Build Prediction Model

Minghe Wang

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Exploratory Data Analysis

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

# no missing data
all(is.na(dat1))
```

```
## [1] FALSE
```

```
all(is.na(dat2))
```

```
## [1] FALSE
```

```
ifelse(all(names(dat1) == names(dat2)), "train and test data have same structure", "train and test data
```

```
## [1] "train and test data have same structure"
```

```
str(dat1)
```

```
## 'data.frame':    5000 obs. of  14 variables:
##  $ id          : int  1 2 3 4 5 6 7 8 9 10 ...
##  $ age         : num  50 71 58 63 56 59 67 62 60 64 ...
##  $ gender      : int  0 1 1 0 1 1 0 1 0 1 ...
##  $ race        : Factor w/ 4 levels "1","2","3","4": 1 1 1 1 1 3 4 1 4 1 ...
##  $ smoking     : Factor w/ 3 levels "0","1","2": 1 1 2 1 1 1 1 1 1 1 ...
##  $ height      : num  176 176 169 167 163 ...
##  $ weight      : num  68.3 69.6 76.9 90 83.9 86.8 91.4 87.7 85.7 76.6 ...
##  $ bmi         : num  22 22.6 27 32.1 31.7 30.8 29.7 28.1 29 31.5 ...
##  $ diabetes    : int  0 0 0 0 0 0 0 0 0 0 ...
##  $ hypertension: num  0 1 0 1 0 1 1 0 0 1 ...
##  $ SBP         : num  130 149 127 138 123 132 133 130 129 134 ...
##  $ LDL         : num  82 129 101 93 97 108 89 96 120 135 ...
##  $ time        : num  76 82 168 105 193 143 63 78 61 88 ...
##  $ log_antibody: num  10.65 9.89 10.9 9.91 9.56 ...
```

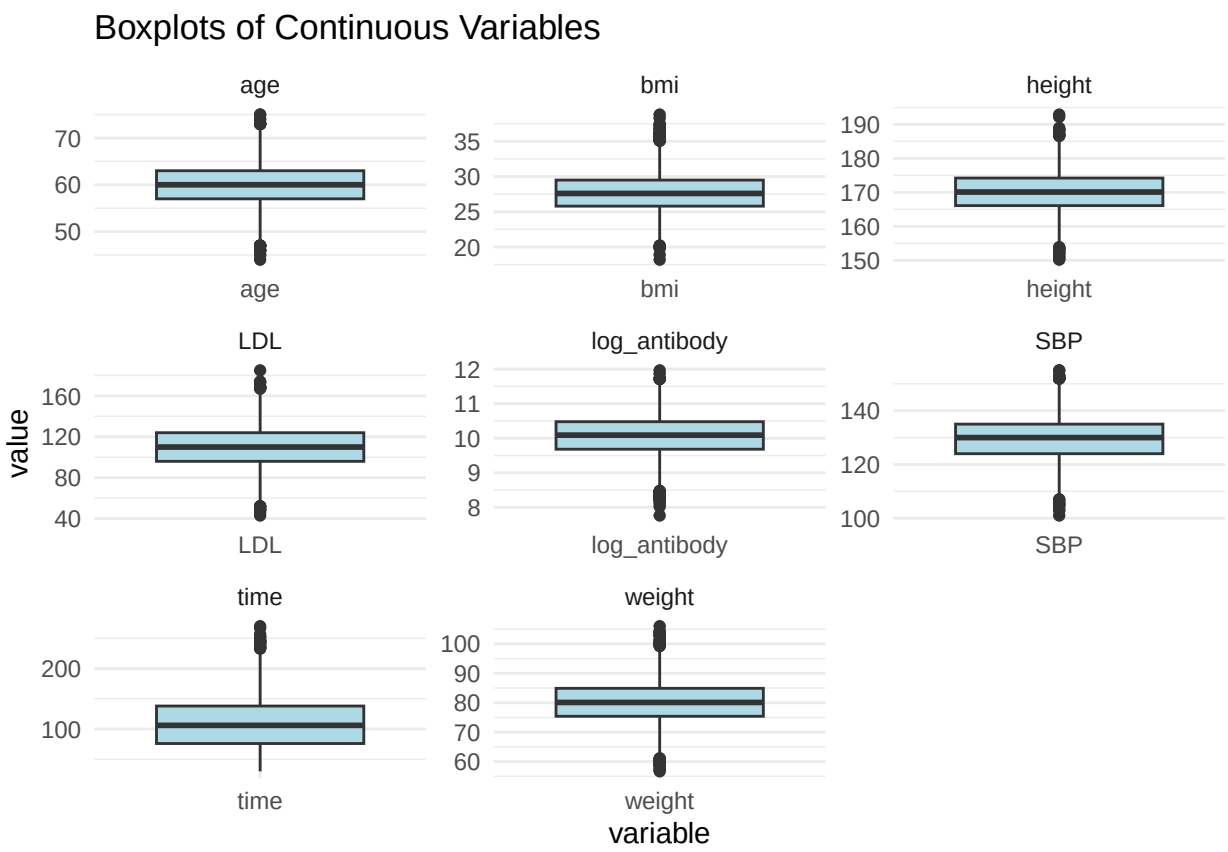
Univariate analysis(continous & categorical)

```
continuous_var <- dat1 %>%
  select(age, height, weight, bmi, SBP, LDL, time, log_antibody)

categorical_var <- dat1 %>%
  select(gender, race, smoking, diabetes, hypertension) %>%
  mutate(
```

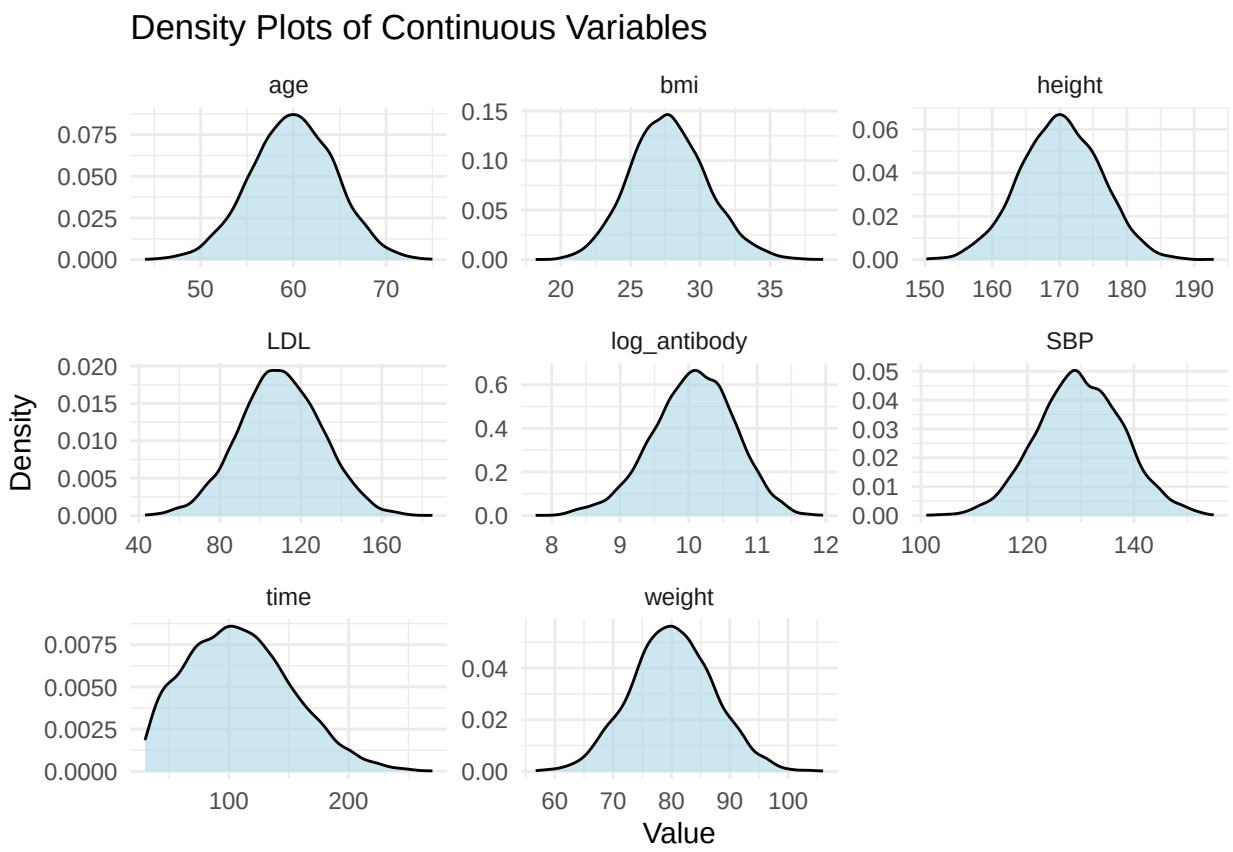
```
    # Convert binary variables to factors with labels
    gender = factor(gender, levels = c(0, 1), labels = c("Female", "Male")),
    diabetes = factor(diabetes, levels = c(0, 1), labels = c("No", "Yes")),
    hypertension = factor(hypertension, levels = c(0, 1), labels = c("No", "Yes"))
  )

# Continuous:
summary(continuous_var)
```

```
##       age             height          weight            bmi
##  Min.   :44.00   Min.   :150.2   Min.   : 56.70   Min.   :18.20
##  1st Qu.:57.00   1st Qu.:166.1   1st Qu.: 75.40   1st Qu.:25.80
##  Median :60.00   Median :170.1   Median : 80.10   Median :27.60
##  Mean   :59.97   Mean   :170.1   Mean   : 80.11   Mean   :27.74
##  3rd Qu.:63.00   3rd Qu.:174.2   3rd Qu.: 84.90   3rd Qu.:29.50
##  Max.   :75.00   Max.   :192.9   Max.   :106.00   Max.   :38.80
##       SBP              LDL              time        log_antibody
##  Min.   :101.0   Min.   : 43.0   Min.   : 30.0   Min.   : 7.765
##  1st Qu.:124.0   1st Qu.: 96.0   1st Qu.: 76.0   1st Qu.: 9.682
##  Median :130.0   Median :110.0   Median :106.0   Median :10.089
##  Mean   :129.9   Mean   :109.9   Mean   :108.9   Mean   :10.064
##  3rd Qu.:135.0   3rd Qu.:124.0   3rd Qu.:138.0   3rd Qu.:10.478
##  Max.   :155.0   Max.   :185.0   Max.   :270.0   Max.   :11.961
```

```
# Boxplots
continuous_var_long <- continuous_var %>%
  tidyr::pivot_longer(cols = everything(), names_to = "variable", values_to = "value")

ggplot(continuous_var_long, aes(x = variable, y = value)) +
  geom_boxplot(fill = "lightblue") +
  facet_wrap(~variable, scales = "free", ncol = 3) +
  theme_minimal() +
  labs(title = "Boxplots of Continuous Variables")
```



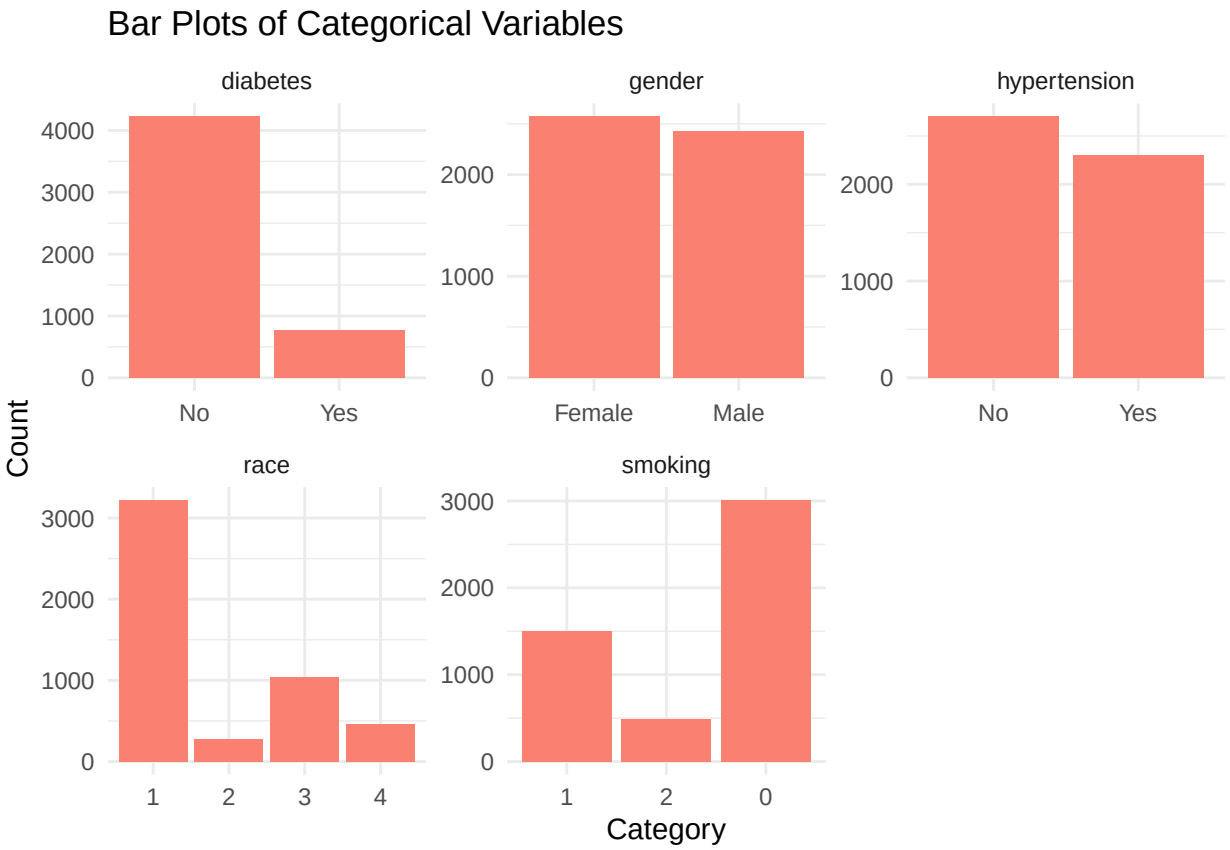

```
ggplot(continuous_var_long, aes(x = value)) +
  geom_density(fill = "lightblue", alpha = 0.6) +
  facet_wrap(~variable, scales = "free", ncol = 3) +
  theme_minimal() +
  labs(title = "Density Plots of Continuous Variables", x = "Value", y = "Density")
```




```
# Categorical:
summary(continuous_var)
```

```
##       age             height          weight           bmi
##  Min.   :44.00   Min.   :150.2   Min.   : 56.70   Min.   :18.20
##  1st Qu.:57.00   1st Qu.:166.1   1st Qu.: 75.40   1st Qu.:25.80
##  Median :60.00   Median :170.1   Median : 80.10   Median :27.60
##  Mean   :59.97   Mean   :170.1   Mean   : 80.11   Mean   :27.74
##  3rd Qu.:63.00   3rd Qu.:174.2   3rd Qu.: 84.90   3rd Qu.:29.50
##  Max.   :75.00   Max.   :192.9   Max.   :106.00   Max.   :38.80
##       SBP              LDL              time        log_antibody
##  Min.   :101.0   Min.   : 43.0   Min.   : 30.0   Min.   : 7.765
##  1st Qu.:124.0   1st Qu.: 96.0   1st Qu.: 76.0   1st Qu.: 9.682
##  Median :130.0   Median :110.0   Median :106.0   Median :10.089
##  Mean   :129.9   Mean   :109.9   Mean   :108.9   Mean   :10.064
##  3rd Qu.:135.0   3rd Qu.:124.0   3rd Qu.:138.0   3rd Qu.:10.478
##  Max.   :155.0   Max.   :185.0   Max.   :270.0   Max.   :11.961
```

```
# bar plots
categorical_var_long <- categorical_var %>%
  tidyr::pivot_longer(cols = everything(), names_to = "variable", values_to = "value")

ggplot(categorical_var_long, aes(x = value)) +
  geom_bar(fill = "salmon") +
  facet_wrap(~variable, scales = "free", ncol = 3) +
  theme_minimal() +
  labs(title = "Bar Plots of Categorical Variables", x = "Category", y = "Count")
```



According to the box plot for continuous variables:

- `Age`, `BMI`, and `SBP` appear reasonably normally distributed, with expected ranges for an adult population; `LDL` cholesterol and `time` since vaccination show a wider range, right-skewness and some outliers, which may impact linear models.
- `log_antibody` (response) appears fairly symmetrical, which supports its use as a continuous response in linear or GAM models.
- Correlations and non-linear trends should be assessed in the next step to guide model form.

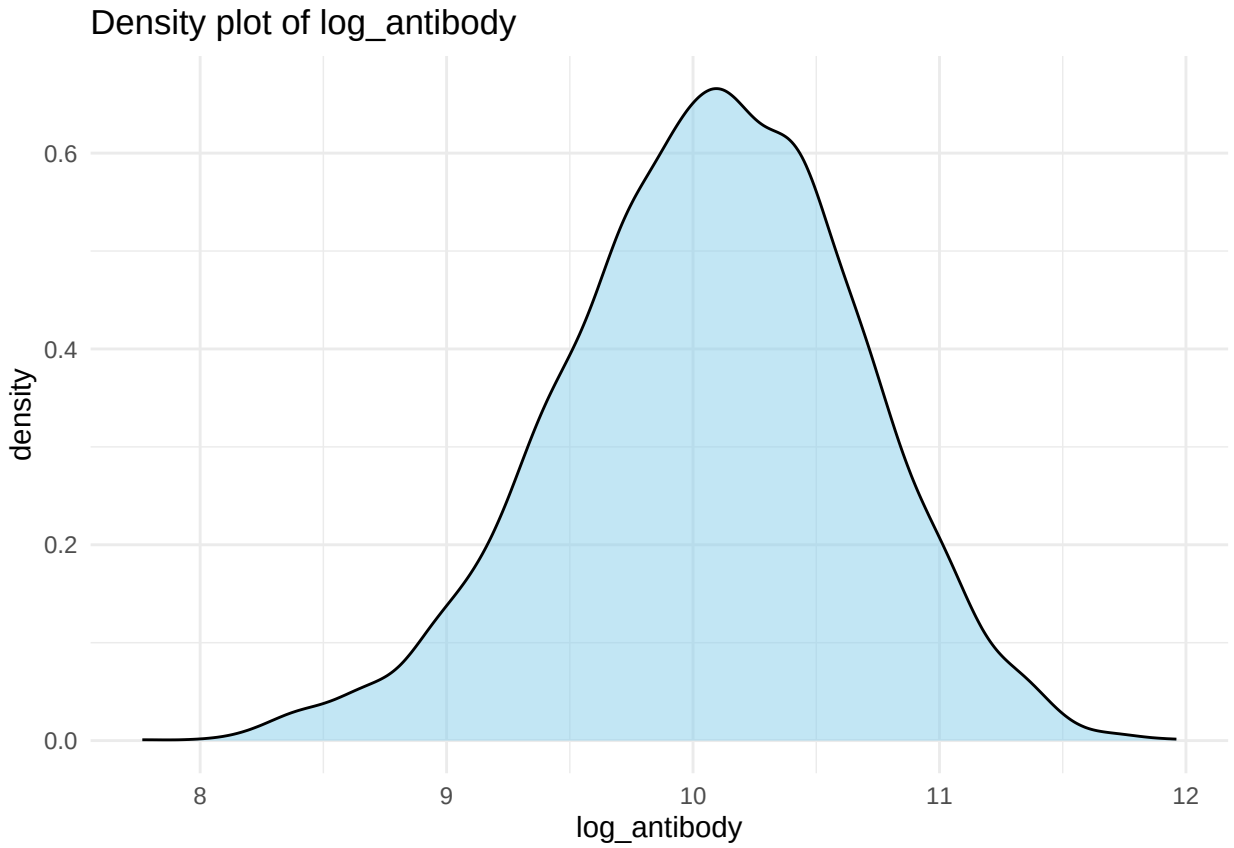
According to the bar plot for categorical variables:

- `Gender` is fairly balanced between Female and Male;
- `Race` is skewed, with a majority of participants identifying as White (Category 1). Other racial/ethnic groups are underrepresented;
- `Smoking` status shows that the majority are never smokers (Category 0), with fewer current and former smokers;
- A large proportion of participants do not have `diabetes`;
- A moderate split exists for `hypertension`, which may contribute meaningfully to clinical outcome variation
- Demographically, the population is balanced by gender but skewed by race and smoking status.

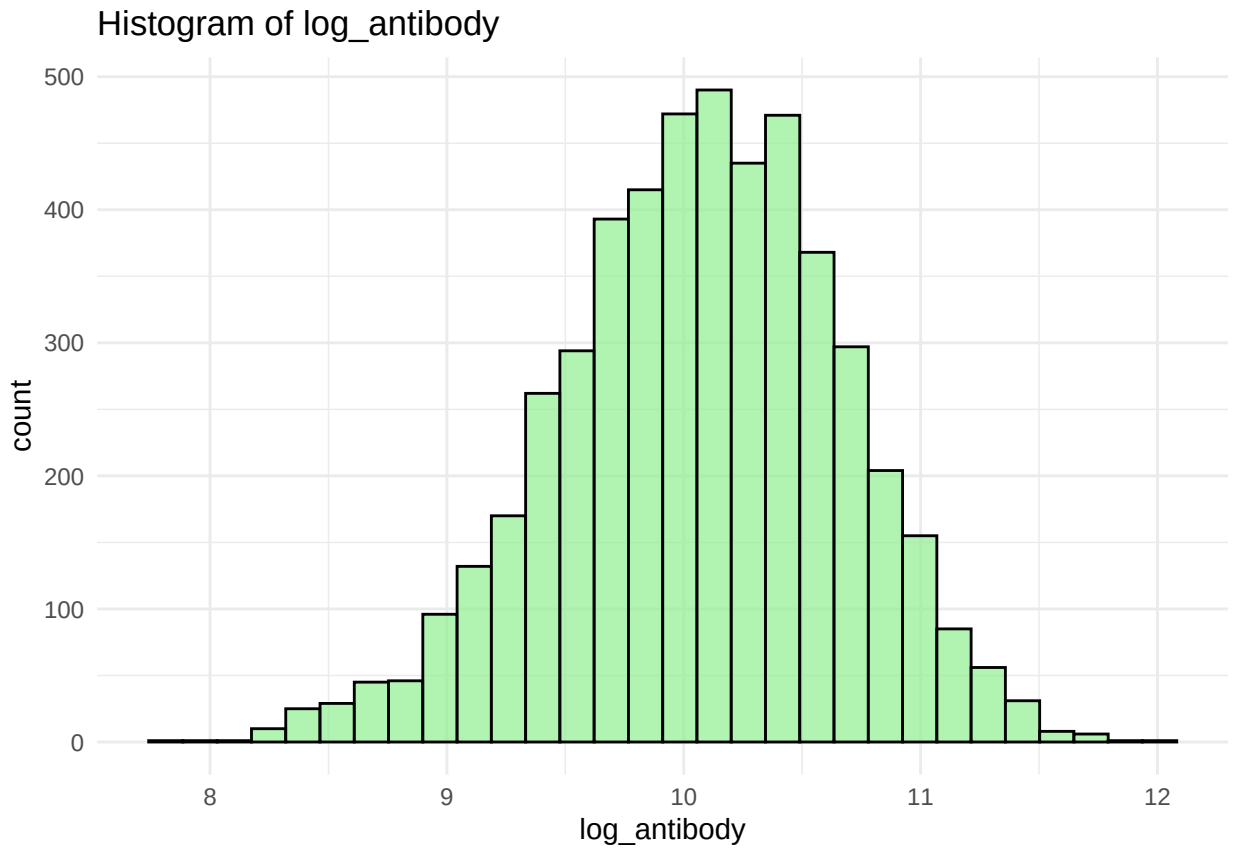
Overall, we believe the response variable `log_antibody` is well-behaved, and further correlation analysis(eg. bivariate) is needed.

```
ggplot(dat1, aes(x = log_antibody)) +
  geom_density(fill = "skyblue", alpha = 0.5) +
```

```
  ggtitle("Density plot of log_antibody") +
  xlab("log_antibody") +
  theme_minimal()
```

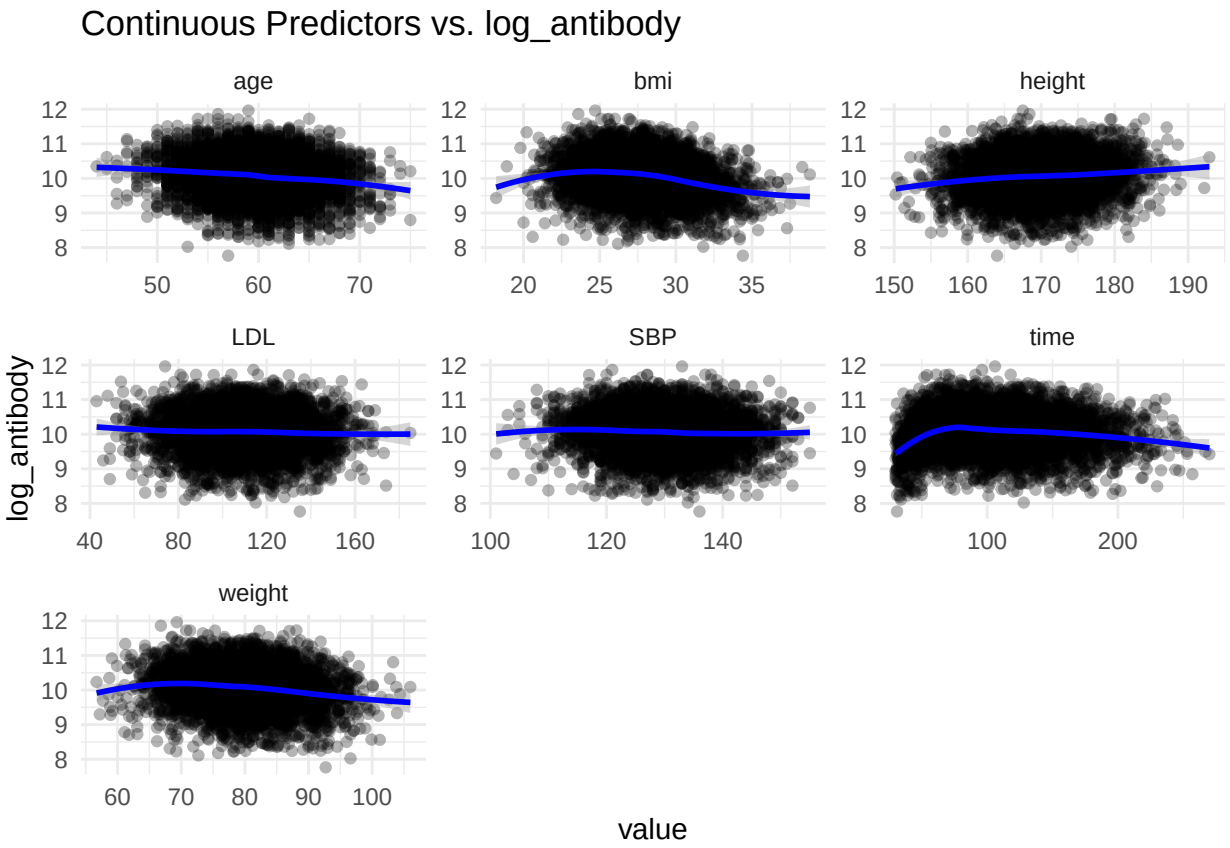



```
ggplot(dat1, aes(x = log_antibody)) +
  geom_histogram(bins = 30, fill = "lightgreen", color = "black", alpha = 0.7) +
  ggtitle("Histogram of log_antibody") +
  xlab("log_antibody") +
  theme_minimal()
```




```
# continous variable
continuous_var_long <- dat1 %>%
  select(age, height, weight, bmi, SBP, LDL, time, log_antibody) %>%
  tidyr::pivot_longer(cols = -log_antibody, names_to = "variable", values_to = "value")

# Scatterplots with smoothing lines
ggplot(continuous_var_long, aes(x = value, y = log_antibody)) +
  geom_point(alpha = 0.3) +
  geom_smooth(method = "loess", color = "blue") +
  facet_wrap(~variable, scales = "free", ncol = 3) +
  theme_minimal() +
  labs(title = "Continuous Predictors vs. log_antibody")
```

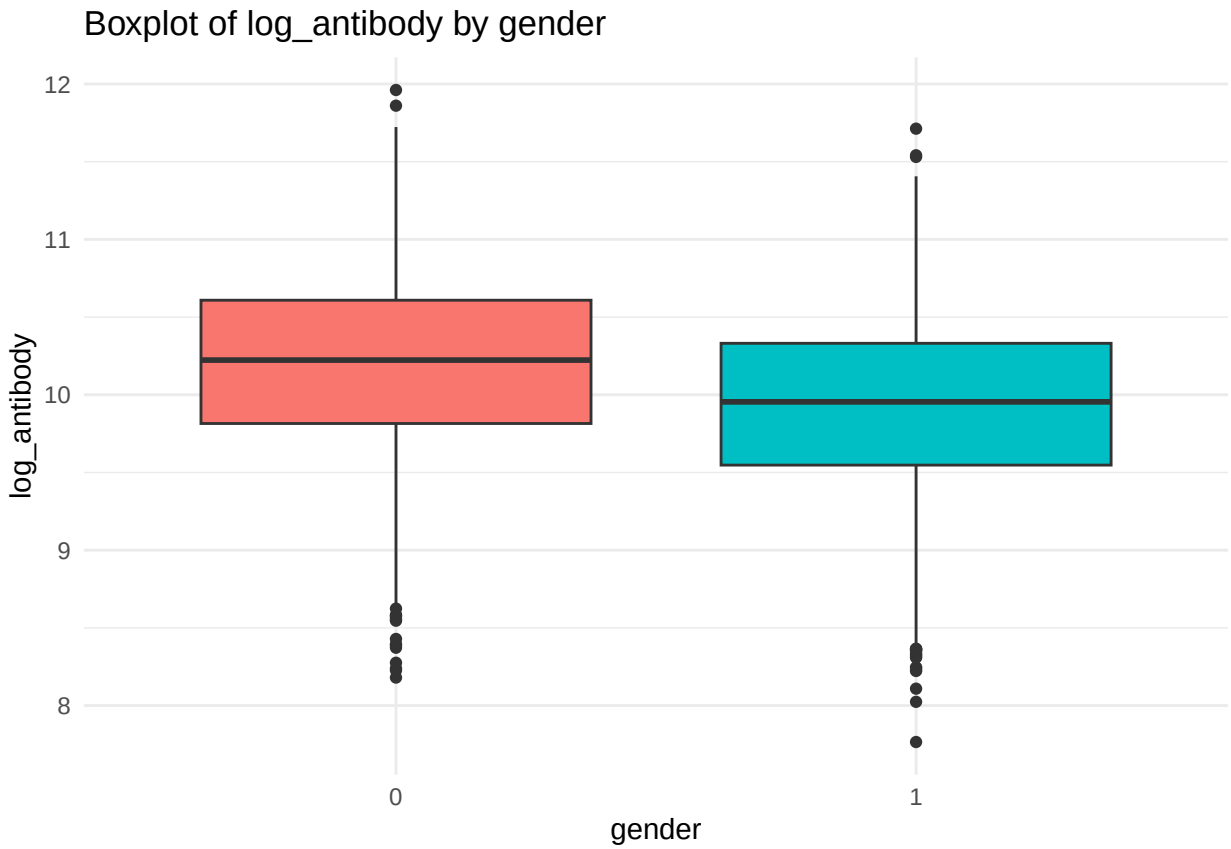
```
## `geom_smooth()` using formula = 'y ~ x'
```

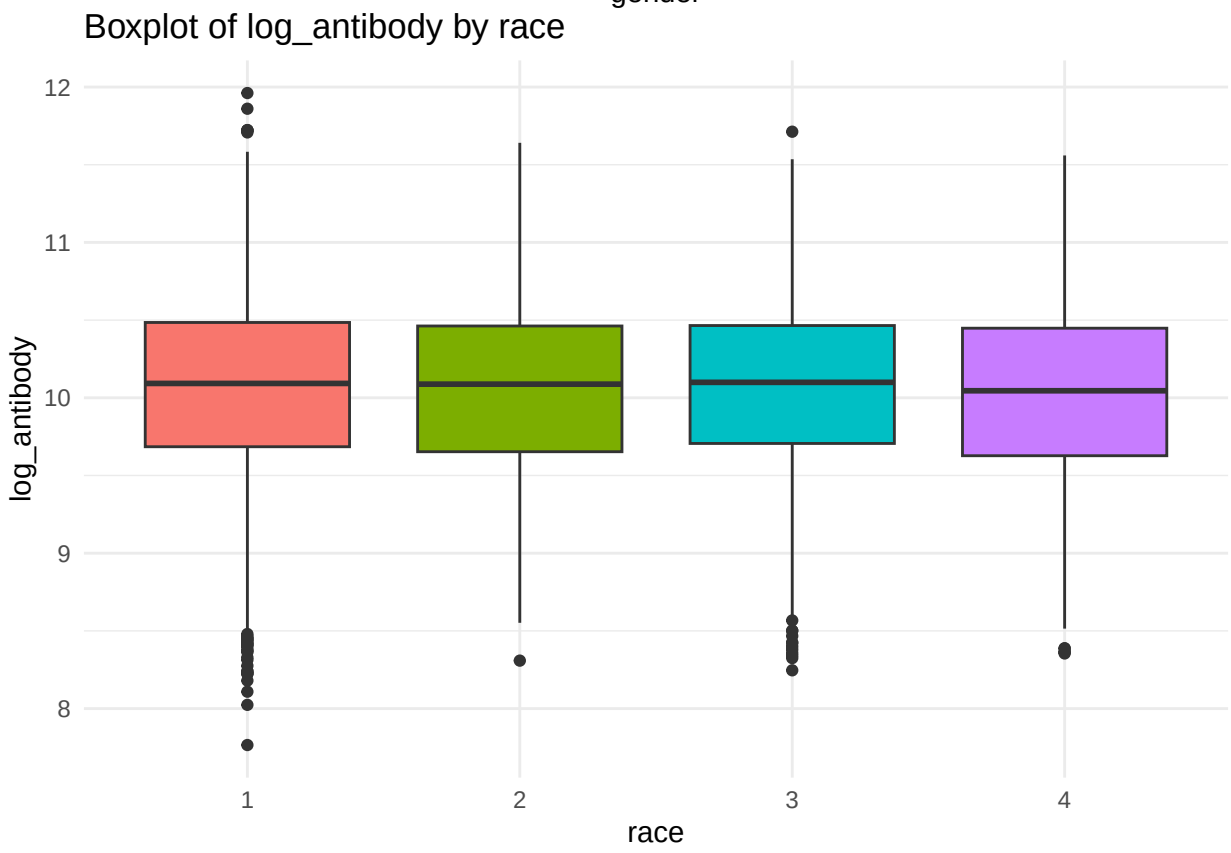


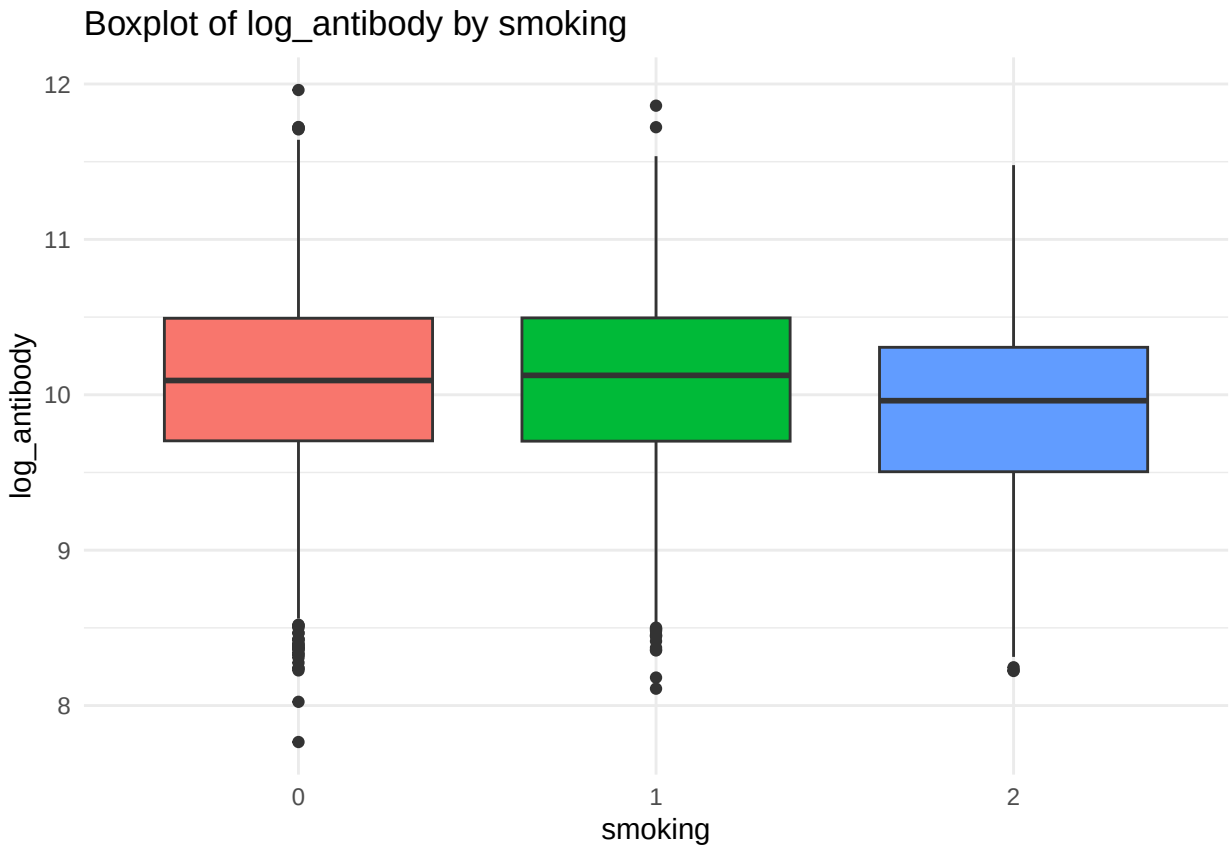
Usin LOESS method, we observe linearity between predictors and the response. The plot shows that `bmi`, `time`, and `weight` has clear non linear trend against resopnse `log_antibody`, indicating potential need to use GAM or non linear model.

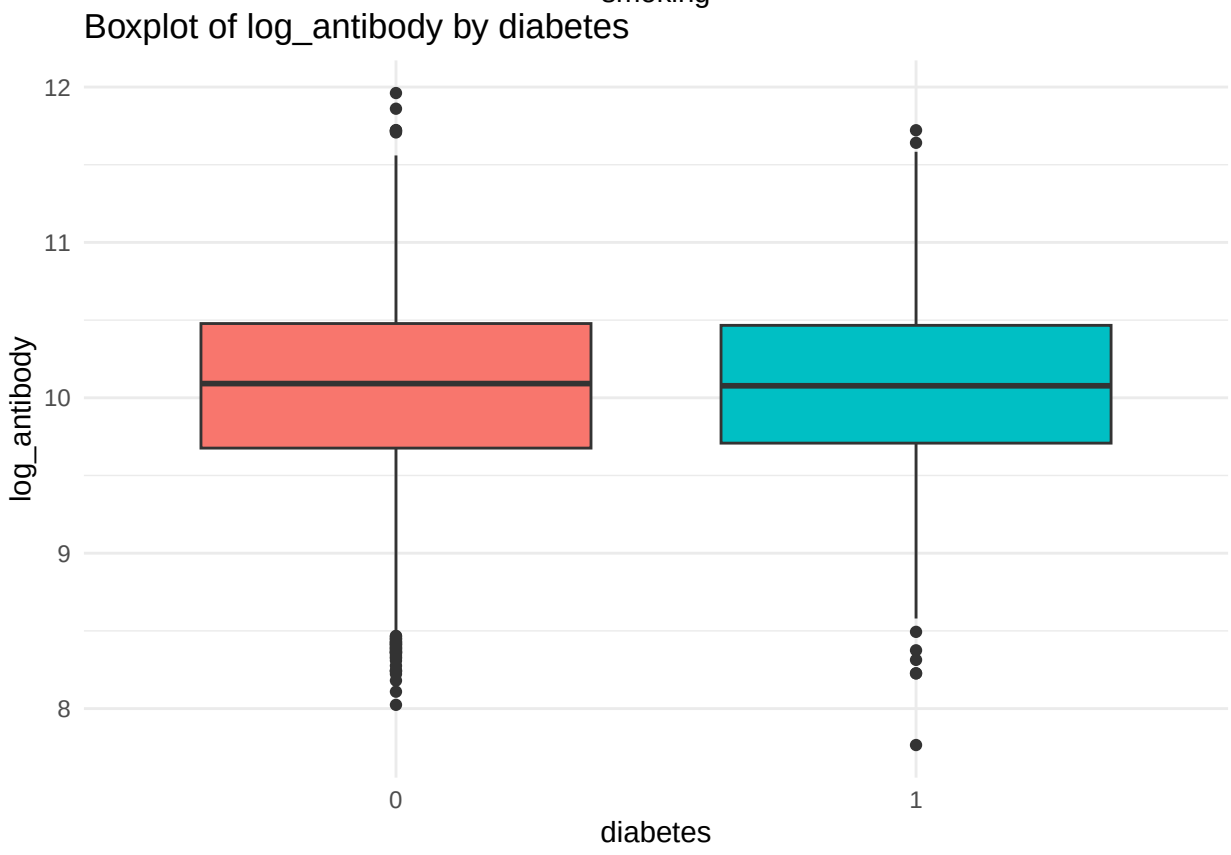
```
# categorical data
categorical_vars <- c("gender", "race", "smoking", "diabetes", "hypertension")
dat1[categorical_vars] <- lapply(dat1[categorical_vars], factor)

for (var in categorical_vars) {
  p <- ggplot(dat1, aes_string(x = var, y = "log_antibody", fill = var)) +
    geom_boxplot() +
    ggtitle(paste("Boxplot of log_antibody by", var)) +
    theme_minimal() +
    theme(legend.position = "none")
  print(p)
}
```

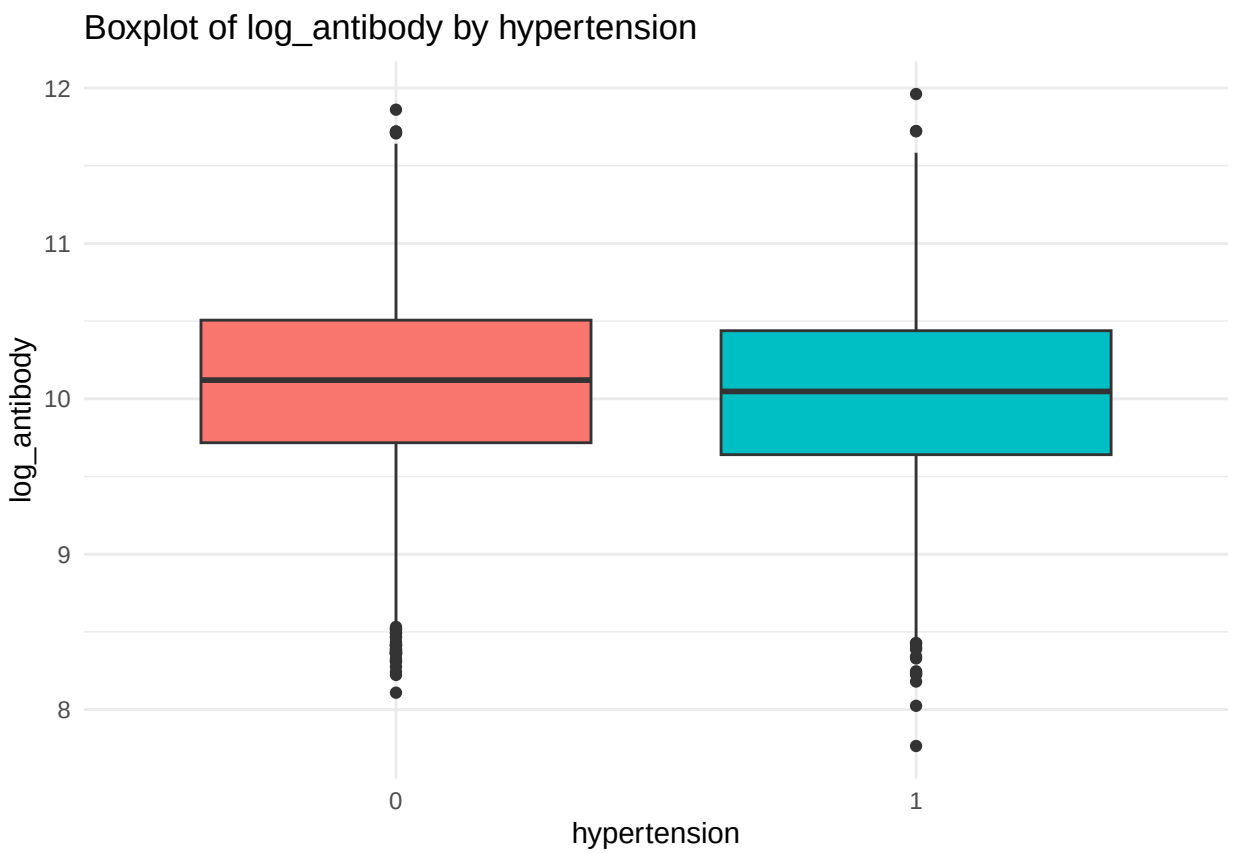
```
## Warning: `aes_string()` was deprecated in ggplot2 3.0.0.
## i Please use tidy evaluation idioms with `aes()`.
## i See also `vignette("ggplot2-in-packages")` for more information.
## This warning is displayed once every 8 hours.
## Call `lifecycle::last_lifecycle_warnings()` to see where this warning was
## generated.
```


Boxplot of log_antibody by gender
log_antibody
12
11
10
9
8
0
1
gender


Boxplot of log_antibody by race
log_antibody
12
11
10
9
8
1
2
3
4
race


Boxplot of log_antibody by smoking
log_antibody
12
11
10
9
8
0
1
2
smoking


Boxplot of log_antibody by diabetes
log_antibody
12
11
10
9
8
0
1
diabetes

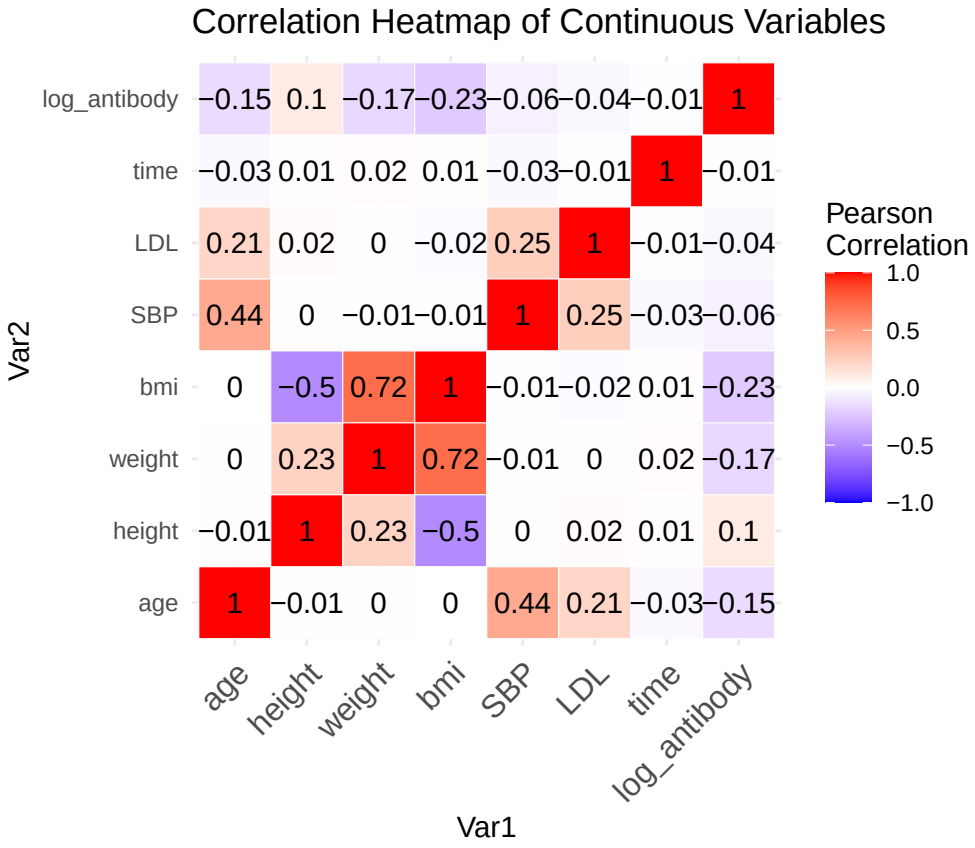



```
continous_vars <- c("age", "height", "weight", "bmi", "SBP", "LDL", "time", "log_antibody")
dat_cont <- dat1[ , continous_vars]

# coefficient matrix
cor_matrix <- cor(dat_cont, use = "complete.obs", method = "pearson")

print(round(cor_matrix, 2))
```

```
##                age height weight   bmi   SBP   LDL  time log_antibody
## age           1.00  -0.01   0.00  0.00  0.44  0.21 -0.03        -0.15
## height       -0.01   1.00   0.23 -0.50  0.00  0.02  0.01         0.10
## weight        0.00   0.23   1.00  0.72 -0.01  0.00  0.02        -0.17
## bmi           0.00  -0.50   0.72  1.00 -0.01 -0.02  0.01        -0.23
## SBP           0.44   0.00  -0.01 -0.01  1.00  0.25 -0.03        -0.06
## LDL           0.21   0.02   0.00 -0.02  0.25  1.00 -0.01        -0.04
## time         -0.03   0.01   0.02  0.01 -0.03 -0.01  1.00        -0.01
## log_antibody -0.15   0.10  -0.17 -0.23 -0.06 -0.04 -0.01         1.00
```

```
cor_melt <- melt(cor_matrix)

ggplot(cor_melt, aes(Var1, Var2, fill = value)) +
  geom_tile(color = "white") +
  scale_fill_gradient2(low = "blue", high = "red", mid = "white",
                       midpoint = 0, limit = c(-1, 1), space = "Lab",
                       name = "Pearson\nCorrelation") +
  geom_text(aes(label = round(value, 2)), color = "black", size = 4) +
  theme_minimal() +
  theme(axis.text.x = element_text(angle = 45, vjust = 1,
```

```
                                    size = 12, hjust = 1)) +
  coord_fixed() +
  ggtitle("Correlation Heatmap of Continuous Variables")
```



Model Training

```
library(caret)
```

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

```
##
## Attaching package: 'caret'
```

```
## The following object is masked from 'package:purrr':
##
##     lift
```

```
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")'.
```

```r
library(pdp)
```

```
##
## Attaching package: 'pdp'
```

```
## The following object is masked from 'package:purrr':
##
##     partial
```

```r
library(earth)
```

```
## Loading required package: Formula
```

```
## Loading required package: plotmo
```

```
## Loading required package: plotrix
```

```r
library(tidyverse)
library(ggplot2)
```

```r
ctrl1 <- trainControl(method = "cv", number = 5)

train_y <- dat1$log_antibody
train_x <- dat1[, -which(names(dat1) == "log_antibody")]


set.seed(2)
gam.fit <- train(train_x, train_y,
                 method = "gam",
                 # tuneGrid = data.frame(method = "GCV.Cp", select = c(TRUE,FALSE)),
                 trControl = ctrl1)

gam.fit$bestTune
```

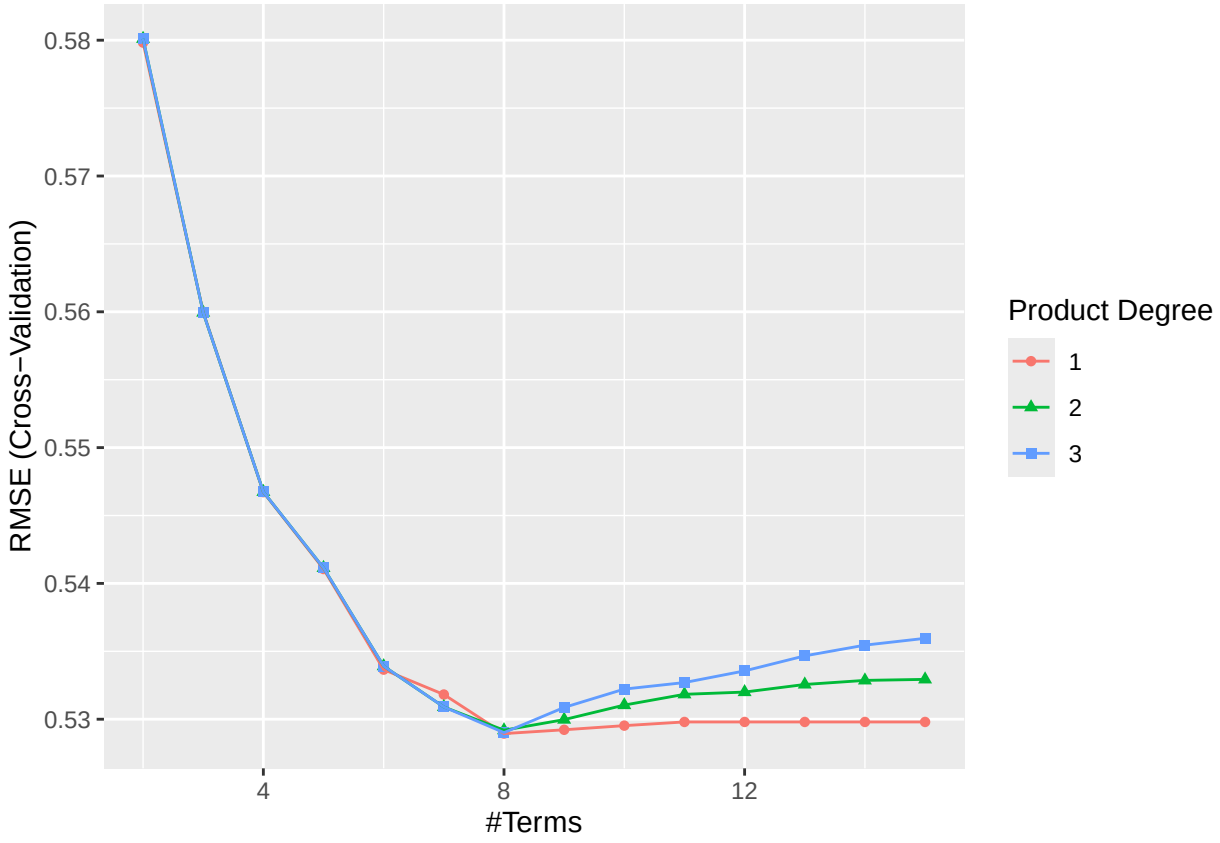
```
##   select method
## 2   TRUE GCV.Cp
```

```r
gam.fit$finalModel
```

```
##
## Family: gaussian
## Link function: identity
##
## Formula:
## .outcome ~ gender + diabetes + hypertension + smoking + race +
##     s(age) + s(SBP) + s(LDL) + s(bmi) + s(time) + s(height) +
##     s(weight) + s(id)
##
## Estimated degrees of freedom:
## 0.991 0.000 0.000 4.661 7.846 1.216 0.000
## 0.000  total = 23.71
##
## GCV score: 0.2786709
```

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

set.seed(2)
```

```
mars.fit <- train(train_x, train_y,
                  method = "earth",
                  tuneGrid = mars_grid,
                  trControl = ctrl1)

ggplot(mars.fit)
```



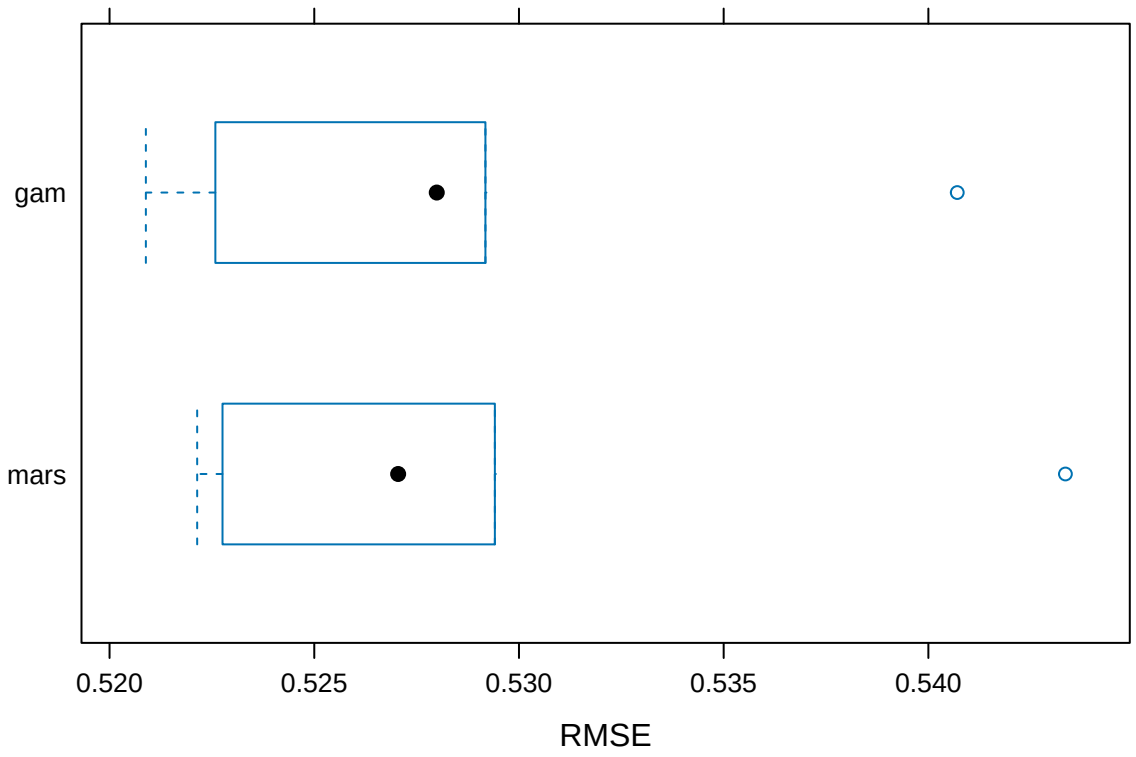

```
mars.fit$bestTune
```

```
##   nprune degree
## 7      8      1
```

```
coef(mars.fit$finalModel)
```

```
##  (Intercept)  h(27.8-bmi)   h(time-57)   h(57-time)      gender1    h(age-59)
## 10.883001065 -0.062038886 -0.002248235 -0.033590729 -0.296365754 -0.028816310
##     smoking2  h(bmi-23.7)
## -0.203269139 -0.084496829
```

```
bwplot(resamples(list(mars = mars.fit,
                      gam = gam.fit)),
                metric = "RMSE")
```


gam
mars
0.520
0.525
0.530
0.535
0.540
RMSE