

Midterm Project

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Library Load

```
library(caret)
```

```
## Loading required package: ggplot2
```

```
## Loading required package: lattice
```

```
library(tidymodels)
```

```
## -- Attaching packages ----- tidymodels 1.3.0 --
```

```
## v broom      1.0.7      v rsample      1.2.1
## v dials      1.4.0      v tibble       3.2.1
## v dplyr      1.1.4      v tidyr        1.3.1
## v infer      1.0.7      v tune         1.3.0
## v modeldata  1.4.0      v workflows    1.2.0
## v parsnip    1.3.1      v workflowsets 1.1.0
## v purrr      1.0.4      v yardstick    1.3.2
## v recipes    1.2.0
```

```
## -- Conflicts ----- tidymodels_conflicts() --
```

```
## x purrr::discard() masks scales::discard()
## x dplyr::filter() masks stats::filter()
## x dplyr::lag() masks stats::lag()
## x purrr::lift() masks caret::lift()
## x yardstick::precision() masks caret::precision()
## x yardstick::recall() masks caret::recall()
## x yardstick::sensitivity() masks caret::sensitivity()
## x yardstick::specificity() masks caret::specificity()
## x recipes::step() masks stats::step()
```

```
library(vtable)
```

```
## Loading required package: kableExtra
```

```
##
```

```
## Attaching package: 'kableExtra'
```

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

```
##
```

```
## group_rows
```

```
library(corrplot)
```

```
## corrplot 0.95 loaded
```

```

library(patchwork)
library(splines)
library(mgcv)

## Loading required package: nlme
##
## Attaching package: 'nlme'
## The following object is masked from 'package:dplyr':
##
##     collapse
## This is mgcv 1.9-1. For overview type 'help("mgcv-package")'.
library(pdp)

##
## Attaching package: 'pdp'
## The following object is masked from 'package:purrr':
##
##     partial
library(earth)

## Loading required package: Formula
## Loading required package: plotmo
## Loading required package: plotrix
##
## Attaching package: 'plotrix'
## The following object is masked from 'package:scales':
##
##     rescale
library(tidyverse)

## -- Attaching core tidyverse packages ----- tidyverse 2.0.0 --
## v forcats   1.0.0      v readr     2.1.5
## v lubridate  1.9.4      v stringr  1.5.1

## -- Conflicts ----- tidyverse_conflicts() --
## x readr::col_factor()      masks scales::col_factor()
## x nlme::collapse()         masks dplyr::collapse()
## x purrr::discard()         masks scales::discard()
## x dplyr::filter()          masks stats::filter()
## x stringr::fixed()         masks recipes::fixed()
## x kableExtra::group_rows() masks dplyr::group_rows()
## x dplyr::lag()             masks stats::lag()
## x purrr::lift()           masks caret::lift()
## x pdp::partial()          masks purrr::partial()
## x readr::spec()           masks yardstick::spec()
## i Use the conflicted package (<http://conflicted.r-lib.org/>) to force all conflicts to become errors
library(ggplot2)
library(glmnet)

```

```
## Loading required package: Matrix
##
## Attaching package: 'Matrix'
##
## The following objects are masked from 'package:tidyr':
##
##     expand, pack, unpack
##
## Loaded glmnet 4.1-8
```

Loading data

```
load("dat1.RData")
load("dat2.RData")
```

Exploratory Data Analysis

Go from labels to variable names

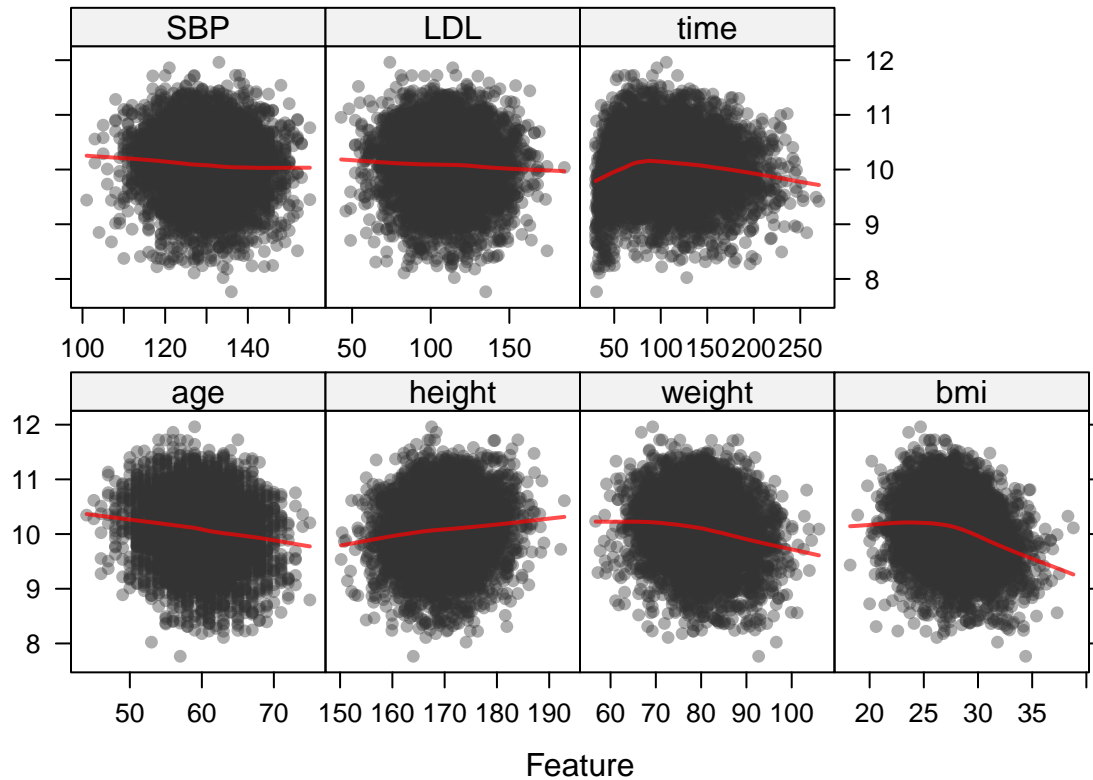
```
dat1 <- dat1 |>
  mutate(gender = factor(gender, levels = c(0,1),
                        labels = c("Female","Male")),
         race = factor(race, levels = c(1,2,3,4),
                      labels = c("White","Asian","Black","Hispanic")),
         smoking = factor(smoking, levels = c(0,1,2),
                         labels = c("Never smoked","Former smoker","Current smoker")),
         diabetes = factor(diabetes, levels = c(0,1),
                          labels = c("No","Yes")),
         hypertension = factor(hypertension, levels = c(0,1),
                              labels = c("No","Yes")),
         ) |>
  dplyr::select(-id)

dat2 <- dat2 |>
  mutate(gender = factor(gender, levels = c(0,1),
                        labels = c("Female","Male")),
         race = factor(race, levels = c(1,2,3,4),
                      labels = c("White","Asian","Black","Hispanic")),
         smoking = factor(smoking, levels = c(0,1,2),
                         labels = c("Never smoked","Former smoker","Current smoker")),
         diabetes = factor(diabetes, levels = c(0,1),
                          labels = c("No","Yes")),
         hypertension = factor(hypertension, levels = c(0,1),
                              labels = c("No","Yes")),
         ) |>
  dplyr::select(-id)
```

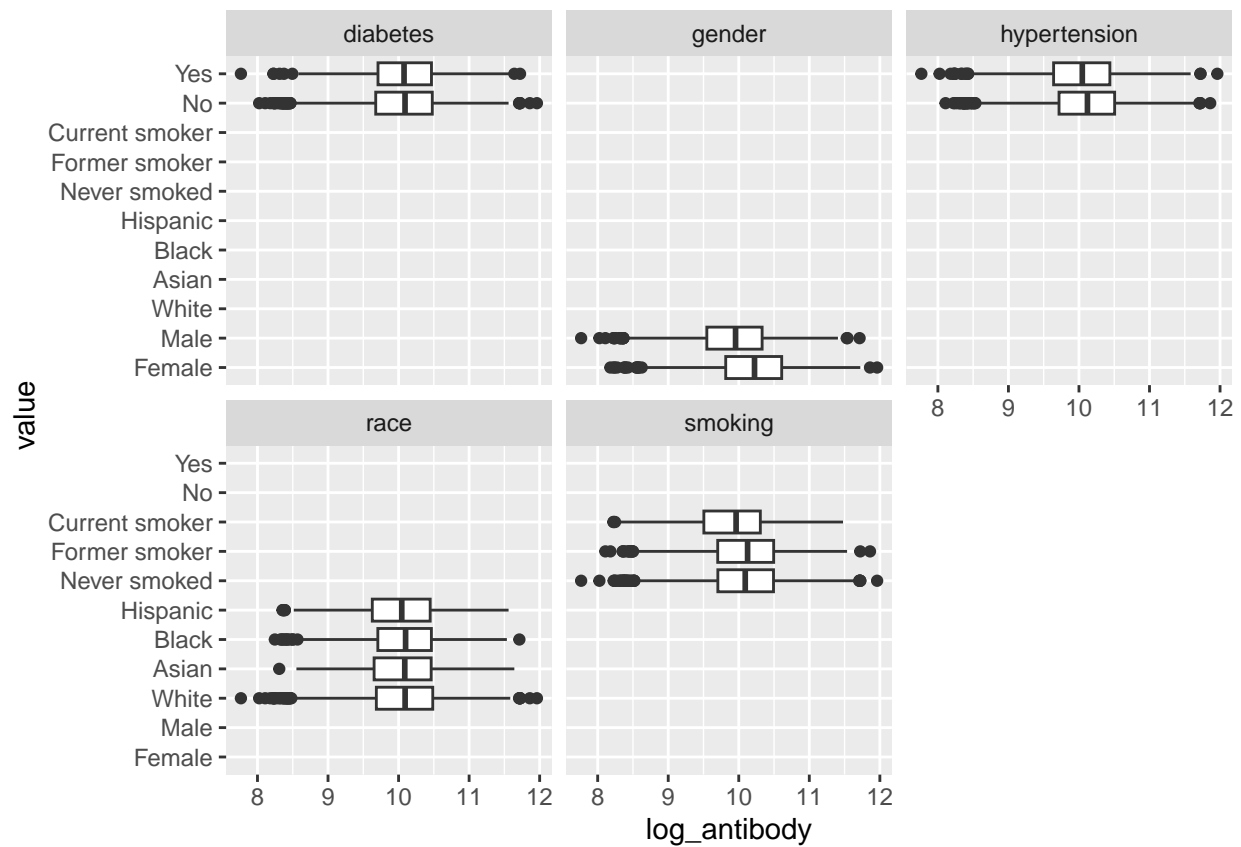
Use featureplot from caret to plot the training data

```
theme1 <- trellis.par.get()
theme1$plot.symbol$col = rgb(.2, .2, .2, .4)
theme1$plot.symbol$pch = 16
theme1$plot.line$col = rgb(1, 0, 0, .7)
theme1$plot.line$lwd <- 2
trellis.par.set(theme1)
```

```
featurePlot(x = dat1 |> dplyr::select(-log_antibody,
                                     -where(is.factor)),
            y = dat1$log_antibody,
            type = c("p", "smooth"))
```

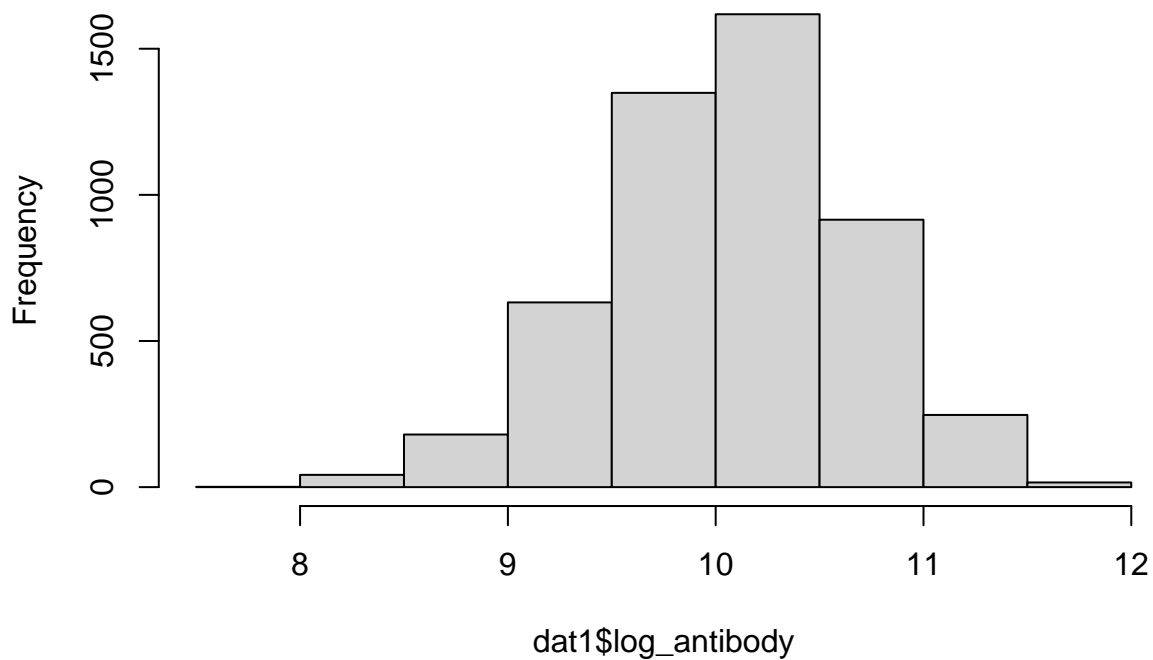


```
dat1 |>
  dplyr::select(log_antibody, gender, race, smoking, diabetes, hypertension) |>
  pivot_longer(cols = 2:6,
               names_to = "variable",
               values_to = "value") |>
  ggplot(aes(y = value, x = log_antibody)) +
  geom_boxplot() +
  facet_wrap(~variable)
```

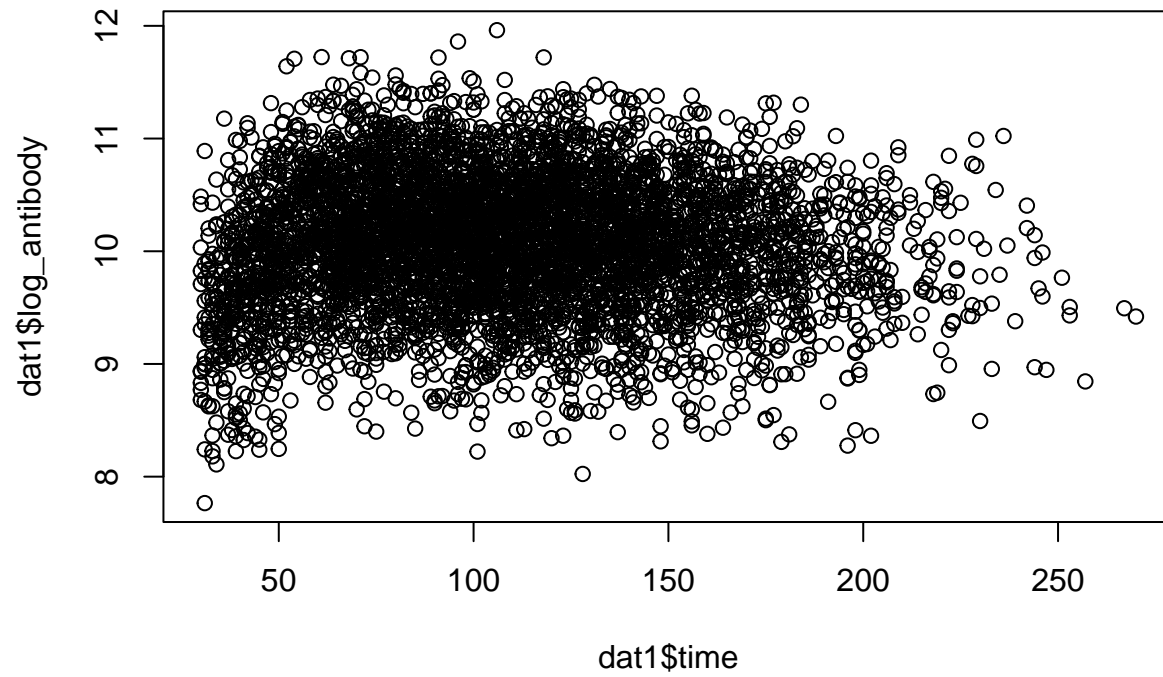


```
antibody_hist = hist(dat1$log_antibody)
```

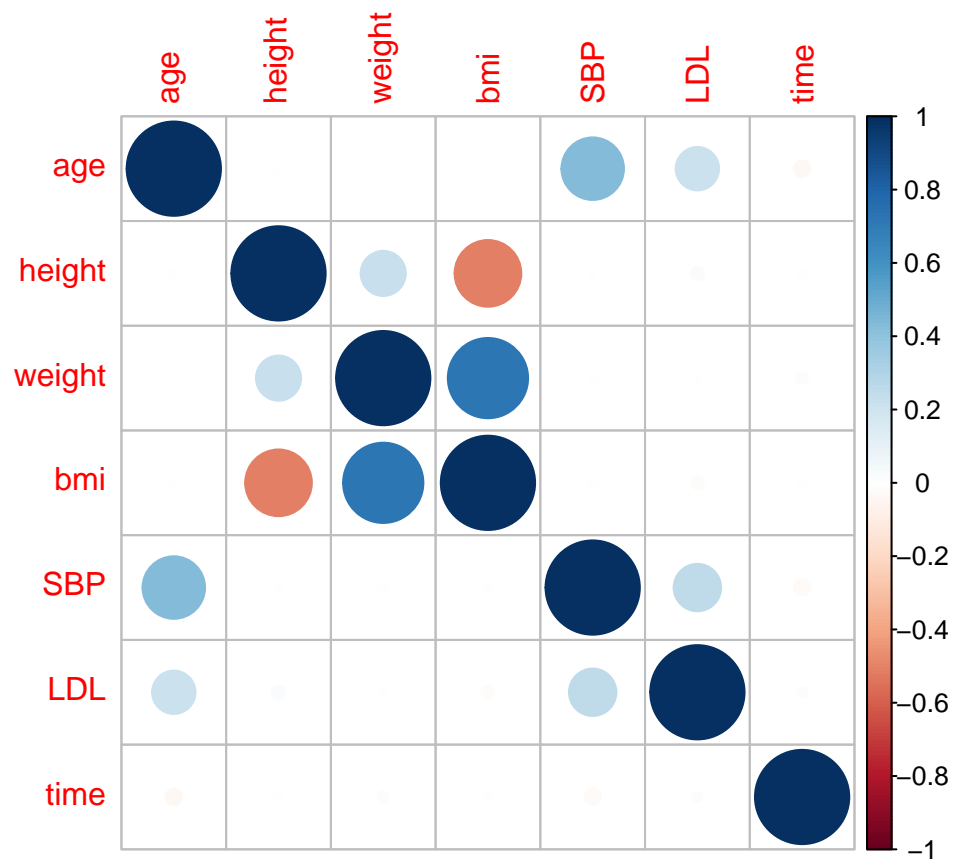
Histogram of dat1\$log_antibody



```
antibody_scatter = plot(x = dat1$time, y = dat1$log_antibody)
```



```
summ_table = sumtable(dat1, out = 'return')  
continuous = dat1[c(1,5:7,10:12)]  
correlations = cor(continuous)  
corr_plot = corrrplot(correlations)
```



```
report_table = sumtable(dat1, out = 'kable')
report_table
```

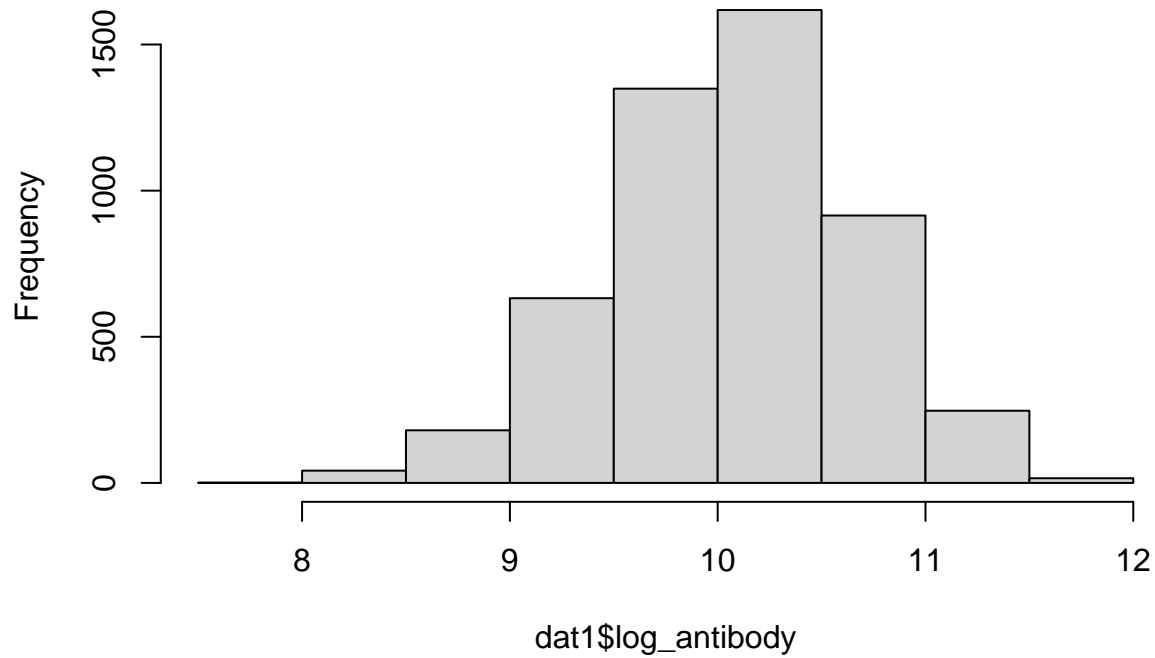
Looking at the second dataset

```
antibody_hist = hist(dat1$log_antibody)
```

Table 1: Summary Statistics

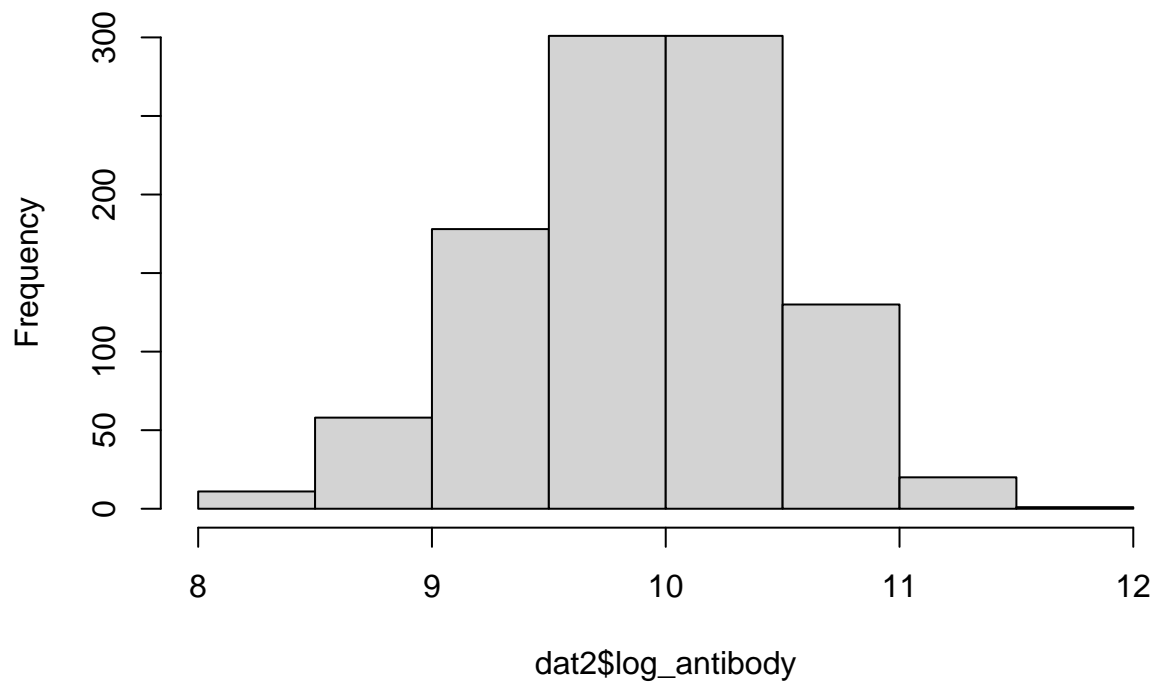
Variable	N	Mean	Std. Dev.	Min	Pctl. 25	Pctl. 75	Max
age	5000	60	4.5	44	57	63	75
gender	5000						
... Female	2573	51%					
... Male	2427	49%					
race	5000						
... White	3221	64%					
... Asian	278	6%					
... Black	1036	21%					
... Hispanic	465	9%					
smoking	5000						
... Never smoked	3010	60%					
... Former smoker	1504	30%					
... Current smoker	486	10%					
height	5000	170	5.9	150	166	174	193
weight	5000	80	7.1	57	75	85	106
bmi	5000	28	2.8	18	26	30	39
diabetes	5000						
... No	4228	85%					
... Yes	772	15%					
hypertension	5000						
... No	2702	54%					
... Yes	2298	46%					
SBP	5000	130	8	101	124	135	155
LDL	5000	110	20	43	96	124	185
time	5000	109	43	30	76	138	270
log_antibody	5000	10	0.6	7.8	9.7	10	12

Histogram of dat1\$log_antibody



```
antibody_hist_data2 = hist(dat2$log_antibody)
```

Histogram of dat2\$log_antibody



```
summ_table_data2 = sumtable(dat2, out = 'return')
```

Model Training

Creating the design Matrix

```
load('dat1.RData')

design_matrix =
  dat1 |>
  mutate(
    race_asian = as.numeric(race == 2),
    race_black = as.numeric(race == 3),
    race_hispanic = as.numeric(race == 4),
    smoking_former = as.numeric(smoking == 1),
    smoking_current = as.numeric(smoking == 2)
  ) %>%
  select(
    age, gender, race_asian, race_black, race_hispanic,
    smoking_former, smoking_current, height, weight,
    bmi, diabetes, hypertension, SBP, LDL, time,
    log_antibody
  )
```

Specify X and Y for model training

```
y = design_matrix$log_antibody
x = select(design_matrix, -log_antibody) %>%
  as.matrix()
```

Specify CV Procedure

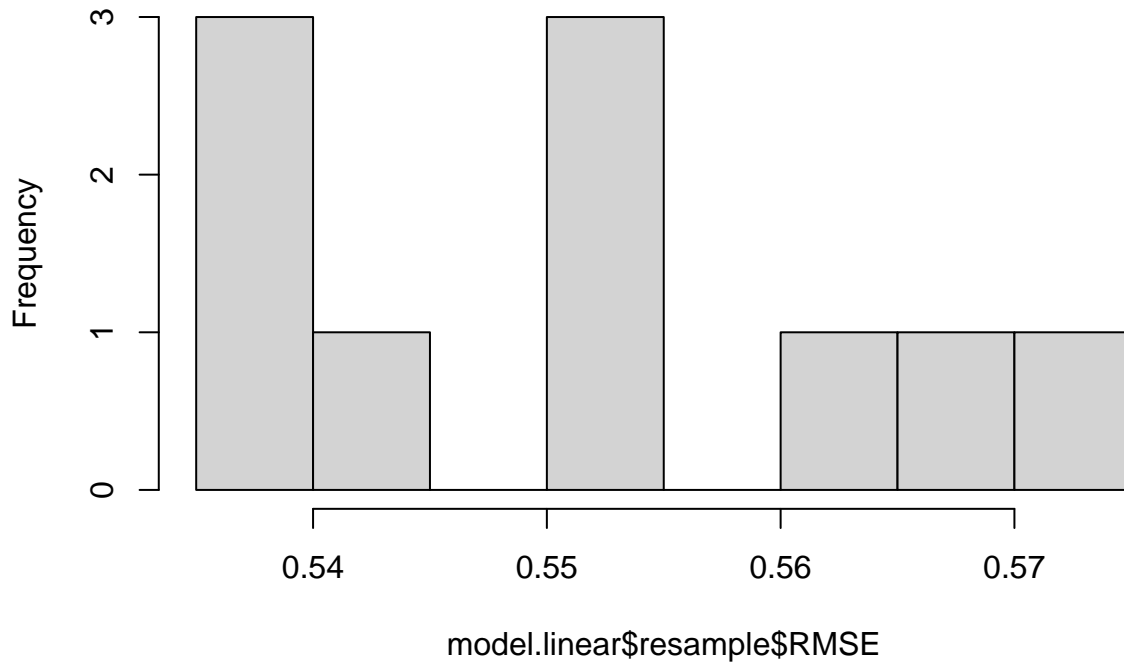
```
ctrl <- trainControl(method = "cv", number = 10)
```

Linear Regression

```
set.seed(1)
model.linear =
  train(x = x,
        y = y,
        method = "lm",
        metric = "RMSE",
        trControl = ctrl)

hist(model.linear$resample$RMSE)
```

Histogram of model.linear\$resample\$RMSE



```
coef(model.linear$finalModel)
```

```
##      (Intercept)          age          gender      race_asian      race_black
## 26.6751961468    -0.0205978746   -0.2974929370   -0.0060422043   -0.0075294859
## race_hispanic smoking_former smoking_current      height      weight
## -0.0417570580    0.0219906714   -0.1934834467   -0.0821380676    0.0859034194
##          bmi      diabetes      hypertension      SBP      LDL
## -0.2977934503    0.0112794933   -0.0179106155    0.0015181119   -0.0001645307
##          time
## -0.0003010641
```

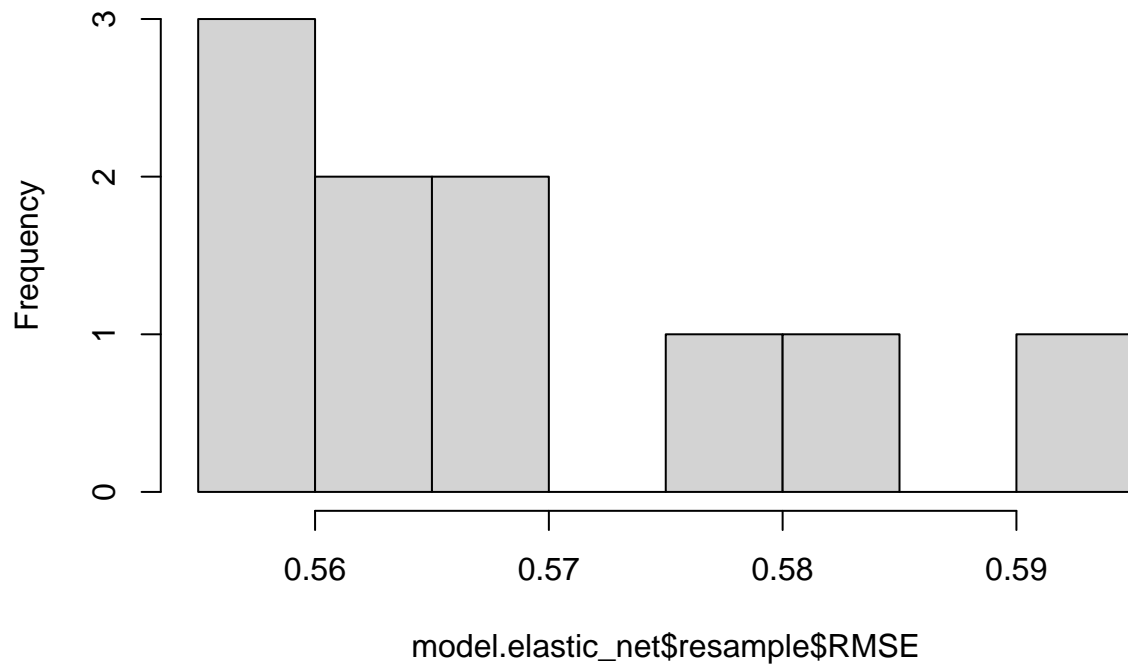
Elastic Net

```
set.seed(1)
model.elastic_net =
  train(x = x,
        y = y,
        method = "glmnet",
        metric = "RMSE",
        trControl = ctrl,
        tuneGrid = expand.grid(.alpha = seq(0,1, length = 21),
                              .lambda = exp(seq(6,0, length = 100))))
```

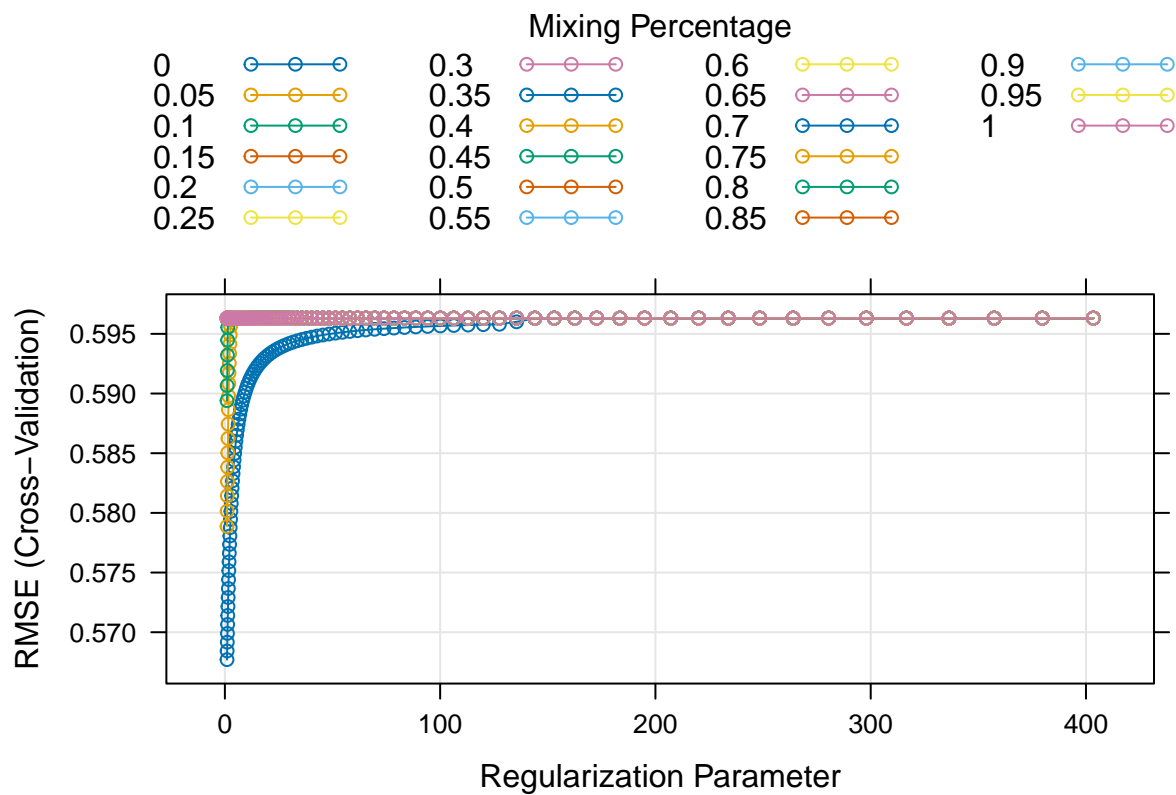
```
## Warning in nominalTrainWorkflow(x = x, y = y, wts = weights, info = trainInfo,
## : There were missing values in resampled performance measures.
```

```
hist(model.elastic_net$resample$RMSE)
```

Histogram of model.elastic_net\$resample\$RMSE



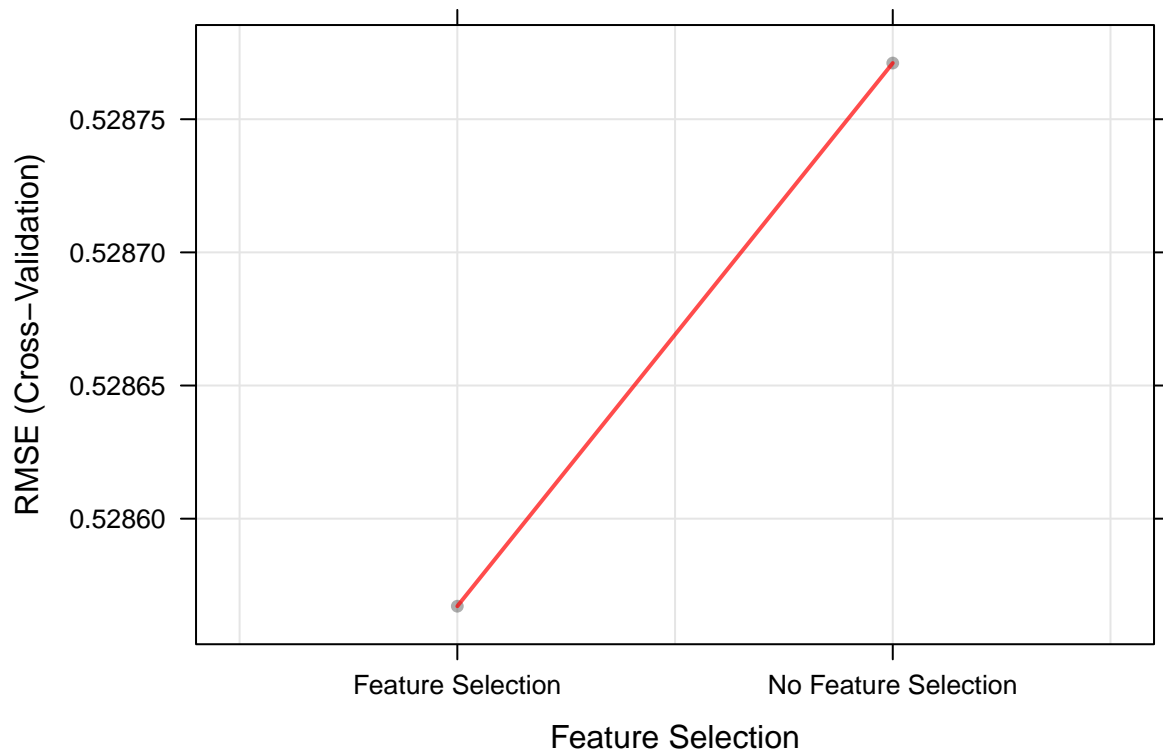
```
plot(model.elastic_net)
```



GAM

```
set.seed(1)
model.gam =
  train(x = x,
        y = y,
        method = "gam",
        metric = "RMSE",
        trControl = ctrl)
```

```
plot(model.gam)
```

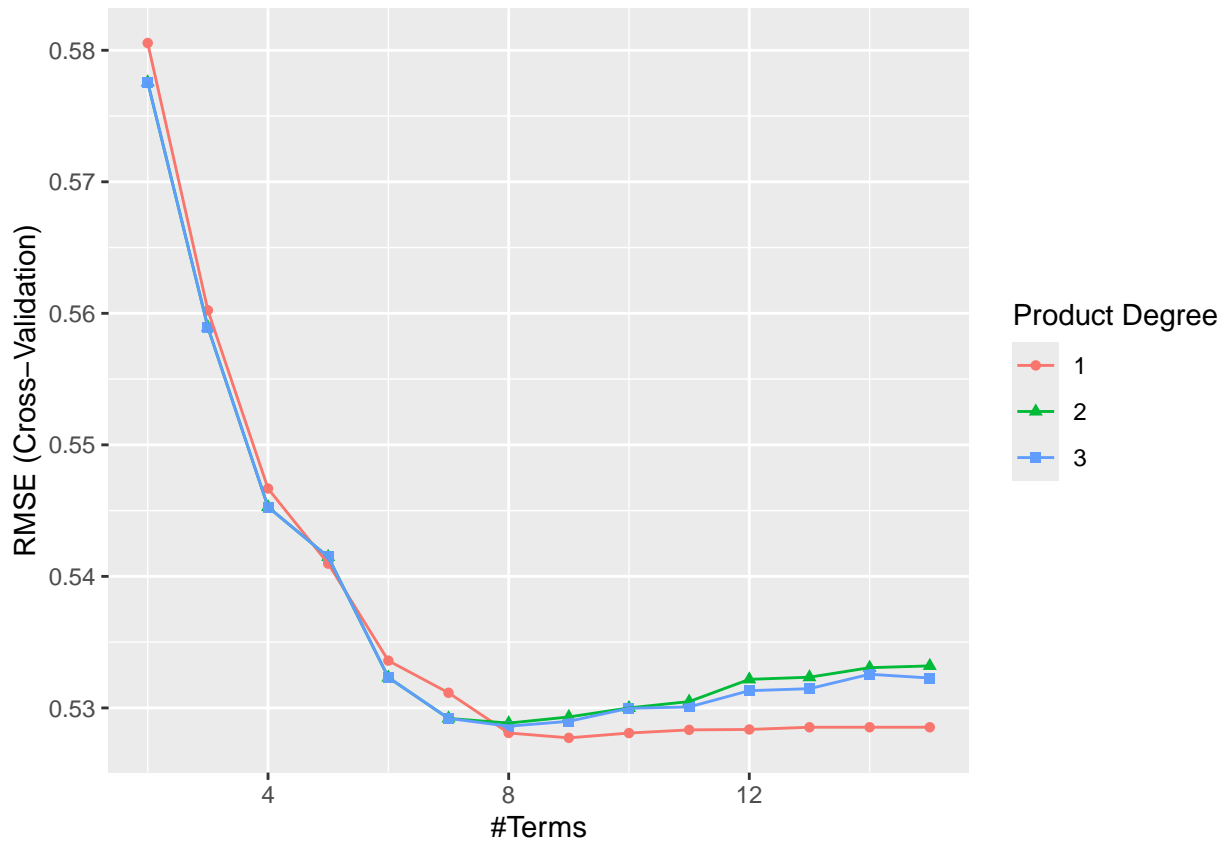


MARS

```
mars_grid =
  expand.grid(degree = 1:3,
             nprune = 2:15)

set.seed(1)
model.mars =
  train(x, y,
        method = "earth",
        tuneGrid = mars_grid,
        trControl = ctrl)

ggplot(model.mars) +
  labs('MARS Model Evaluation')
```



Comparing Cross Validated RMSE

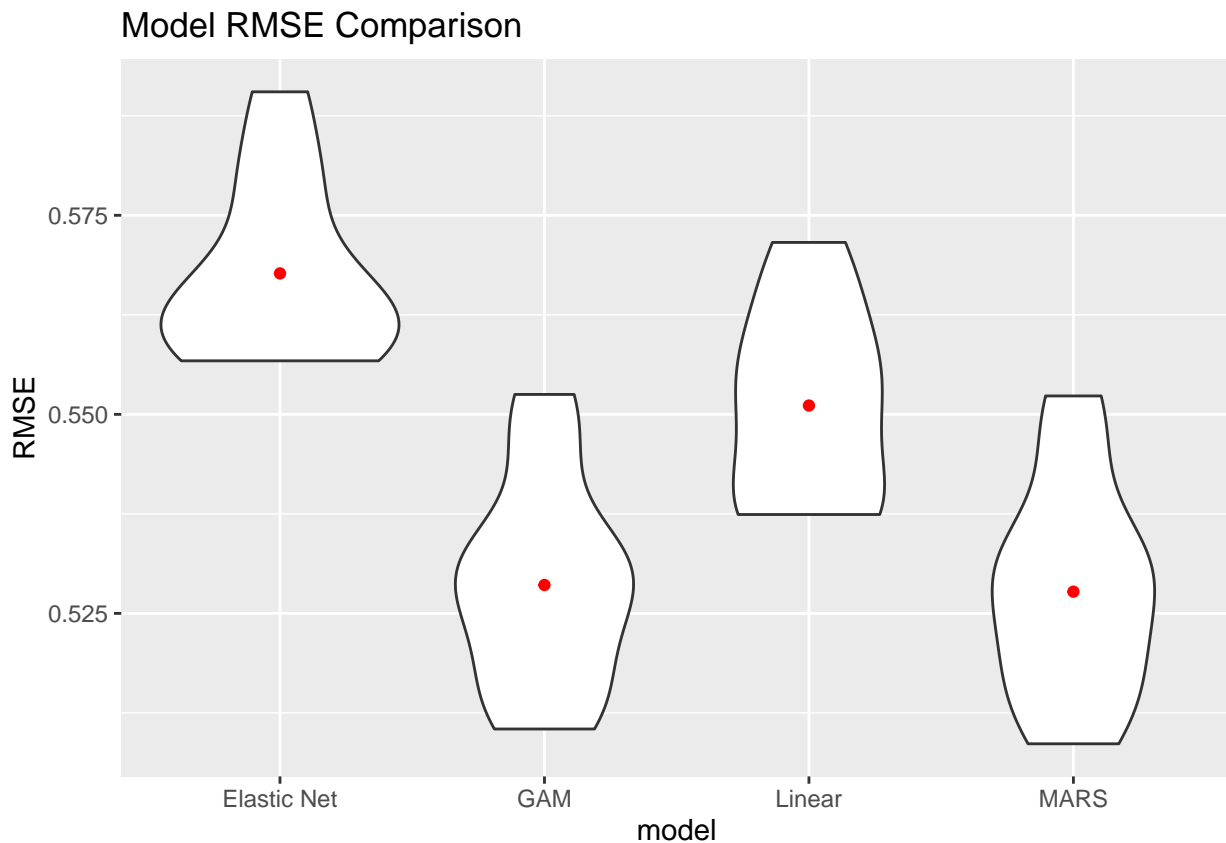
```
model.RMSE=
  rbind(
    data.frame(
      model = 'Linear',
      RMSE = model.linear$resample$RMSE
    ),
    data.frame(
      model = 'Elastic Net',
      RMSE = model.elastic_net$resample$RMSE),
    data.frame(
      model = 'GAM',
      RMSE = model.gam$resample$RMSE
    ),
    data.frame(
      model = 'MARS',
      RMSE = model.mars$resample$RMSE
    )
  )
```

```
model.RMSE %>%
  group_by(model) %>%
  summarize(mean(RMSE))
```

```
## # A tibble: 4 x 2
##   model      `mean(RMSE)`
```

```
##   <chr>           <dbl>
## 1 Elastic Net    0.568
## 2 GAM            0.529
## 3 Linear         0.551
## 4 MARS           0.528
```

```
model.RMSE |>
  ggplot(aes(x = model, y = RMSE)) +
  geom_violin() +
  stat_summary(
    fun = "mean",
    geom = "point",
    color = "red") +
  labs(title = "Model RMSE Comparison", xlab = "Model")
```



Model Evaluation

Clean new data set

```
load('dat2.RData')

design_matrix2 =
  dat2 |>
  mutate(
    race_asian = as.numeric(race == 2),
    race_black = as.numeric(race == 3),
    race_hispanic = as.numeric(race == 4),
    smoking_former = as.numeric(smoking == 1),
```

```

    smoking_current = as.numeric(smoking ==2)
  ) %>%
  select(
    age, gender, race_asian, race_black, race_hispanic,
    smoking_former, smoking_current, height, weight,
    bmi, diabetes, hypertension, SBP, LDL, time,
    log_antibody
  )

x2 = as.matrix(dplyr::select(design_matrix2, -log_antibody))
y2 = design_matrix2$log_antibody

```

```
head(x)
```

```

##   age gender race_asian race_black race_hispanic smoking_former smoking_current
## 1  50      0          0          0          0          0          0
## 2  71      1          0          0          0          0          0
## 3  58      1          0          0          0          1          0
## 4  63      0          0          0          0          0          0
## 5  56      1          0          0          0          0          0
## 6  59      1          0          1          0          0          0
##   height weight  bmi diabetes hypertension SBP LDL time
## 1  176.1  68.3 22.0         0          0 130 82  76
## 2  175.7  69.6 22.6         0          1 149 129 82
## 3  168.7  76.9 27.0         0          0 127 101 168
## 4  167.4  90.0 32.1         0          1 138  93 105
## 5  162.7  83.9 31.7         0          0 123  97 193
## 6  167.8  86.8 30.8         0          1 132 108 143

```

```
head(x2)
```

```

##      age gender race_asian race_black race_hispanic smoking_former
## 5001  58      0          0          0          1          1
## 5002  62      0          0          0          0          1
## 5003  71      0          0          0          1          0
## 5004  59      1          0          0          0          0
## 5005  69      1          0          0          0          0
## 5006  56      0          0          0          0          0
##      smoking_current height weight  bmi diabetes hypertension SBP LDL time
## 5001              0  176.4  86.4 27.7         0          0 130 115 205
## 5002              0  167.5  82.4 29.4         1          0 123 118 229
## 5003              0  179.3  79.2 24.6         1          1 145 149 206
## 5004              0  170.0  81.0 28.0         0          0 123 119 163
## 5005              0  166.5  74.8 27.0         1          1 150 142 240
## 5006              0  167.6  74.8 26.6         0          0 121 112 206

```

Make predictions and get test set RMSE

```

pred = predict(model.gam, x2)

dat2_rmse = sqrt(mean((pred - y2)^2))

dat2_rmse

## [1] 0.5691192

```