Data Science II Midterm

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Libraries

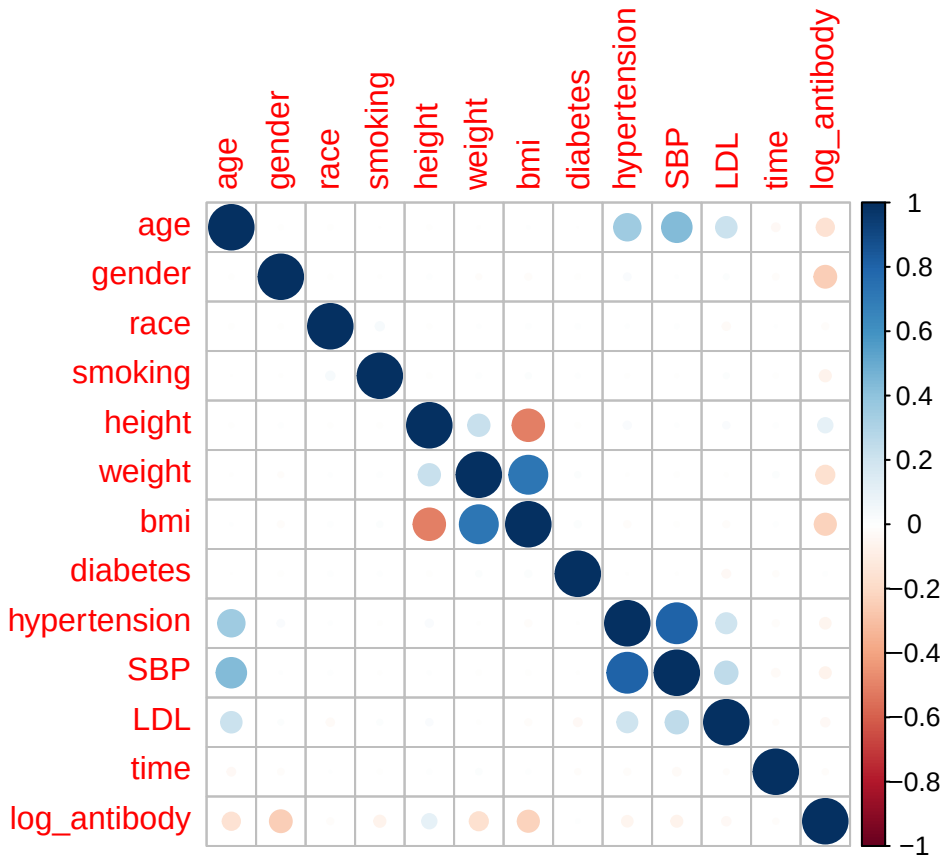
```
library(readxl) # to import excel files
library(tidyverse)
library(corrplot)
library(ggplot2)
library(tidymodels)
library(glmnet)
library(caret)
library(splines)
library(mgcv)
library(pROC)
library(vip)
library(AppliedPredictiveModeling)
library(tidymodels)
library(earth)
library(pdp)
```

Importing and Organizing Data

```
load("./data/dat1.RData") #importing training data
  # Log-transformed antibody level (log_antibody) --> y
initial_training = dat1 #renaming the original training data name

load("./data/dat2.RData") #importing training data
initial_test = dat2 #renaming the original training data name

set.seed(2222)

# partition data into training and validation data sets
datSplit = initial_split(data = initial_training, prop = 0.8)
training = training(datSplit)
validation = testing(datSplit)
```

Exploratory Analysis

```
Exploratory_train <- initial_training
Exploratory_train$race <- as.numeric(Exploratory_train$race)
Exploratory_train$smoking <- as.numeric(Exploratory_train$smoking)


train_cor_matrix <- cor(Exploratory_train[, !names(Exploratory_train) %in% c("id")],use = "complete.obs
corrplot(train_cor_matrix, method = "circle")
```




```
round(train_cor_matrix, 2)
```

```
##                 age gender  race smoking height weight   bmi diabetes
## age            1.00  -0.01 -0.01    0.00  -0.01   0.00  0.00     0.00
## gender        -0.01   1.00 -0.01    0.00   0.01  -0.01 -0.02    -0.01
## race          -0.01  -0.01  1.00    0.04  -0.01   0.00  0.01     0.01
## smoking        0.00   0.00  0.04    1.00  -0.01   0.01  0.01     0.01
## height        -0.01   0.01 -0.01   -0.01   1.00   0.23 -0.50    -0.01
## weight         0.00  -0.01  0.00    0.01   0.23   1.00  0.72     0.01
## bmi            0.00  -0.02  0.01    0.01  -0.50   0.72  1.00     0.02
## diabetes       0.00  -0.01  0.01    0.01  -0.01   0.01  0.02     1.00
## hypertension   0.35   0.02  0.00   -0.01   0.03   0.00 -0.02     0.00
## SBP            0.44   0.00  0.01    0.00   0.00  -0.01 -0.01     0.00
## LDL            0.21   0.01 -0.03    0.01   0.02   0.00 -0.02    -0.03
## time          -0.03  -0.02  0.00   -0.01   0.01   0.02  0.01    -0.01
## log_antibody -0.15  -0.24 -0.02   -0.06   0.10  -0.17 -0.23     0.01
```

```
##              hypertension   SBP   LDL  time log_antibody
## age                  0.35  0.44  0.21 -0.03        -0.15
## gender               0.02  0.00  0.01 -0.02        -0.24
## race                 0.00  0.01 -0.03  0.00        -0.02
## smoking             -0.01  0.00  0.01 -0.01        -0.06
## height               0.03  0.00  0.02  0.01         0.10
## weight               0.00 -0.01  0.00  0.02        -0.17
## bmi                 -0.02 -0.01 -0.02  0.01        -0.23
## diabetes             0.00  0.00 -0.03 -0.01         0.01
## hypertension         1.00  0.80  0.20 -0.02        -0.06
## SBP                  0.80  1.00  0.25 -0.03        -0.06
## LDL                  0.20  0.25  1.00 -0.01        -0.04
## time                -0.02 -0.03 -0.01  1.00        -0.01
## log_antibody        -0.06 -0.06 -0.04 -0.01         1.00
```

```
Exploratory_test <- initial_test
Exploratory_test$race <- as.numeric(Exploratory_test$race)
Exploratory_test$smoking <- as.numeric(Exploratory_test$smoking)
str(Exploratory_test)
```

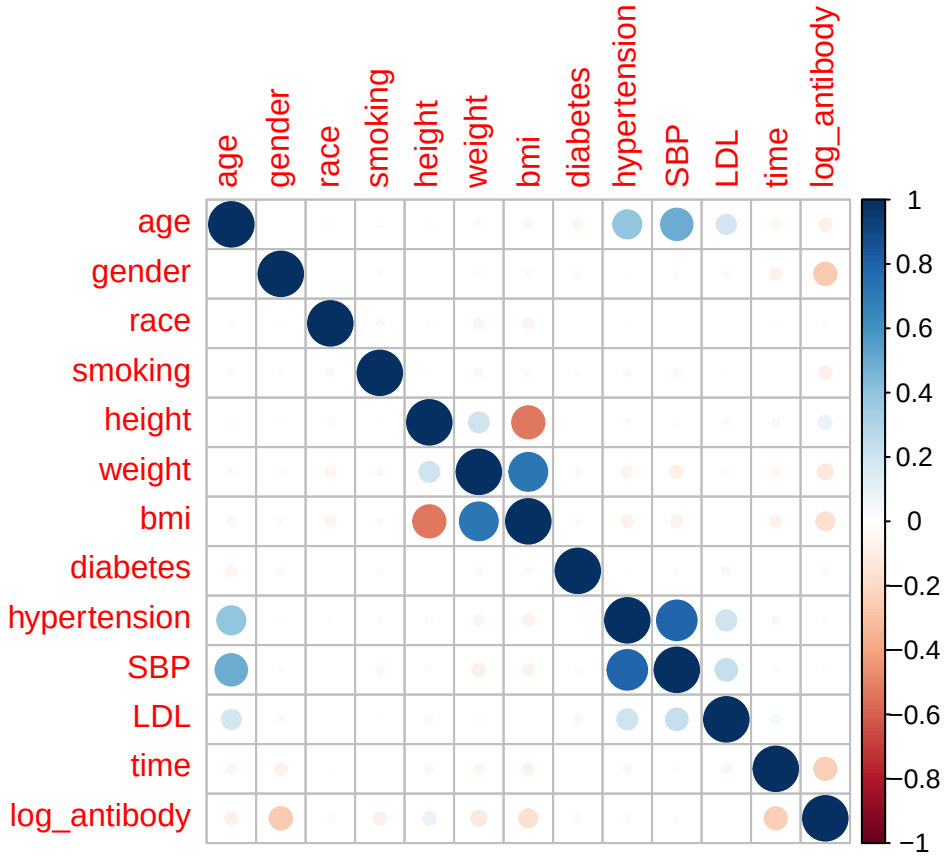
```
## 'data.frame':    1000 obs. of  14 variables:
##  $ id          : int  5001 5002 5003 5004 5005 5006 5007 5008 5009 5010 ...
##  $ age         : num  58 62 71 59 69 56 65 61 62 68 ...
##  $ gender      : int  0 0 0 1 1 0 0 1 0 0 ...
##  $ race        : num  4 1 4 1 1 1 1 1 1 4 ...
##  $ smoking     : num  2 2 1 1 1 1 1 2 1 1 ...
##  $ height      : num  176 168 179 170 166 ...
##  $ weight      : num  86.4 82.4 79.2 81 74.8 74.8 69.2 81.3 82.1 74.4 ...
##  $ bmi         : num  27.7 29.4 24.6 28 27 26.6 22.4 27.4 30.7 26.7 ...
##  $ diabetes    : int  0 1 1 0 1 0 0 0 0 0 ...
##  $ hypertension: num  0 0 1 0 1 0 1 0 1 1 ...
##  $ SBP         : num  130 123 145 123 150 121 132 120 142 137 ...
##  $ LDL         : num  115 118 149 119 142 112 127 76 86 123 ...
##  $ time        : num  205 229 206 163 240 206 285 185 124 127 ...
##  $ log_antibody: num  9.81 9.08 10.43 9.83 9.07 ...
```

```
test_cor_matrix <- cor(Exploratory_test[, !names(Exploratory_test) %in% c("id")],use = "complete.obs")
round(test_cor_matrix, 2)
```

```
##                age gender  race smoking height weight   bmi diabetes
## age           1.00   0.00  0.02   -0.02   0.02  -0.02 -0.03    -0.05
## gender        0.00   1.00 -0.01   -0.01   0.01  -0.02 -0.02    -0.03
## race          0.02  -0.01  1.00    0.03   0.02  -0.05 -0.06     0.00
## smoking      -0.02  -0.01  0.03    1.00   0.00   0.03  0.02    -0.02
## height        0.02   0.01  0.02    0.00   1.00   0.20 -0.53    -0.01
## weight       -0.02  -0.02 -0.05    0.03   0.20   1.00  0.72    -0.03
## bmi          -0.03  -0.02 -0.06    0.02  -0.53   0.72  1.00    -0.02
## diabetes     -0.05  -0.03  0.00   -0.02  -0.01  -0.03 -0.02     1.00
## hypertension  0.40   0.00 -0.01   -0.02   0.02  -0.06 -0.07    -0.01
## SBP           0.50   0.02  0.00   -0.03  -0.01  -0.08 -0.06    -0.01
## LDL           0.19  -0.02  0.00    0.00  -0.02  -0.02  0.00     0.04
## time         -0.04  -0.07 -0.01    0.00   0.03  -0.05 -0.06     0.00
## log_antibody -0.08  -0.25 -0.01   -0.08   0.08  -0.11 -0.16     0.03
```

```
##                hypertension   SBP   LDL  time log_antibody
## age                    0.40  0.50  0.19 -0.04        -0.08
## gender                 0.00  0.02 -0.02 -0.07        -0.25
## race                  -0.01  0.00  0.00 -0.01        -0.01
## smoking               -0.02 -0.03  0.00  0.00        -0.08
## height                 0.02 -0.01 -0.02  0.03         0.08
## weight                -0.06 -0.08 -0.02 -0.05        -0.11
## bmi                   -0.07 -0.06  0.00 -0.06        -0.16
## diabetes              -0.01 -0.01  0.04  0.00         0.03
## hypertension           1.00  0.79  0.21  0.03         0.02
## SBP                    0.79  1.00  0.24  0.02        -0.01
## LDL                    0.21  0.24  1.00  0.04         0.00
## time                   0.03  0.02  0.04  1.00        -0.25
## log_antibody           0.02 -0.01  0.00 -0.25         1.00
```

```r
corrplot(test_cor_matrix, method = "circle")
```



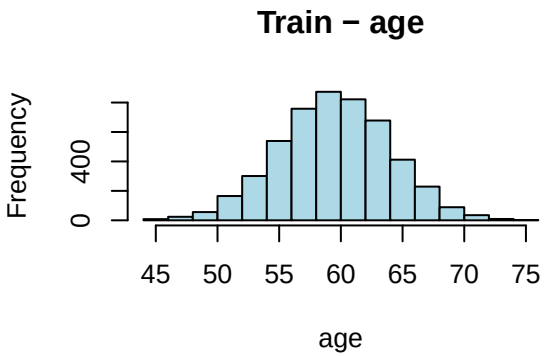

```r
measurement<-data.frame(
 Train_Mean = sapply(Exploratory_train, mean, na.rm = TRUE),
 Test_Mean = sapply(Exploratory_test, mean, na.rm = TRUE),
 Train_SD   = sapply(Exploratory_train, sd, na.rm = TRUE),
 Test_SD   = sapply(Exploratory_test, sd, na.rm = TRUE),
 Train_Min  = sapply(Exploratory_train, min, na.rm = TRUE),
 Train_Max  = sapply(Exploratory_train, max, na.rm = TRUE),
 Test_Min  = sapply(Exploratory_test, min, na.rm = TRUE),
```

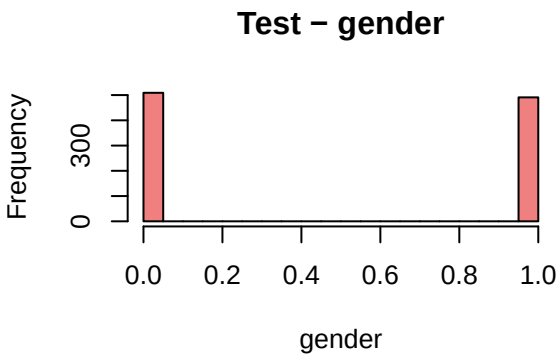
```
  Test_Max  = sapply(Exploratory_test, max, na.rm = TRUE))
round(measurement, 2)
```

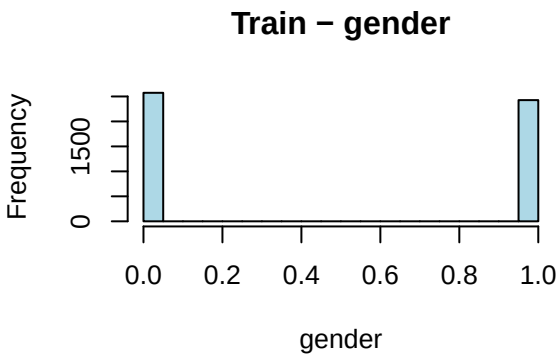
```
##              Train_Mean Test_Mean Train_SD Test_SD Train_Min Train_Max Test_Min
## id              2500.50   5500.50  1443.52  288.82      1.00   5000.00  5001.00
## age               59.97     60.02     4.50    4.45     44.00     75.00    46.00
## gender             0.49      0.49     0.50    0.50      0.00      1.00     0.00
## race               1.75      1.70     1.08    1.05      1.00      4.00     1.00
## smoking            1.50      1.50     0.67    0.68      1.00      3.00     1.00
## height           170.13    170.22     5.94    6.02    150.20    192.90   149.40
## weight            80.11     80.13     7.06    7.05     56.70    106.00    58.80
## bmi               27.74     27.72     2.76    2.82     18.20     38.80    19.80
## diabetes           0.15      0.16     0.36    0.36      0.00      1.00     0.00
## hypertension       0.46      0.46     0.50    0.50      0.00      1.00     0.00
## SBP              129.90    129.61     8.00    8.20    101.00    155.00   106.00
## LDL              109.91    110.25    20.15   20.32     43.00    185.00    46.00
## time             108.86    173.77    43.42   46.78     30.00    270.00    61.00
## log_antibody      10.06      9.90     0.60    0.59      7.77     11.96     8.05
##              Test_Max
## id            6000.00
## age             75.00
## gender           1.00
## race             4.00
## smoking          3.00
## height         190.60
## weight         101.60
## bmi             35.80
## diabetes         1.00
## hypertension     1.00
## SBP            156.00
## LDL            174.00
## time           330.00
## log_antibody    11.85
```

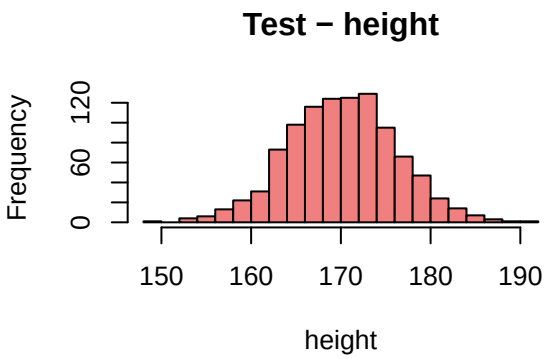
```
train_vars <- initial_training[, !names(initial_training) %in% c("id", "race", "smoking")]
test_vars  <- initial_test[, !names(initial_test) %in% c("id", "race", "smoking")]
par(mfrow = c(2, 2))
for (var in names(train_vars)) {
  hist(test_vars[[var]],
       main = paste("Test -", var),
       xlab = var,
       col = "lightcoral",
       breaks = 20)
  hist(train_vars[[var]],
       main = paste("Train -", var),
       xlab = var,
       col = "lightblue",
       breaks = 20)
}
```

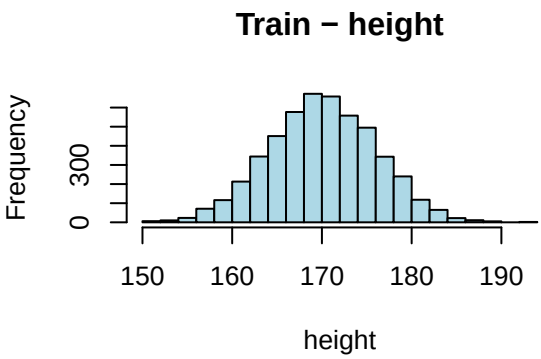

Test − age
Frequency
0
100
45
50
55
60
65
70
75
age

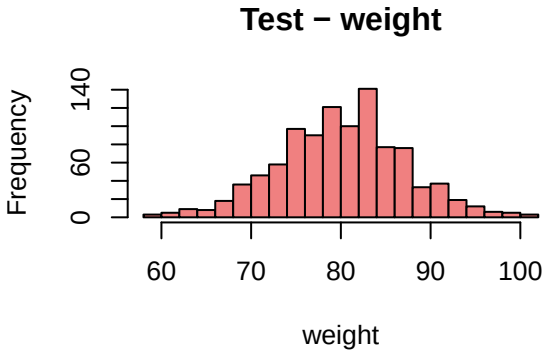

Train − age
Frequency
0
400
45
50
55
60
65
70
75
age

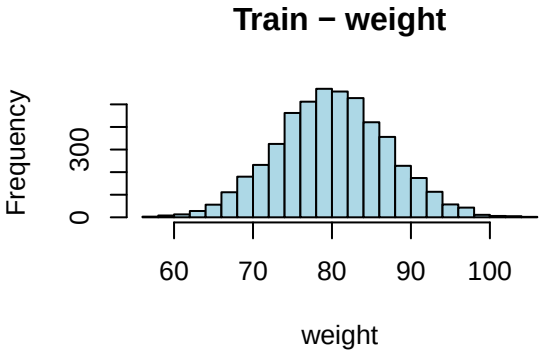

Test − gender
Frequency
0
300
0.0
0.2
0.4
0.6
0.8
1.0
gender

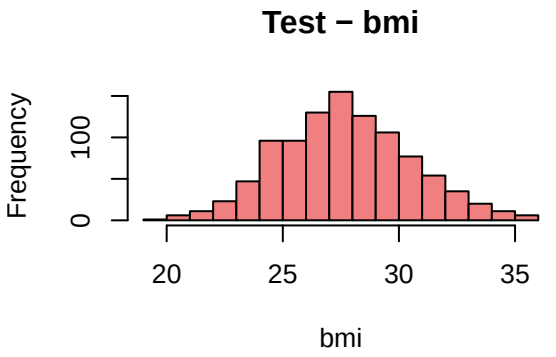

Train − gender
Frequency
0
1500
0.0
0.2
0.4
0.6
0.8
1.0
gender

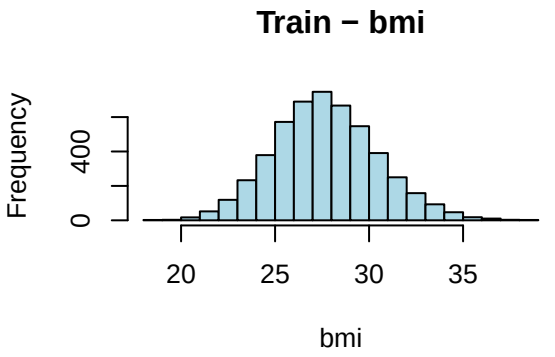

Test − height
Frequency
0
60
120
150
160
170
180
190
height

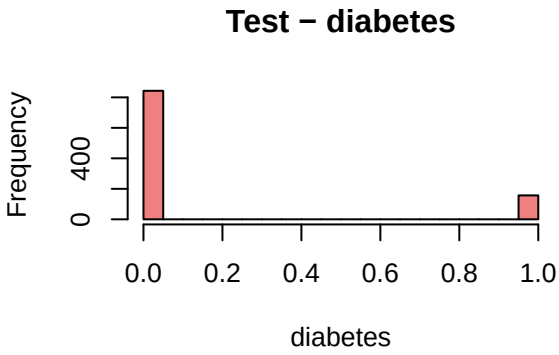

Train − height
Frequency
0
300
150
160
170
180
190
height

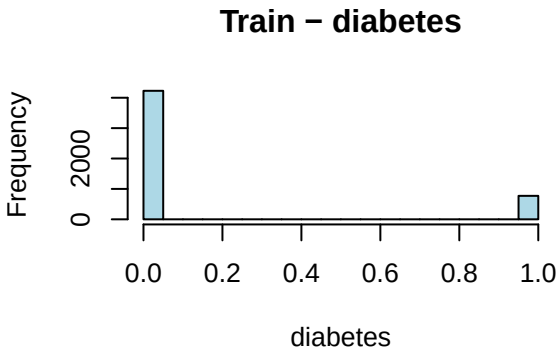

Test − weight
Frequency
0
60
140
60
70
80
90
100
weight

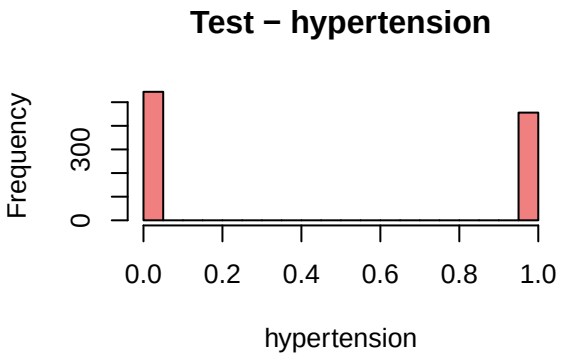

Train − weight
Frequency
0
300
60
70
80
90
100
weight

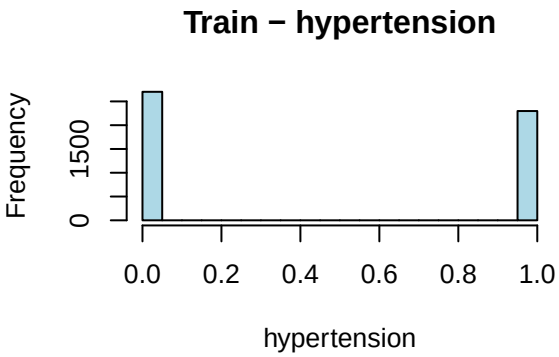

Test − bmi
Frequency
0
100
20
25
30
35
bmi

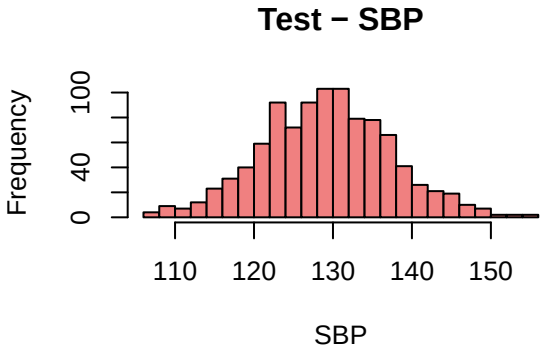

Train − bmi
Frequency
0
400
20
25
30
35
bmi

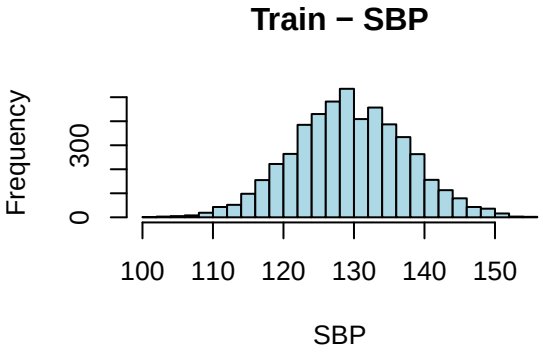

Test − diabetes
Frequency
0
400
0.0
0.2
0.4
0.6
0.8
1.0
diabetes

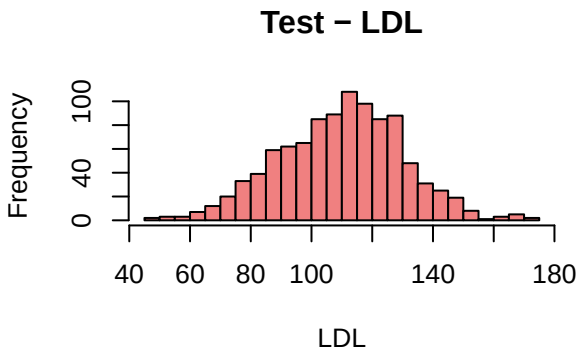

Train − diabetes
Frequency
0
2000
0.0
0.2
0.4
0.6
0.8
1.0
diabetes

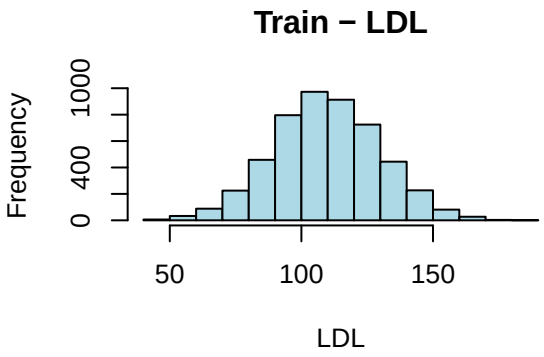

Test − hypertension
Frequency
0
300
0.0
0.2
0.4
0.6
0.8
1.0
hypertension

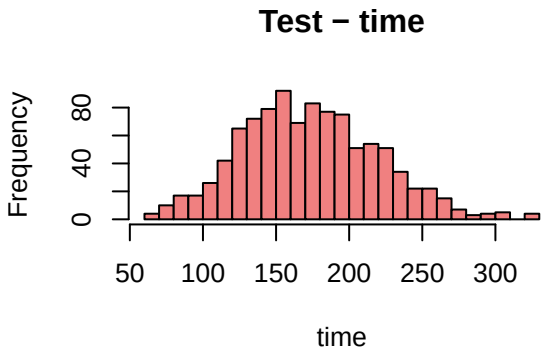

Train − hypertension
Frequency
0
1500
0.0
0.2
0.4
0.6
0.8
1.0
hypertension

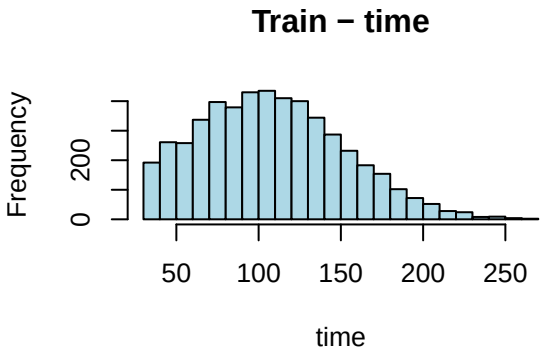

Test − SBP
Frequency
0
40
100
110
120
130
140
150
SBP


Train − SBP
Frequency
0
300
100
110
120
130
140
150
SBP

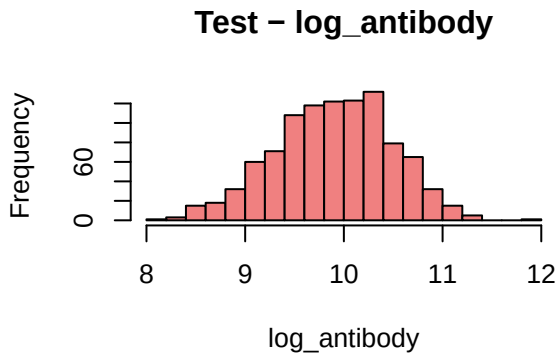


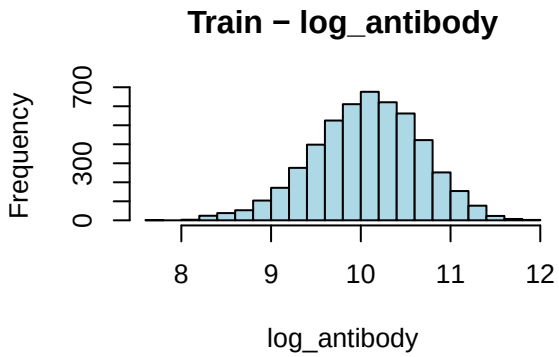


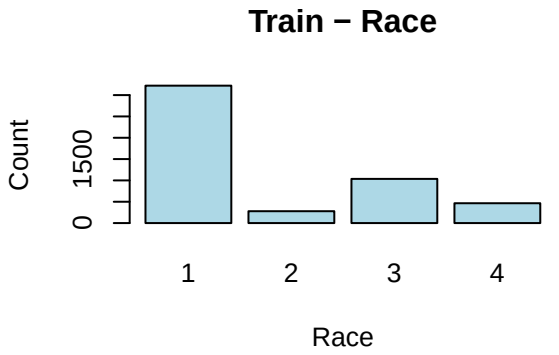




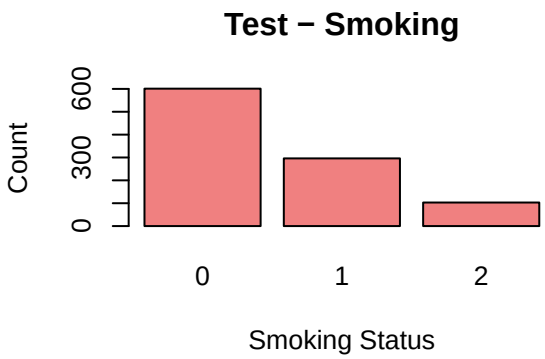

```r
barplot(table(initial_test$race),
        main = "Test - Race",
        col = "lightcoral",
        xlab = "Race",
        ylab = "Count")

barplot(table(initial_training$race),
        main = "Train - Race",
        col = "lightblue",
        xlab = "Race",
        ylab = "Count")
```

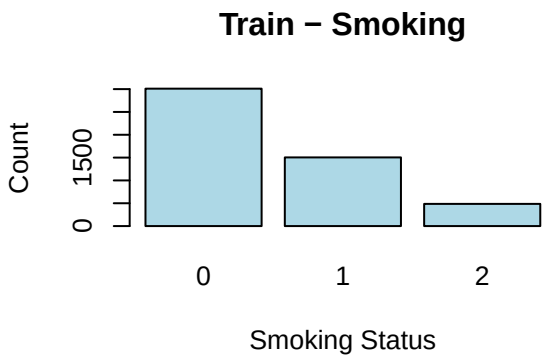







```r
barplot(table(initial_test$smoking),
        main = "Test - Smoking",
        col = "lightcoral",
        xlab = "Smoking Status",
        ylab = "Count")

barplot(table(initial_training$smoking),
        main = "Train - Smoking",
        col = "lightblue",
        xlab = "Smoking Status",
        ylab = "Count")
```





Linear Regression

```
model = lm(log_antibody ~ age + gender + race + smoking + bmi + diabetes +
             hypertension + LDL + time, data = training)

# View the model summary
summary(model)
```

```
##
## Call:
## lm(formula = log_antibody ~ age + gender + race + smoking + bmi +
##     diabetes + hypertension + LDL + time, data = training)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -2.13184 -0.35446  0.03155  0.38071  1.57178
##
## Coefficients:
##                Estimate Std. Error t value Pr(>|t|)
## (Intercept)   1.279e+01  1.540e-01  83.056  < 2e-16 ***
## age          -1.873e-02  2.094e-03  -8.945  < 2e-16 ***
## gender       -2.770e-01  1.741e-02 -15.916  < 2e-16 ***
## race2        -1.263e-02  3.877e-02  -0.326   0.7447
```

```
## race3        -8.852e-03  2.193e-02  -0.404   0.6864
## race4        -4.747e-02  3.027e-02  -1.569   0.1168
## smoking1      2.452e-02  1.944e-02   1.262   0.2072
## smoking2     -1.757e-01  2.986e-02  -5.885  4.3e-09 ***
## bmi          -5.054e-02  3.170e-03 -15.941  < 2e-16 ***
## diabetes      1.688e-03  2.445e-02   0.069   0.9450
## hypertension -3.728e-03  1.882e-02  -0.198   0.8430
## LDL          -8.155e-05  4.500e-04  -0.181   0.8562
## time         -3.720e-04  1.996e-04  -1.864   0.0624 .
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.5495 on 3987 degrees of freedom
## Multiple R-squared:  0.139,  Adjusted R-squared:  0.1364
## F-statistic: 53.62 on 12 and 3987 DF,  p-value: < 2.2e-16
```

```
predictions_train = predict(model, newdata = validation)

# RMSE
rmse_train = sqrt(mean((predictions_train - validation$log_antibody)^2))
rmse_train
```

```
## [1] 0.5636857
```

```
# R^2
rsq_train = 1 - sum((predictions_train - validation$log_antibody)^2) /
  sum((mean(training$log_antibody) - validation$log_antibody)^2)
rsq_train
```

```
## [1] 0.1648078
```

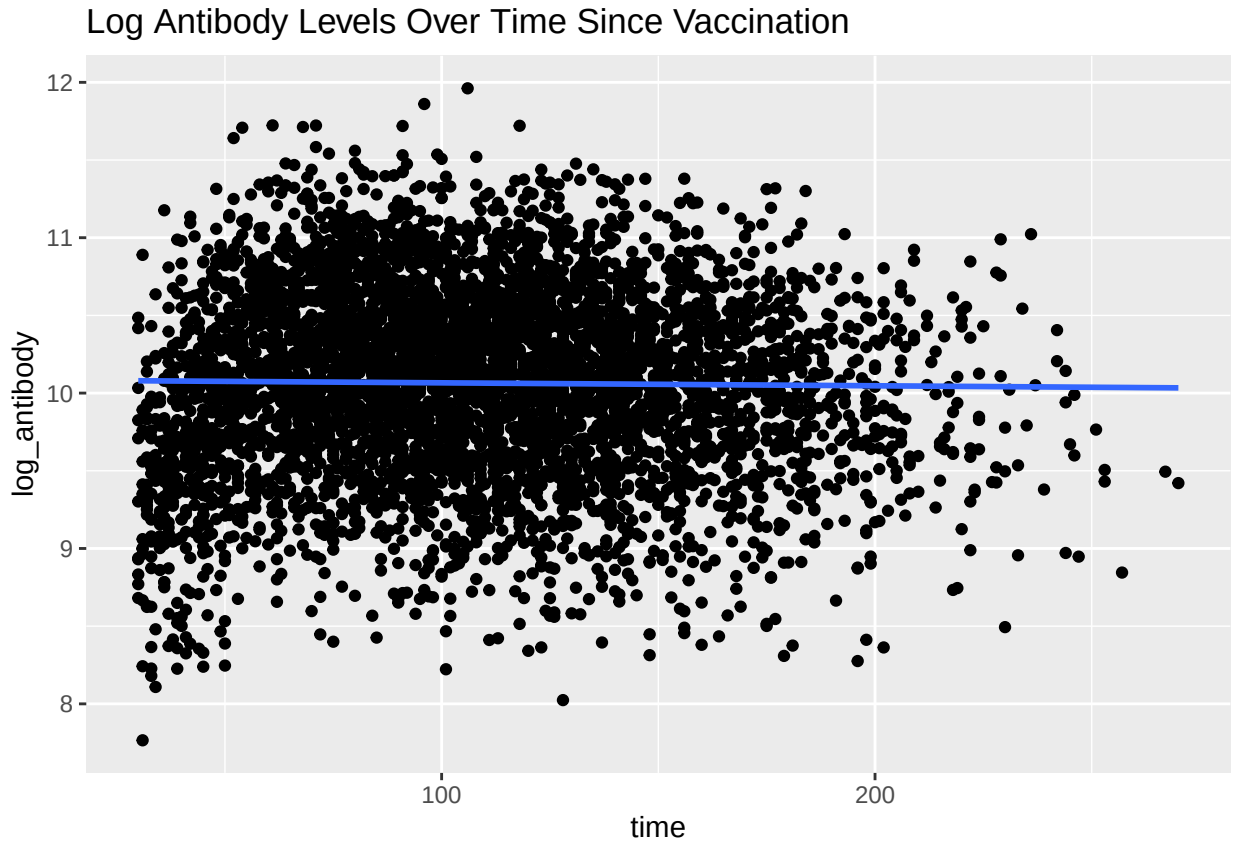
```
generalization = predict(model, newdata = initial_test)

# Calculate RMSE for dat2
rmse_dat2 = sqrt(mean((generalization - initial_test$log_antibody)^2))
rmse_dat2
```

```
## [1] 0.568555
```

```
# Calculate R-squared for dat2
rsq_dat2 = 1 - sum((generalization - initial_test$log_antibody)^2) /
  sum((mean(initial_test$log_antibody) - initial_test$log_antibody)^2)
rsq_dat2
```

```
## [1] 0.06204078
```

```
ggplot(initial_training, aes(x = time, y = log_antibody)) +
  geom_point() +
  geom_smooth(method = "lm", se = FALSE) +
  labs(title = "Log Antibody Levels Over Time Since Vaccination")
```



GAM MODEL

```
##########################GAM MODEL#########################

#converted some of the variables to factor for smoother flow

training <- training %>% mutate(across(c(race, smoking, gender), as.factor))
validation <- validation %>% mutate(across(c(race, smoking, gender), as.factor))
dat2 <- dat2 %>% mutate(across(c(race, smoking, gender), as.factor))

set.seed(2222)
cv_folds <- vfold_cv(training, v = 10)

fit_gam_fold <- function(split, id) {
  train_data <- analysis(split)
  val_data <- assessment(split)
  model <- gam(log_antibody ~ s(age) + s(bmi) + s(time) + gender + race + smoking +diabetes + hypertensi

  val_data$.pred <- predict(model, newdata = val_data)
  rmse_val <- yardstick::rmse(val_data, truth = log_antibody, estimate = .pred)$.estimate
  rsq_val <- yardstick::rsq(val_data, truth = log_antibody, estimate = .pred)$.estimate
  tibble(
    fold = id,
    model = list(model),
    rmse = rmse_val,
    rsq = rsq_val
  )
```

```
}

cv_model_results <- map2_dfr(cv_folds$splits, cv_folds$id, fit_gam_fold)

best_model_row <- cv_model_results %>%
  arrange(rmse) %>%
  slice(1)
best_gam_model <- best_model_row$model[[1]]
best_model_row$rmse
```

```
## [1] 0.4927833
```

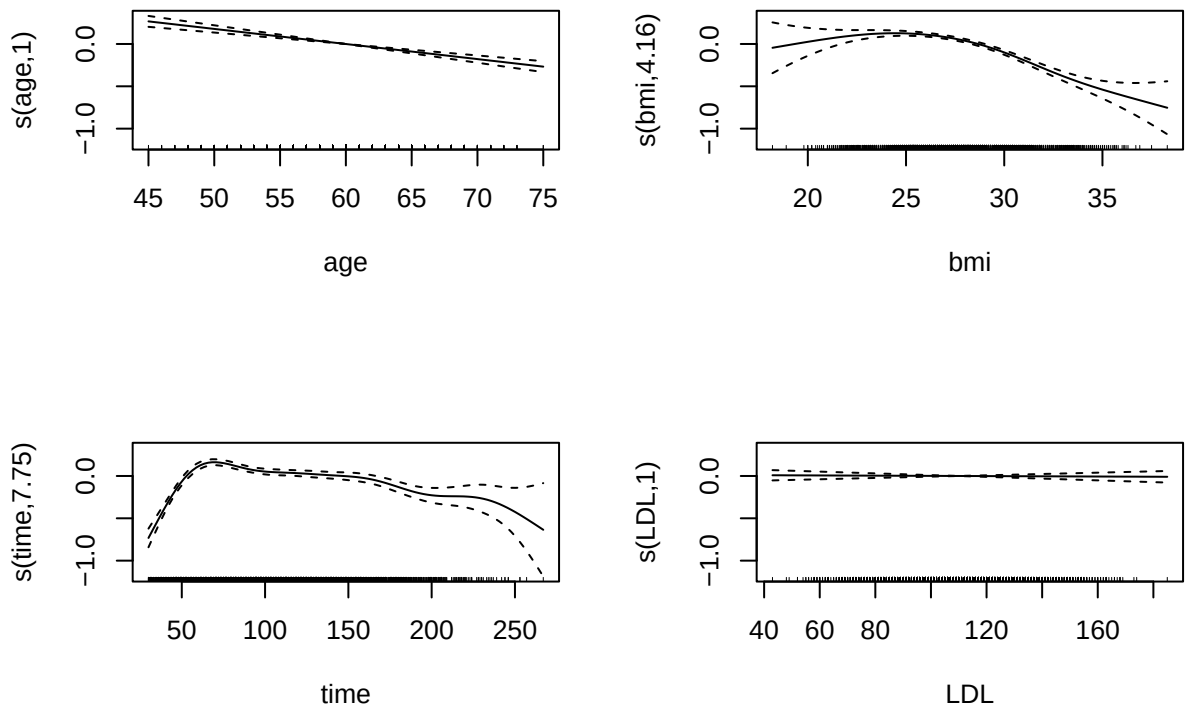
```
best_model_row$rsq
```

```
## [1] 0.3095418
```

```
summary(best_gam_model)
```

```
##
## Family: gaussian
## Link function: identity
##
## Formula:
## log_antibody ~ s(age) + s(bmi) + s(time) + gender + race + smoking +
##     diabetes + hypertension + s(LDL)
##
## Parametric coefficients:
##               Estimate Std. Error t value Pr(>|t|)
## (Intercept)  10.224719   0.018191 562.074  < 2e-16 ***
## gender1      -0.275874   0.017644 -15.636  < 2e-16 ***
## race2        -0.004582   0.038591  -0.119    0.905
## race3        -0.005678   0.022175  -0.256    0.798
## race4        -0.040430   0.030715  -1.316    0.188
## smoking1      0.028018   0.019659   1.425    0.154
## smoking2     -0.203533   0.030414  -6.692 2.54e-11 ***
## diabetes      0.002432   0.024623   0.099    0.921
## hypertension -0.008015   0.019048  -0.421    0.674
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Approximate significance of smooth terms:
##           edf Ref.df      F p-value
## s(age)  1.001  1.003 68.895  <2e-16 ***
## s(bmi)  4.164  5.162 55.653  <2e-16 ***
## s(time) 7.753  8.510 33.749  <2e-16 ***
## s(LDL)  1.002  1.005  0.077   0.784
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## R-sq.(adj) =  0.204   Deviance explained = 20.9%
## -REML = 2855.8  Scale est. = 0.27818   n = 3600
```

```r
#visual
plot(best_gam_model, pages = 1)
```




```r
dat2$.pred_gam <- predict(best_gam_model, newdata = dat2)

# Evaluate performance
rmse_gam_dat2 <- yardstick::rmse(dat2, truth = log_antibody, estimate = .pred_gam)
rsq_gam_dat2 <- yardstick::rsq(dat2, truth = log_antibody, estimate = .pred_gam)

print(rmse_gam_dat2)
```

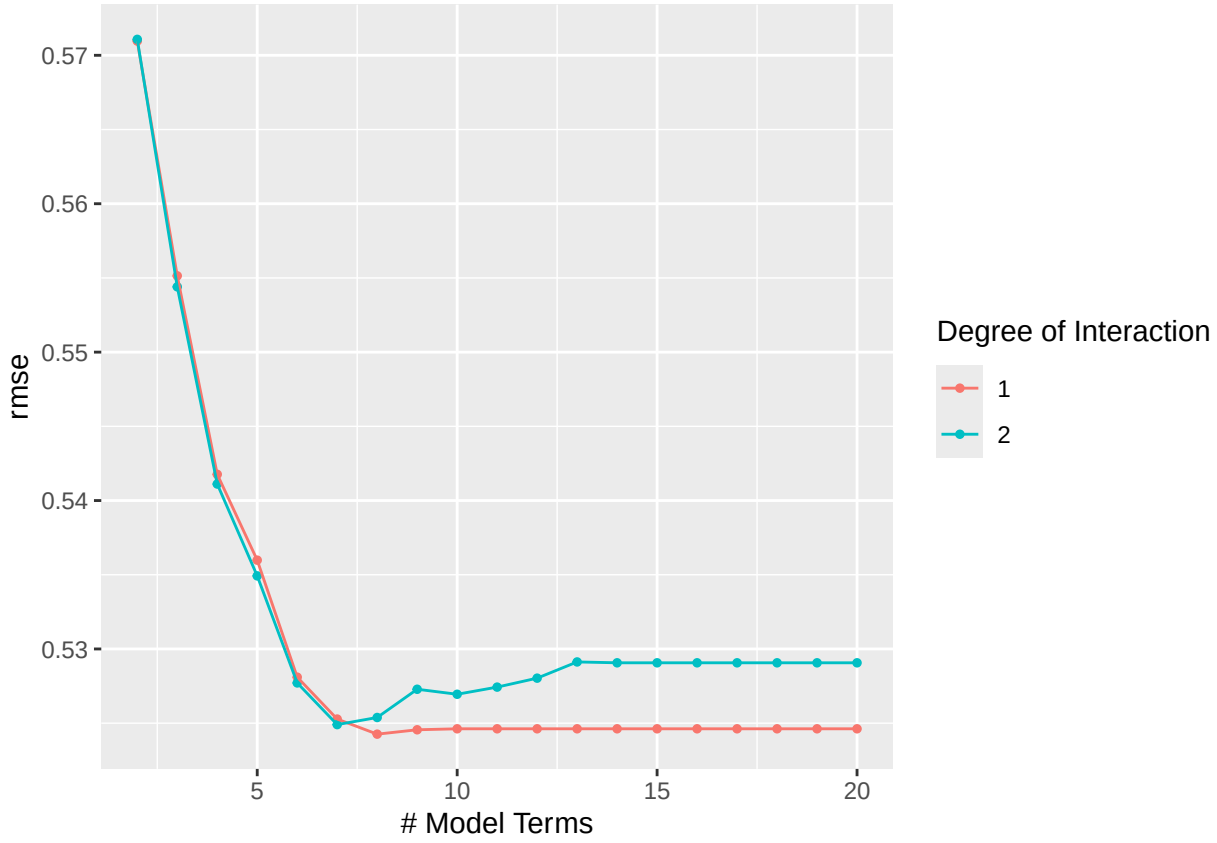
```
## # A tibble: 1 x 3
##   .metric .estimator .estimate
##   <chr>   <chr>          <dbl>
## 1 rmse    standard       0.534
```

```r
print(rsq_gam_dat2)
```

```
## # A tibble: 1 x 3
##   .metric .estimator .estimate
##   <chr>   <chr>          <dbl>
## 1 rsq     standard       0.181
```

MARS MODEL

```
###RESOLVE THIS BEFORE WE SUBMIT###
## I did this in both of my parts --> if you guys are okay with it maybe we can do this in the data prep

training <- training %>% mutate(across(c(race, smoking, gender), as.factor))
validation <- validation %>% mutate(across(c(race, smoking, gender), as.factor))
dat2 <- dat2 %>% mutate(across(c(race, smoking, gender), as.factor))

## Cross-Validation Setup
set.seed(2222)
cv_folds <- vfold_cv(training, v = 10)

## MARS Model Specification
mars_spec <- mars(num_terms = tune(), prod_degree = tune()) %>%
  set_engine("earth") %>%
  set_mode("regression")

## Hyperparameter Grid
mars_grid_set <- parameters(num_terms(range = c(2, 20)), prod_degree(range = c(1, 2)))
mars_grid <- grid_regular(mars_grid_set, levels = c(20, 4))

## setting up the workflow
mars_workflow <- workflow() %>%
  add_model(mars_spec) %>%
  add_formula(log_antibody ~ age + gender + race + smoking +
                bmi + diabetes + hypertension + LDL + time)

## Hyperparameter Tuning
set.seed(2222)
mars_tune <- tune_grid(
  mars_workflow,
  resamples = cv_folds,
  grid = mars_grid
)

# Visualizing the tuning results
autoplot(mars_tune, metric = "rmse")
```



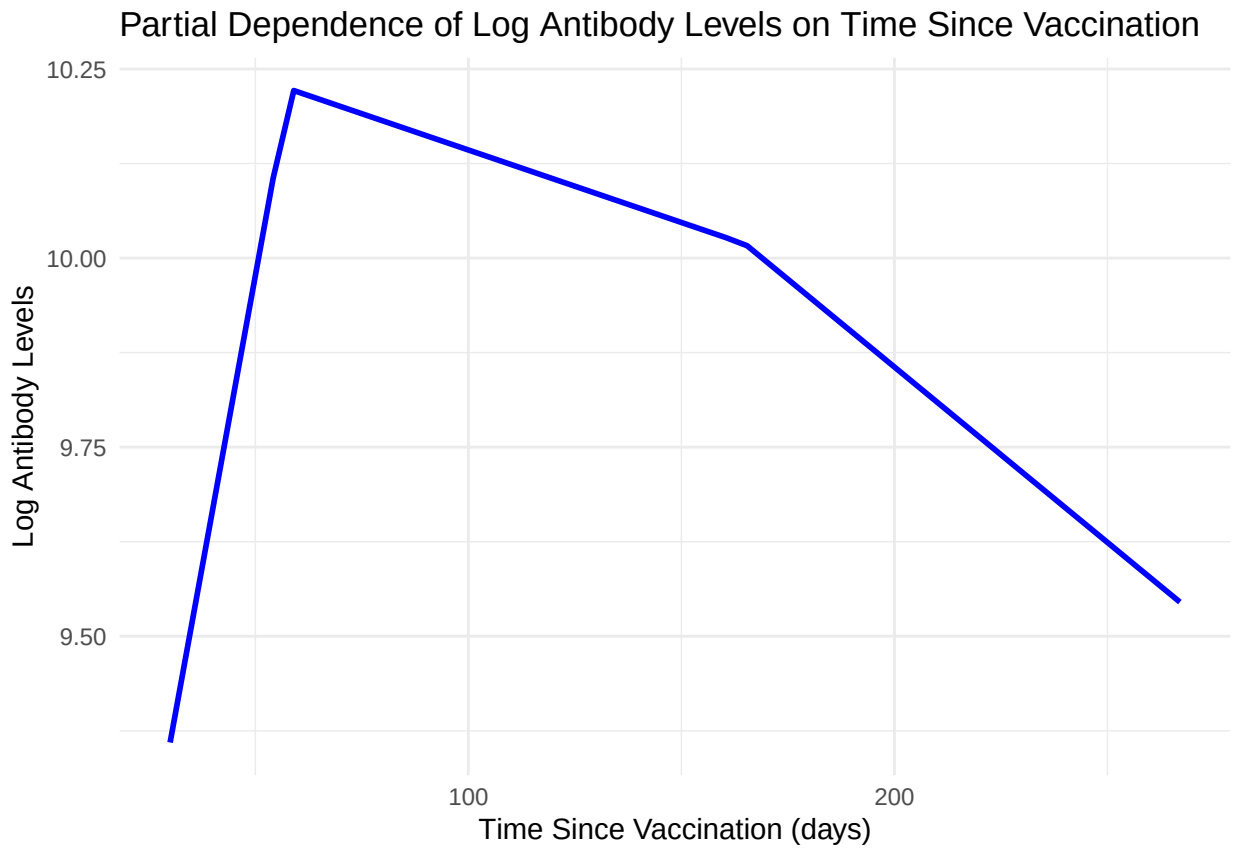

```
# best hyperparameters Based on RMSE
mars_best <- select_best(mars_tune, metric = "rmse")

## Updated model using best tune
final_mars_spec <- mars_spec %>%
  update(num_terms = mars_best$num_terms,
         prod_degree = mars_best$prod_degree)

##Final MARS
mars_fit <- fit(final_mars_spec,
                formula = log_antibody ~ age + gender + race + smoking +
                  bmi + diabetes + hypertension + LDL + time,
                data = training)

## Extracting fitted MARS and Coefficients
mars_model <- extract_fit_engine(mars_fit)
coef(mars_model)
```

```
##  (Intercept)  h(bmi-27.8)   h(time-58)   h(58-time)      gender1    h(70-age)
## 10.288401336 -0.094250784 -0.001917226 -0.030854679 -0.280399107  0.018948596
##     smoking2  h(time-165)
## -0.200881611 -0.002721176
```

```
## Partial Dependence Plot for 'time'
pdp_plot <- partial(mars_fit, pred.var = "time", grid.resolution = 50, train = training)
```

```r
ggplot(pdp_plot, aes(x = time, y = yhat)) +
  geom_line(color = "blue", size = 1) +
  labs(title = "Partial Dependence of Log Antibody Levels on Time Since Vaccination",
       x = "Time Since Vaccination (days)",
       y = "Log Antibody Levels") +
  theme_minimal()
```

```
## Warning: Using ‘size‘ aesthetic for lines was deprecated in ggplot2 3.4.0.
## i Please use ‘linewidth‘ instead.
## This warning is displayed once every 8 hours.
## Call ‘lifecycle::last_lifecycle_warnings()‘ to see where this warning was
## generated.
```




```r
# Testing MARS model with the test data
test.pred = predict(mars_fit, new_data = initial_test)
```

```
## Warning in model.frame.default(terms.without.response, data = data, na.action =
## na.pass, : variable 'gender' is not a factor
```

```
## Error : variable 'gender' was fitted with type "factor" but type "numeric" was supplied
## Continuing anyway, first few rows of modelframe are
##      age gender race smoking  bmi diabetes hypertension LDL time
## 5001  58      0    4       1 27.7        0            0 115  205
## 5002  62      0    1       1 29.4        1            0 118  229
```

```
## 5003  71      0    4       0 24.6        1            1 149  206
## 5004  59      1    1       0 28.0        0            0 119  163
## 5005  69      1    1       0 27.0        1            1 142  240
## 5006  56      0    1       0 26.6        0            0 112  206
```

```r
# Calculating RMSE of the test data
rmse = sqrt(mean((test.pred$.pred - initial_test$log_antibody)^2))
rmse # 0.5276064
```

```
## [1] 0.5276064
```