of these

improvements over all the trees. (“Gradient Boosting Machines · UC Business Analytics R Programming Guide” 2019) Table 7.9 shows the relative influence of each variable in the GBM.

4.1.2 Dest

Based on my best GBM model with a shrinkage of 0.01 and 8192 trees, ‘dest’ was the most important feature, with 30.23130 relative influence. ‘dest’ refers to which airport a given plane was flying to. Other high relative influence explanatory variables include ‘model’ and ‘sched_dep_time_num_minute’.

4.1.3 Final Holdout Test Set Performance

When we tested our final GBM model on the final holdout test set, we achieved an RMSE of 7.88805. The improvement in performance over testing on the validation set could be because our final GBM model was trained on a larger dataset (both the training set and the validation set), and then tested on the holdout test set.

4.2 Linear Regression

The one-hot encoded versions of the variable ‘carrier’ were some of the most important features for regression. On the other hand, ‘dest’ does appear as an important feature in linear regression as well but it is not the most important feature. If we could somehow sum up all the contributions from each of the one-hot-encoded variables derived from ‘dest’, then it might appear as the most important feature for linear regression as well. We use ANOVA to measure the statistical significance of ‘dest’. Performing ANOVA to compare linear regression models with and without ‘dest’ yielded a low p-value of 0.0001863, meaning that keeping at least one of the one-hot-encoded variables derived from ‘dest’ is beneficial with high statistical significance for the linear regression model.

4.3 Comparison

‘dest’ appeared to be a more important feature in GBM than in linear regression, which may be because the GBM can capture interaction effects between ‘dest’ and other variables, whereas our simple linear regression model cannot.

5 Discussion

5.1 Data Preprocessing

We considered removing outliers in terms of ‘dep_delay’ in train but not in validation, then use k-folds cross validation on test to determine how many outliers we should remove to boost performance on the validation set. We considered removing highly influential points in order to train a better model. In this case, we consider highly influential points to be points with high Cook’s distances. However, this was infeasible as we did not have enough computational resources available and it took too long. We compromised by excluding data which has a departure delay of more than 30 minutes late as a proxy for excluding outliers, which reduced the dataset from 200,000 rows to approximately 170,000. This is because we consider extreme delays of over 30 minutes late to be freak accidents which cannot be accurately predicted by the available explanatory variables. If we keep outliers, we would be learning relationships between the response variable and the explanatory variables for a particular outlier observation which do not generalize well to other observations. However, when we are removing 30,000 points, we are probably removing many points that would help the model generalize to new data if kept. The threshold of 30 minutes was probably too low, and we may have

benefited from picking a higher threshold. We could have tuned the threshold by using validation sets that do not have points removed according to the threshold.

We drop columns which consist of over 50% NAs, which includes the speed column. However, it should be noted that a rule of thumb suggested by Professor McNeney is to drop any columns with over 5% NAs. We use a different threshold for dropping columns leading to us keeping columns such as model instead of dropping it.

We impute the missing values. However, there are limitations to this approach of imputing the missing values. It is possible, that the missingness of the plane model variable is related to ‘dep_delay’. In this scenario, we may be creating an inferior feature set by keeping the variable ‘model’ and imputing it. For example, say a highly unreliable plane model that frequently causes long delays has a high probability of being labeled as NA and represents the majority of NAs in the dataset. We would not be able to capture the relationship between this plane ‘model’ and ‘dep_delay’ if we imputed the model with the mode. To counteract this affect, we imputed NAs for the remaining columns using the ‘imputeMissings’ library, adding a boolean flag which indicates 0 if the associated value was present and 1 if the associated value was NA. For example, the ‘model_flag’ for a given row is 1 if the ‘model’ value was NA for that given row. Hence, no information is lost from our imputation.

6 Conclusion

None of the models that we tried performed particularly well. We believe that this is intrinsically a difficult problem. If departure delays were easy to predict, the flight schedules would be designed to prevent them and therefore there would be no departure delays. This difficulty may be compounded by poor explanatory variables having weak relationships with the ‘dep_delay’. Specifically, information about the condition of a particular flight before it reaches New York City is missing. Instead, we get information about where the flight is going next, which would reveal less information about the current condition of the plane and what kind of maintenance it would need, and therefore what ‘dep_delay’ it would have. Out of all the models, that we tried, gradient boosted regression models yielded the best performance based on having the lowest root mean squared error on the validation set. We believe that this makes sense because GBMs are able to capture non-linear relationships between the explanatory variables and ‘dep_delay’ whereas our simple linear regression model could not.

7 Code

The R version used was R version 3.6.1 (2019-07-05). The following packages were used: tidyverse nycflights13 Hmisc lubridate imputeMissings dplyr gbm

Time to Run: Takes 2+ hours to knit the code, mostly because GBM takes a long time to train.

7.1 Preparing the programming environment

7.1.1 Loading Libraries

```
library(tidyverse)
```

7.2 Data Preprocessing

7.2.1 Loading the data

```
library(nycflights13)
library(Hmisc)

## Loading required package: lattice
## Loading required package: survival
## Loading required package: Formula
##
## Attaching package: 'Hmisc'
## The following objects are masked from 'package:dplyr':
##   src, summarize
## The following objects are masked from 'package:base':
##   format.pval, units
set.seed(42)
original_data <- read_csv("fltrain.csv.gz")

## Parsed with column specification:
## cols(
##   .default = col_double(),
##   carrier = col_character(),
##   tailnum = col_character(),
##   origin = col_character(),
##   dest = col_character(),
##   time_hour = col_datetime(format = ""),
##   name = col_character(),
##   dst = col_character(),
##   tzone = col_character(),
##   type = col_character(),
##   manufacturer = col_character(),
##   model = col_character(),
##   engine = col_character()
## )
## See spec(...) for full column specifications.
DF <- original_data
```

7.2.2 turning all columns with datatype characters to factors.

```
DF[sapply(DF, is.character)] <- lapply(DF[sapply(DF, is.character)],
                                         as.factor)
DF$flight <- as.factor(DF$flight)
```

Table 2: A table of the first few rows of the nycflights13 data.

year.x	month	day	dep_time	sched_dep_time	dep_delay	arr_time	sched_arr_time	arr_delay	carrier	f
2013	11	7	600	600	0	826	825	-1	WN	
2013	10	30	1252	1250	2	1356	1400	-4	AA	
2013	12	18	1723	1715	8	2008	2020	-12	DL	
2013	11	20	2029	2030	-1	2141	2205	-24	WN	
2013	10	21	1620	1625	-5	1818	1831	-13	DL	
2013	11	7	852	900	-8	1139	1157	-18	B6	

7.2.3 parsing times from strings and calculating scheduled air time

```

library(lubridate)

##
## Attaching package: 'lubridate'

## The following object is masked from 'package:base':
##
##     date

DF$sched_arr_time_posix <- as.POSIXct(str_pad(as.character(DF$sched_arr_time), 4, pad="0"),format="%H%M")
DF$sched_arr_time_hour <- hour(DF$sched_arr_time_posix)
DF$sched_arr_time_minute <- minute(DF$sched_arr_time_posix)

#num minute is number of minutes since start of day for scheduled arrival time
DF$sched_arr_time_num_minute <- 60*DF$sched_arr_time_hour + DF$sched_arr_time_minute

DF$sched_dep_time_posix <- as.POSIXct(str_pad(as.character(DF$sched_dep_time), 4 , pad="0"),format="%H%M")
DF$sched_dep_time_hour <- hour(DF$sched_dep_time_posix)
DF$sched_dep_time_minute <- minute(DF$sched_dep_time_posix)
#num minute is number of minutes since start of day for scheduled depival time
DF$sched_dep_time_num_minute <- 60*DF$sched_dep_time_hour + DF$sched_dep_time_minute

select(original_data, time_hour, sched_dep_time, sched_arr_time, tz, tzone)
select(DF, sched_arr_time, sched_arr_time_hour)

DF$sched_air_time <- DF$sched_arr_time_posix - DF$sched_dep_time_posix
drops <- c('sched_arr_time_posix', 'sched_arr_time_hour', 'sched_dep_time_posix', 'sched_dep_time_hour')
DF <- DF[ , !(names(DF) %in% drops)]

drops <- c("dep_time", "arr_time", "air_time", "arr_delay", "year.x", 'tailnum')
DF <- DF[ , !(names(DF) %in% drops)]

## Remove columns with more than 50% NA
DF <- DF[, -which(colMeans(is.na(DF)) > 0.5)] 

DF$sched_air_time <- as.numeric(DF$sched_air_time)

```

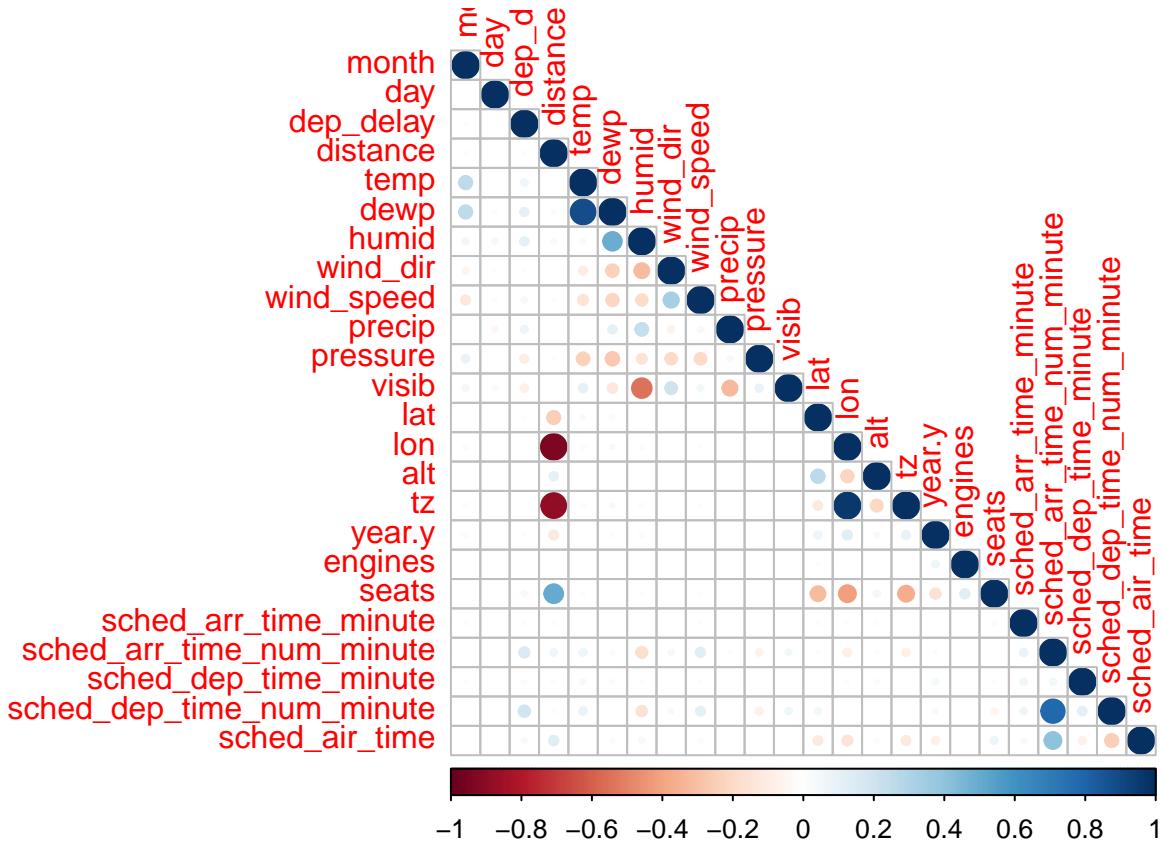


Figure 1: grid depicting correlation amongst all numerical variables

7.2.4 Imputing Variables

```

library(imputeMissings)

##
## Attaching package: 'imputeMissings'

## The following object is masked from 'package:Hmisc':
##
##     impute

## The following object is masked from 'package:dplyr':
##
##     compute

impute_model <- imputeMissings::compute(DF, method="median/mode")
DF <- impute(DF, object=impute_model, flag=TRUE)
DF <- DF[!duplicated(as.list(DF))] #remove all redundant flag columns that are identical to each other

numeric_only_df <- dplyr::select_if(DF, is.numeric)
library(corrplot)

## corrplot 0.84 loaded

```

Table 3: proportion of variance explained by each principal component

	x
PC1	0.135269
PC2	0.106195
PC3	0.086279
PC4	0.068886
PC5	0.060590
PC6	0.058295

7.3 Feature Scaling

```
dep_delay_vec <- DF$dep_delay
DF$dep_delay <- NULL
head(DF)

library(dplyr)
DF <- DF %>% mutate_if(is.numeric, scale)
head(DF)
DF$dep_delay <- dep_delay_vec
```

7.4 Exploratory Data Analysis

```
numeric_DF <- dplyr::select_if(DF, is.numeric) %>% scale()

prcomp_res <- prcomp(numeric_DF)
sdev <- prcomp_res$sdev
sdev
```

7.4.1 all four components at same time

proportion of variance explained by each component

```
pve <- colSums(prcomp_res$x^2)/sum(numeric_DF^2)

rotation <- as.data.frame(prcomp_res$rotation)
rotation[order(-abs(rotation$PC1)),]

pca_rotation <- head(rotation[order(-abs(rotation$PC1)),])
```

7.4.2 take out extreme departure delays

```
DF<-DF[DF$dep_delay < 30,]

set.seed(42)
DF$flight <- NULL
train_index <- sample(1:nrow(DF), size=2*nrow(DF)/3, replace=FALSE)
train_df <- DF[train_index,]
test_df <- DF[-train_index,]
```

Table 4: coefficients for each variable on each principal component

	PC1	PC2	PC3	PC4	PC5	PC6	PC7	PC8	P
lon	0.534262	0.008228	-0.011813	-0.007181	-0.141255	0.021195	0.014172	-0.023885	-0.0224
distance	-0.530322	-0.013673	0.042091	0.000606	-0.042942	-0.005943	-0.122736	0.043705	0.0200
tz	0.515232	0.003918	-0.003819	-0.009390	-0.207494	0.030490	0.001420	-0.017610	-0.0442
seats	-0.326797	-0.021807	0.092398	0.007581	-0.299155	-0.009582	-0.206563	-0.144397	0.0156
alt	-0.129118	0.001274	-0.022431	0.017906	0.466078	-0.062307	0.241778	-0.082761	-0.1384
sched_air_time	-0.126932	-0.059262	-0.046756	-0.053512	-0.299113	0.151635	0.696202	-0.179246	-0.1491

save entire dataset for later

```
train_and_validation_df <- DF
```

7.5 predicting 0

```
benchmark_df <- data.frame(model_description = character(), rmse = numeric(), stringsAsFactors = FALSE)
rmse = mean((test_df$dep_delay-0)^2) %>% sqrt()
model_description = "predicting 0"
benchmark_df <- rbind(benchmark_df, data.frame(model_description = model_description, rmse=rmse))
```

7.6 predicting the mean

```
rmse = mean((test_df$dep_delay-mean(train_df$dep_delay))^2)%>% sqrt()
rmse
model_description <- 'predicting the mean'
benchmark_df <- rbind(benchmark_df, data.frame(model_description = model_description, rmse=rmse))
benchmark_df
```

7.7 predicting the median

```
rmse = mean((test_df$dep_delay-median(train_df$dep_delay))^2)%>% sqrt()
rmse
model_description <- 'predicting the median'
benchmark_df <- rbind(benchmark_df, data.frame(model_description = model_description, rmse=rmse))
```

7.8 linear regression with dest

```
model <- lm(dep_delay ~ ., data=train_df)
model_without_dest <- lm(dep_delay ~ .-dest, data=train_df)
anova(model, model_without_dest)
summary <- round(summary(model)$coefficients,6)
sorteddf <- summary[order(summary[, ncol(summary)]),]
head(sorteddf)
```

```

lm_test_df <- test_df

in_test_but_not_train <- setdiff(unique(lm_test_df$model), unique(train_df$model))
lm_test_df <- lm_test_df[ !lm_test_df$model %in% in_test_but_not_train, ]

in_test_but_not_train <- setdiff(unique(lm_test_df$dest), unique(train_df$dest))
lm_test_df <- lm_test_df[ !lm_test_df$dest %in% in_test_but_not_train, ]

preds = predict(model, newdata=lm_test_df)

## Warning in predict.lm(model, newdata = lm_test_df): prediction from a rank-
## deficient fit may be misleading
rmse = sqrt(mean((lm_test_df$dep_delay - preds)^2))
rmse
model_description <- 'linear regression'
benchmark_df <- rbind(benchmark_df, data.frame(model_description = model_description, rmse=rmse))

```

7.9 GBM

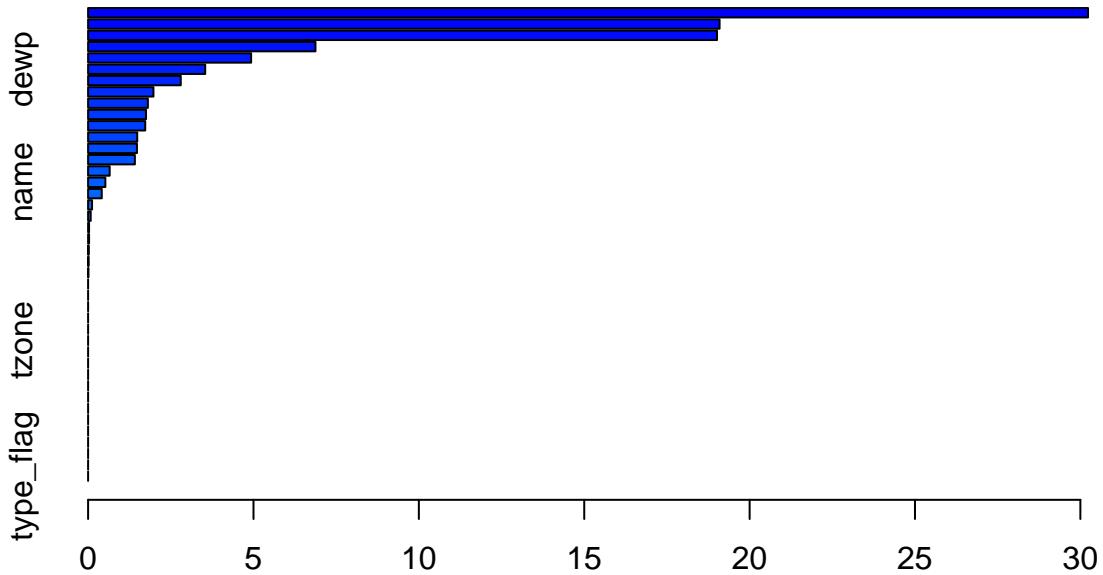
```

library(gbm)

## Loaded gbm 2.1.5
train_gbm <- function(filename){
  num_trees <- 2^13
  set.seed(42)
  model <- gbm(dep_delay ~ ., data=train_df,
                n.trees=num_trees, shrinkage=0.01) # default shrinkage = 0.1
  preds = predict(model, newdata=test_df, n.trees=num_trees)
  rmse = sqrt(mean((test_df$dep_delay - preds)^2))
  summary(model)
  saveRDS(model, filename)
  return(model)
}

destfile <- "models2/gbm_shrinkage_0point01_ntrees_8192_v2.rds"
if (!file.exists(destfile)) {
  train_gbm(destfile)
}
model <- readRDS(destfile)

```



Relative influence

```
\begin{table}
\caption{GBM relative influence; dest is the destination airport code. sched_dep_time_num_minute is the number of minutes since the beginning of a given day for that flight. model is the plane model.}
```

	var	rel.inf
dest	dest	30.23130
model	model	19.09165
sched_dep_time_num_minute	sched_dep_time_num_minute	19.01377
month	month	6.87392
carrier	carrier	4.92863
dewp	dewp	3.54021

\end{table}

Chunk below takes 2+ hours to run on an average laptop.

```
library(gbm)
train_gbm_rmse_vs_num_trees <- function(shrinkage, rerun, num_trees_2_exp=16) {
  #rerun <- TRUE
  set.seed(42)
  x <- 2 ^ seq(5, num_trees_2_exp, by = 1)
  rmse_vec <- numeric(length(x))
  count <- 1
  filename_vec1 <- c("models2/gbm_shrinkage_")
  filename_vec1 <-
    append(filename_vec1, gsub('\\.', 'point', toString(shrinkage)))
  filename_vec1 <- append(filename_vec1, "_ntrees_")
  filename_prefix1 <- paste(filename_vec1, collapse = '')

  for (val in x) {
    filename_vec2 <- append(filename_prefix1, val)
    filename_vec2 <- append(filename_vec2, "_v2.rds")
    filename <- paste(filename_vec2, collapse = '')
```

```

if (!file.exists(filename) | rerun) {
  hboost <- gbm(
    dep_delay ~ .,
    data = train_df,
    n.trees = val,
    shrinkage = shrinkage
  ) # default shrinkage = 0.1
  saveRDS(hboost, filename)
  hboost <- readRDS(filename)
} else {
  print("reading saved model")
  hboost <- readRDS(filename)
}

preds = predict(hboost, n.trees = val, newdata = test_df)
mse = mean((test_df$dep_delay - preds) ^ 2)
rmse <- sqrt(mse)
rmse_vec[count] <- rmse
print(val)
print(rmse)
count = count + 1
}

filename_vec1 <- c("performance2/gbm_shrinkage_")
filename_vec1 <-
  append(filename_vec1, gsub('\\.', 'point', toString(shrinkage)))
#filename_vec1 <- append(filename_vec1, "_ntrees_")
#filename_prefix1 <- paste(filename_vec1, collapse = '')
#filename_vec2 <- append(filename_prefix1, x[length(x)])

#summary filename
filename_vec_summary <- append(filename_vec1, "_v2_summary.csv")
filename_summary <- paste(filename_vec_summary, collapse = '')

#rmse_vs_num_trees filename
filename_vec_rmse_vs_num_trees <- append(filename_vec1, "_v2_rmse_vs_num_trees.csv")
filename_rmse_vs_num_trees <- paste(filename_vec_rmse_vs_num_trees, collapse = '')

summary <- summary(hboost)
write.csv(summary, filename_summary)

num_trees_vs_rmse <-
  data.frame("num_trees" = x, "rmse" = rmse_vec)
write.csv(
  num_trees_vs_rmse, filename_rmse_vs_num_trees
)
}

train_gbm_rmse_vs_num_trees(shrinkage = 0.01, rerun = FALSE, num_trees_2_exp=17)
train_gbm_rmse_vs_num_trees(shrinkage = 0.001, rerun = FALSE, num_trees_2_exp=17)

shrinkage_Opoint01_bench <- read.csv('performance2/gbm_shrinkage_Opoint01_v2_rmse_vs_num_trees.csv')
shrinkage_Opoint01_bench$x <- NULL
shrinkage_Opoint01_bench <- shrinkage_Opoint01_bench %>%

```

GBM: RMSE vs. Number of Trees for Different Shrinkage

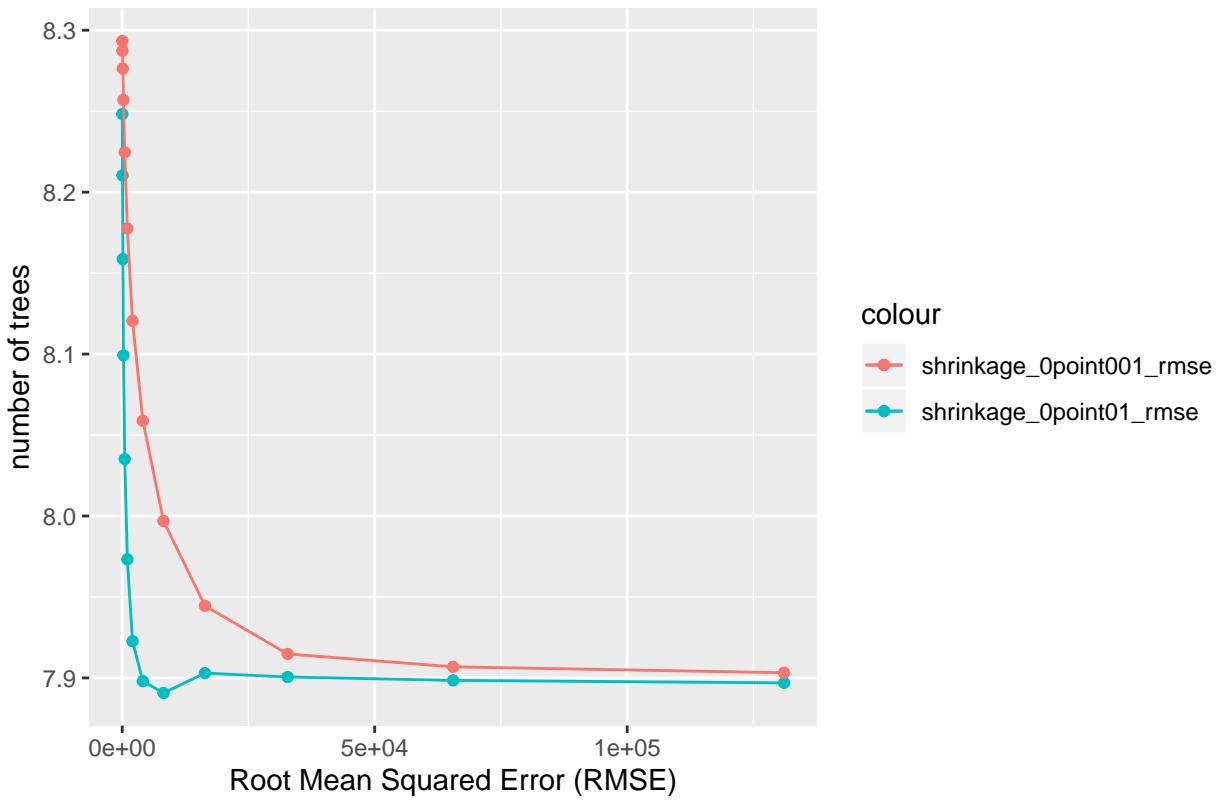


Figure 2: plot of RMSE vs number of trees for shrinkage = 0.01 and shrinkage = 0.001

```
dplyr::rename(
  "shrinkage_0point01_rmse" = rmse
)
shrinkage_0point01_bench

shrinkage_0point01_bench <- read.csv('performance2/gbm_shrinkage_0point001_v2_rmse_vs_num_trees.csv')
shrinkage_0point01_bench$X <- NULL
shrinkage_0point01_bench <- shrinkage_0point01_bench %>%
  dplyr::rename(
    "shrinkage_0point001_rmse" = rmse
  )
shrinkage_0point01_bench

gbm_merge_df <- merge(shrinkage_0point01_bench, shrinkage_0point01_bench, all.x = TRUE)
gbm_merge_df

benchmark_df <- rbind(benchmark_df, data.frame(model_description = 'GBM (tuned)', rmse=7.89071))
write_csv(benchmark_df, 'performance/benchmark_df.csv')
```

Final training on entire dataset to prepare for test set.

```
library(gbm)
num_trees <- 2^13
train_final_gbm <- function(filename, num_trees){
  set.seed(42)
```

Table 5: RMSE on the validation set, benchmark comparing all the models that we tried

model_description	rmse
predicting 0	8.30571
predicting the mean	8.29977
predicting the median	8.46926
linear regression	7.98999
GBM (tuned)	7.89071

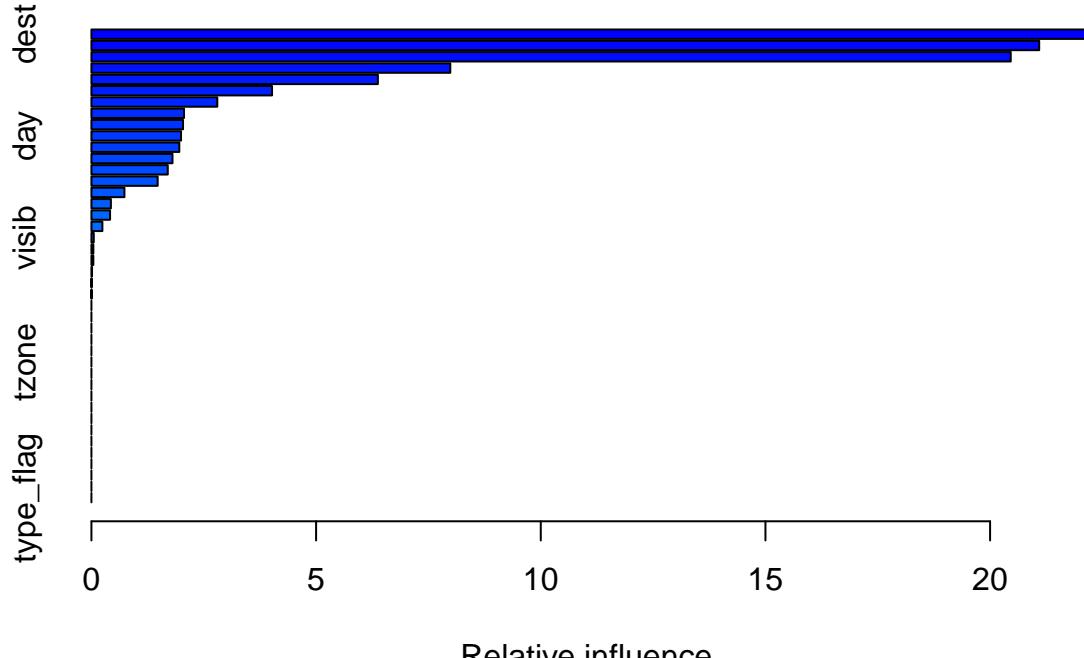
```

model <- gbm(dep_delay ~ ., data=train_and_validation_df,
               n.trees=num_trees, shrinkage=0.01) # default shrinkage = 0.1
saveRDS(model, filename)
return(model)
}

destfile <- "models_ultimate/final_train_on_train_and_validation_gbm_v1.rds"
if (!file.exists(destfile)) {
  train_final_gbm(destfile)
}

final_model <- readRDS(destfile)
final_preds = predict(final_model, newdata=train_and_validation_df, n.trees=num_trees)
final_rmse = sqrt(mean((train_and_validation_df$dep_delay - final_preds)^2))
summary(final_model)

```



```

rmse
## [1] 7.98999

```

8 test on final test data

```
library(tidyverse)
library(nycflights13)
library(Hmisc)
library(lubridate)
library(imputeMissing)
library(dplyr)

preprocess_data <- function(filepath) {
  set.seed(42)
  original_data <- read_csv(filepath)
  DF <- original_data
  DF[sapply(DF, is.character)] <-
    lapply(DF[sapply(DF, is.character)], as.factor)
  DF$flight <- as.factor(DF$flight)
  DF$sched_arr_time_posix <-
    as.POSIXct(str_pad(as.character(DF$sched_arr_time), 4, pad = "0"), format =
      "%H%M")
  DF$sched_arr_time_hour <- hour(DF$sched_arr_time_posix)
  DF$sched_arr_time_minute <- minute(DF$sched_arr_time_posix)

  #num minute is number of minutes since start of day for scheduled arrival time
  DF$sched_arr_time_num_minute <-
    60 * DF$sched_arr_time_hour + DF$sched_arr_time_minute
  DF$sched_dep_time_posix <-
    as.POSIXct(str_pad(as.character(DF$sched_dep_time), 4 , pad = "0"), format =
      "%H%M")
  DF$sched_dep_time_hour <- hour(DF$sched_dep_time_posix)
  DF$sched_dep_time_minute <- minute(DF$sched_dep_time_posix)

  #num minute is number of minutes since start of day for scheduled depival time
  DF$sched_dep_time_num_minute <-
    60 * DF$sched_dep_time_hour + DF$sched_dep_time_minute
  DF$sched_air_time <-
    DF$sched_arr_time_posix - DF$sched_dep_time_posix
  drops <-
  c(
    'sched_arr_time_posix',
    'sched_arr_time_hour',
    'sched_dep_time_posix',
    'sched_dep_time_hour',
    'sched_dep_time',
    'sched_arr_time',
    'hour',
    'time',
    'minute',
    'time_hour',
    "dep_time",
    "arr_time",
    "air_time",
```

```

    "arr_delay",
    "year.x",
    'tailnum'
)
DF <- DF[, !(names(DF) %in% drops)]

## Remove columns with more than 50% NA
DF <- DF[, -which(colMeans(is.na(DF)) > 0.5)]

DF$sched_air_time <- as.numeric(DF$sched_air_time)

# impute
impute_model <- imputeMissings::compute(DF, method = "median/mode")
DF <- impute(DF, object = impute_model, flag = TRUE)
DF <-
  DF[!duplicated(as.list(DF))] #remove all redundant flag columns that are identical to each other.

# scale all but dep_delay
dep_delay_vec <- DF$dep_delay
DF$dep_delay <- NULL
DF <- DF %>% mutate_if(is.numeric, scale)
DF$dep_delay <- dep_delay_vec

# exclude dep_delay >= 30
DF <- DF[DF$dep_delay < 30,]
DF$flight <- NULL

return(DF)
}

final_test_df <- preprocess_data('fltest.csv.gz')

## Parsed with column specification:
## cols(
##   .default = col_double(),
##   carrier = col_character(),
##   tailnum = col_character(),
##   origin = col_character(),
##   dest = col_character(),
##   time_hour = col_datetime(format = ""),
##   name = col_character(),
##   dst = col_character(),
##   tzone = col_character(),
##   type = col_character(),
##   manufacturer = col_character(),
##   model = col_character(),
##   engine = col_character()
## )

## See spec(...) for full column specifications.
num_trees <- 2^13
set.seed(42)

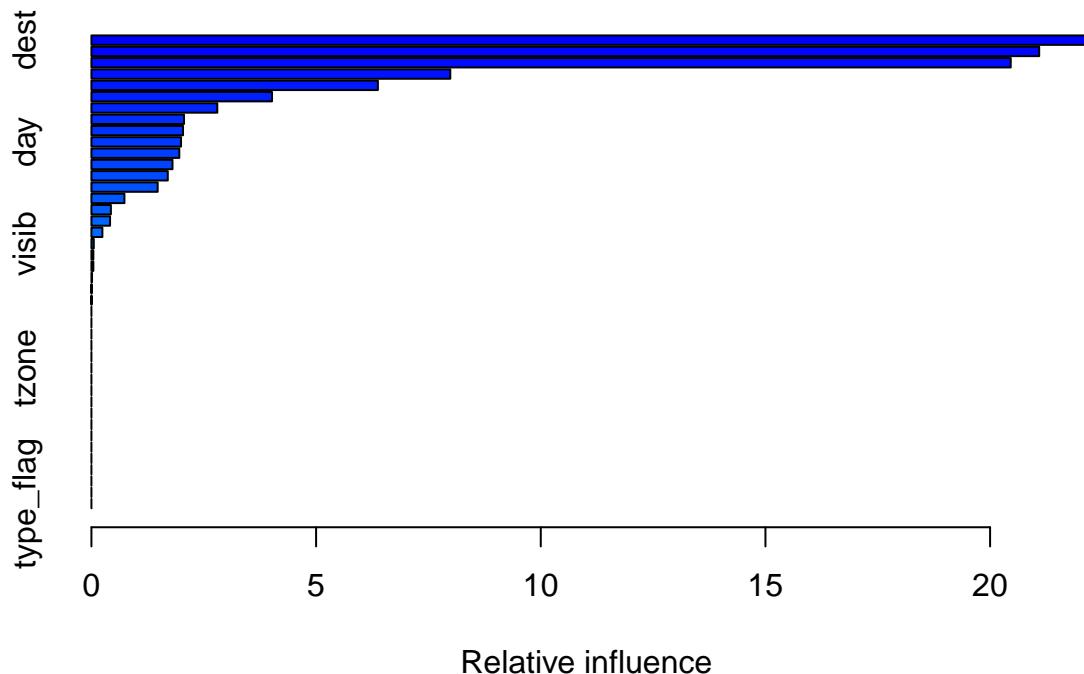
```

```

destfile <- "models_ultimate/final_train_on_train_and_validation_gbm_v1.rds"
if (!file.exists(destfile)) {
  train_final_gbm(destfile)
}

final_model <- readRDS(destfile)
final_preds = predict(final_model, newdata=final_test_df, n.trees=num_trees)
final_rmse = sqrt(mean((final_test_df$dep_delay - final_preds)^2))
summary(final_model)

```



```

##                                     var      rel.inf
## dest                               dest 22.25381765
## sched_dep_time_num_minute sched_dep_time_num_minute 21.09228564
## model                             model 20.45894347
## month                            month  7.98661863
## carrier                           carrier 6.37527061
## dewp                                dewp  4.01976517
## origin                             origin 2.80117601
## precip                            precip 2.06055864
## pressure                           pressure 2.03864363
## day                                 day  1.99401600
## sched_arr_time_num_minute sched_arr_time_num_minute 1.95561859
## dep_delay_flag                   dep_delay_flag 1.80418829
## humid                                humid 1.69910915
## temp                                 temp  1.47431690
## wind_speed                          wind_speed 0.73476017
## sched_dep_time_minute sched_dep_time_minute 0.43305222
## name                                name  0.41477025
## pressure_flag                      pressure_flag 0.24412420
## visib                                visib 0.05216855
## sched_arr_time_minute sched_arr_time_minute 0.04287644
## wind_dir                            wind_dir 0.04284273

```

```

## manufacturer          manufacturer  0.01357422
## sched_air_time        sched_air_time 0.00389522
## distance              distance    0.00360764
## lat                   lat         0.00000000
## lon                   lon         0.00000000
## alt                   alt         0.00000000
## tz                    tz          0.00000000
## dst                   dst         0.00000000
## tzone                 tzone      0.00000000
## year.y                year.y     0.00000000
## type                  type      0.00000000
## engines               engines   0.00000000
## seats                 seats     0.00000000
## engine                engine   0.00000000
## temp_flag              temp_flag  0.00000000
## wind_dir_flag          wind_dir_flag 0.00000000
## wind_speed_flag        wind_speed_flag 0.00000000
## precip_flag            precip_flag 0.00000000
## name_flag              name_flag  0.00000000
## year.y_flag            year.y_flag 0.00000000
## type_flag              type_flag  0.00000000

print(final_rmse)

## [1] 7.88805

## `geom_smooth()` using method = 'gam' and formula 'y ~ s(x, bs = "cs")'
## Warning: Removed 19882 rows containing non-finite values (stat_smooth).
## Warning: Removed 19882 rows containing missing values (geom_point).

print("done")

## [1] "done"

```

References

“Gradient Boosting Machines · UC Business Analytics R Programming Guide.” 2019.
http://uc-r.github.io/gbm_regression#h2o.

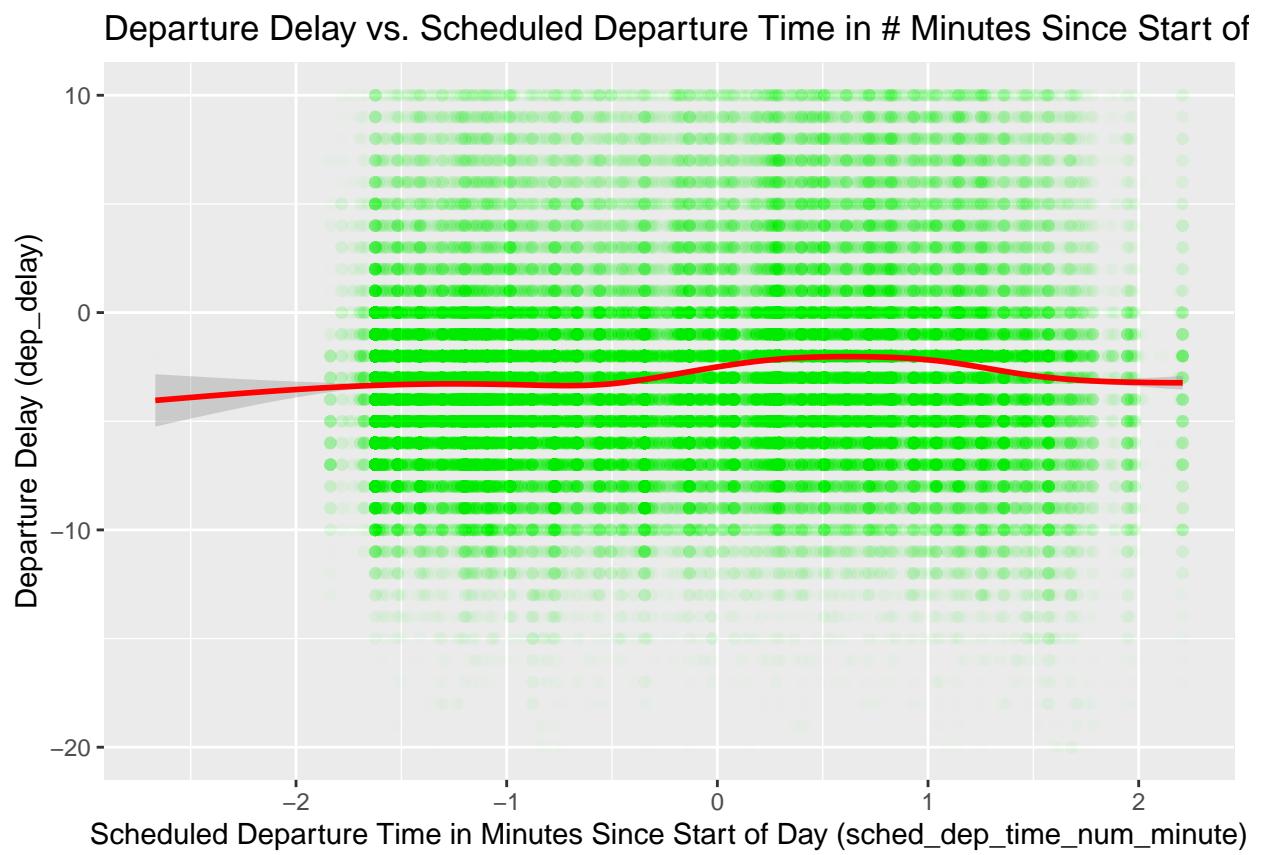


Figure 3: Departure Delay vs. Scheduled Departure Time in # Minutes Since Start of Day with Spline Plotted on Top Depicting Possible Non-Linear Relationship