P8106 Data Science II Homework 2: Predicting Out-of-State Tuition Costs

Sarah Forrest - sef2183

3/12/2023

Contents

Data

In this exercise, we build nonlinear models using the “College” data. The dataset contains statistics for 565 US Colleges from a previous issue of US News and World Report. The response variable is the out-of-state tuition (Outstate).

```
# read in test data
College = read.csv("data/College.csv")
```

Partition the dataset into two parts: training data (80%) and test data (20%).

```
set.seed(1)

# specify rows of training data (80% of the dataset)
trRows <- createDataPartition(College$Outstate,
                              p = .8,
                              list = F)

# training data
College_train <- College[trRows, ]
## matrix of predictors
x <- model.matrix(Outstate~.,College)[trRows,-1]
## vector of response
y <- College$Outstate[trRows]

# test data
College_test <- College[-trRows, ]
## matrix of predictors
x2 <- model.matrix(Outstate~.,College)[-trRows,-1]
## vector of response
y2 <- College$Outstate[-trRows]
```

(a) Fit smoothing spline models using the training data set and perc.alumni as the only predictor of Outstate

For a range of degrees of freedom (df):

```
set.seed(1)

# fit smoothing spline model with df = 5
fit.ss_df5 <- smooth.spline(College_train$perc.alumni, College_train$Outstate, df = 5)

# fit smoothing spline model with df = 2
fit.ss_df2 <- smooth.spline(College_train$perc.alumni, College_train$Outstate, df = 2)

# fit smoothing spline model with df = 8
fit.ss_df8 <- smooth.spline(College_train$perc.alumni, College_train$Outstate, df = 8)
```

For the degree of freedom obtained by generalized cross-validation:

```
set.seed(1)

# fit smoothing spline model with df obtained by generalized cross-validation
fit.ss <- smooth.spline(College_train$perc.alumni, College_train$Outstate)

# retrieve df obtained by generalized cross-validation
fit.ss$df
```

```
## [1] 3.779231
```

The degree of freedom obtained by generalized cross-validation is 3.779231.

```
set.seed(1)

# Note that the range of perc.alumni is [2,64], and this is only for
# illustrating fitted curve beyond the boundary knots
perc.alumni.grid <- seq(from = -8, to = 74, by = 1)

# df = 5
pred.ss_df5 <- predict(fit.ss_df5,
                   x = perc.alumni.grid)

pred.ss.df_5 <- data.frame(pred = pred.ss_df5$y,
                         perc.alumni = perc.alumni.grid)

# df = 2
pred.ss_df2 <- predict(fit.ss_df2,
                   x = perc.alumni.grid)

pred.ss.df_2 <- data.frame(pred = pred.ss_df2$y,
                         perc.alumni = perc.alumni.grid)

# df = 8
pred.ss_df8 <- predict(fit.ss_df8,
                   x = perc.alumni.grid)

pred.ss.df_8 <- data.frame(pred = pred.ss_df8$y,
                         perc.alumni = perc.alumni.grid)

# df obtained by generalized cross-validation
pred.ss <- predict(fit.ss,
                   x = perc.alumni.grid)

pred.ss.df <- data.frame(pred = pred.ss$y,
                         perc.alumni = perc.alumni.grid)
```

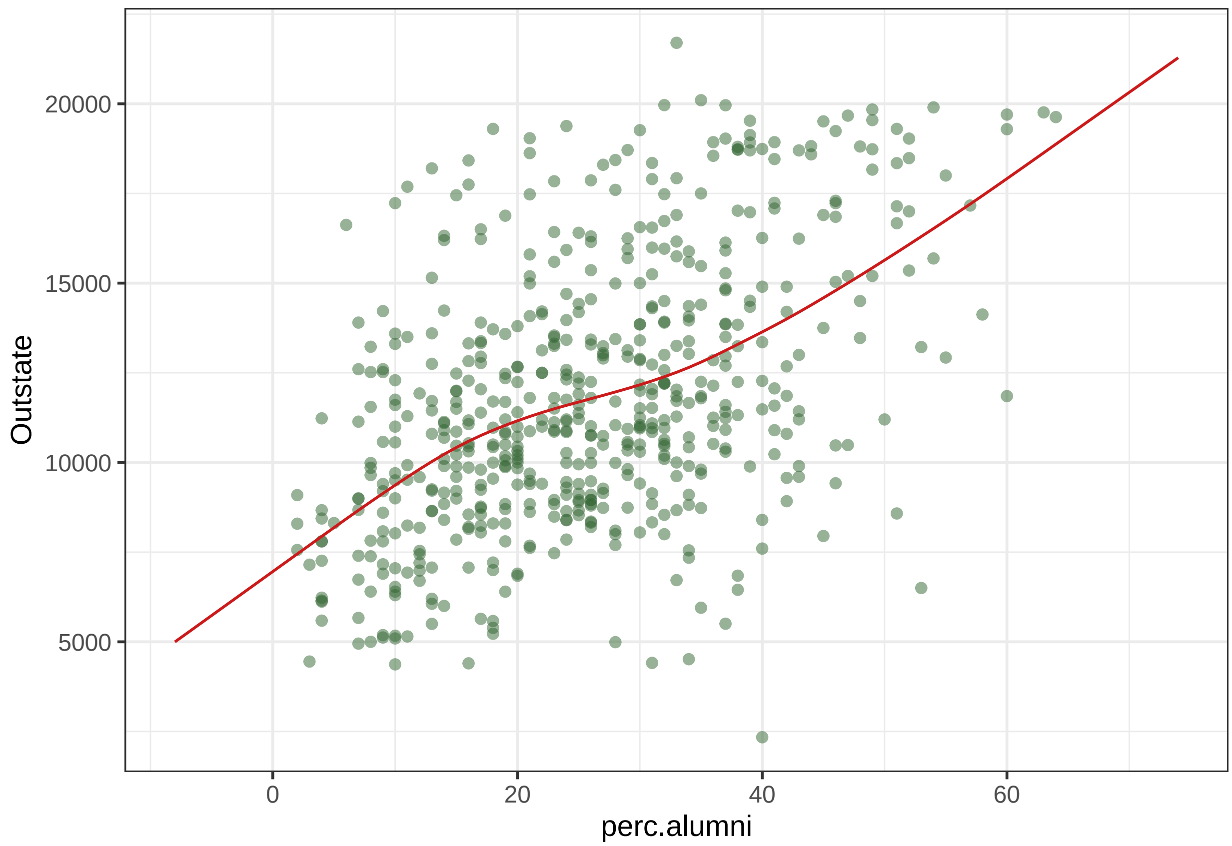
Plot of the resulting fits

```
# create scatter plot object 'p' of the data points
# perc.alumni on the x-axis and Outstate on the y-axis
```

```
p <- ggplot(data = College, aes(x = perc.alumni, y = Outstate)) +
  geom_point(color = rgb(.2, .4, .2, .5))
```

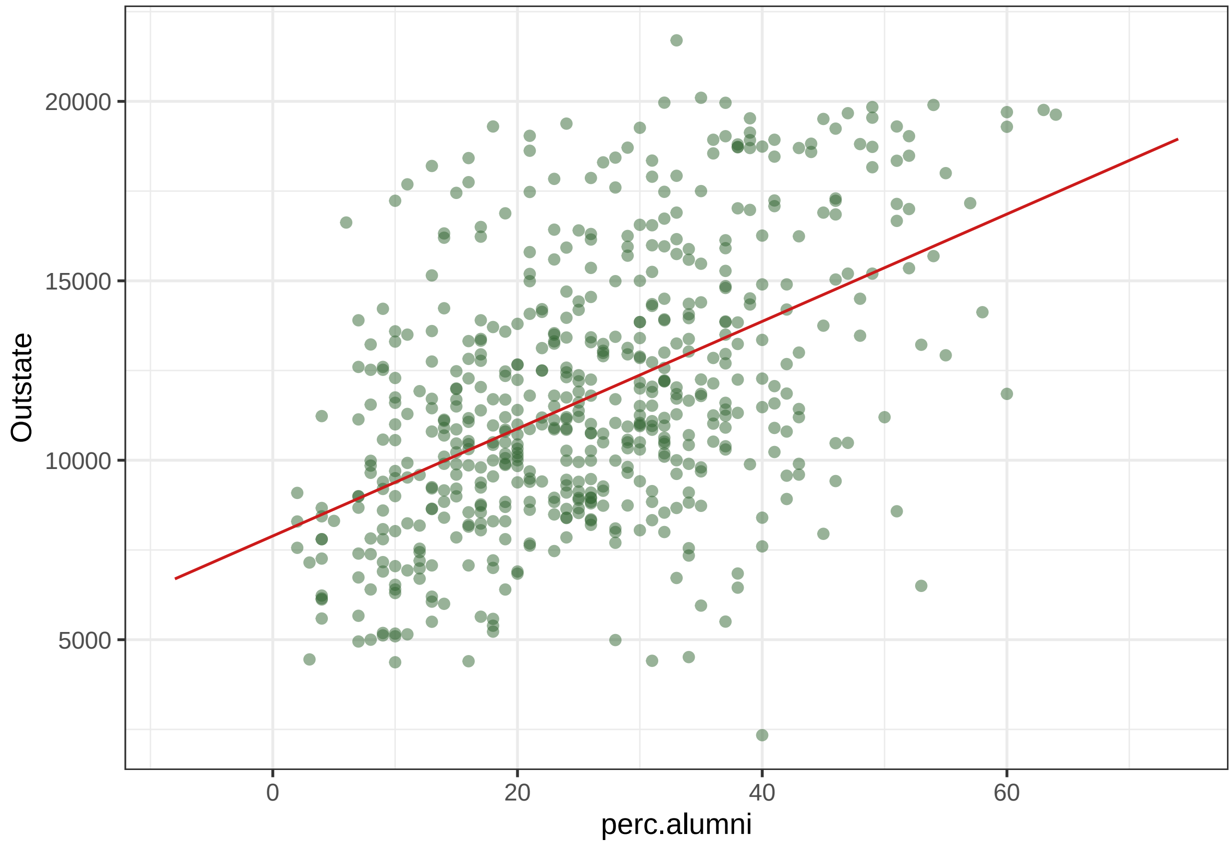
Plot for df = 5

```
p +
  geom_line(aes(x = perc.alumni, y = pred), data = pred.ss.df_5,
            color = rgb(.8, .1, .1, 1)) + theme_bw()
```



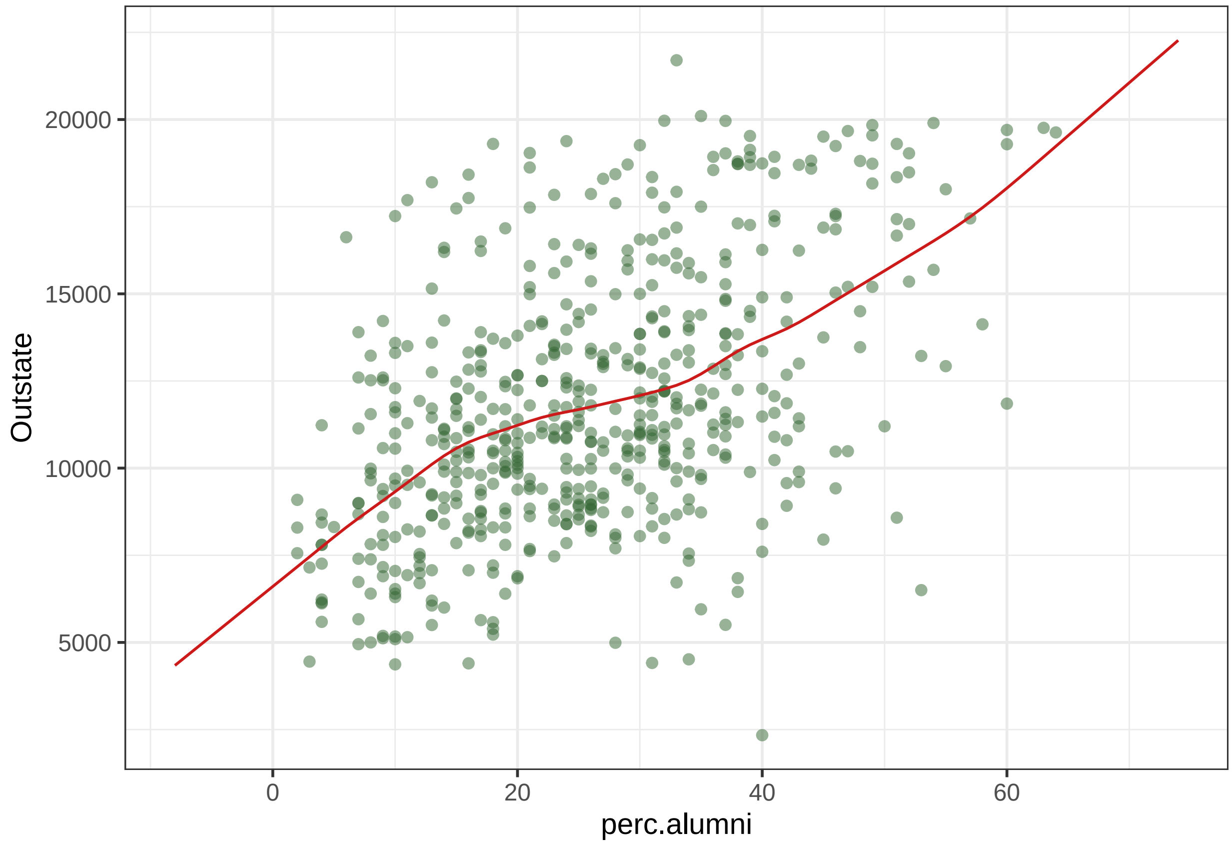
Plot for df = 2

```
p +
  geom_line(aes(x = perc.alumni, y = pred), data = pred.ss.df_2,
            color = rgb(.8, .1, .1, 1)) + theme_bw()
```



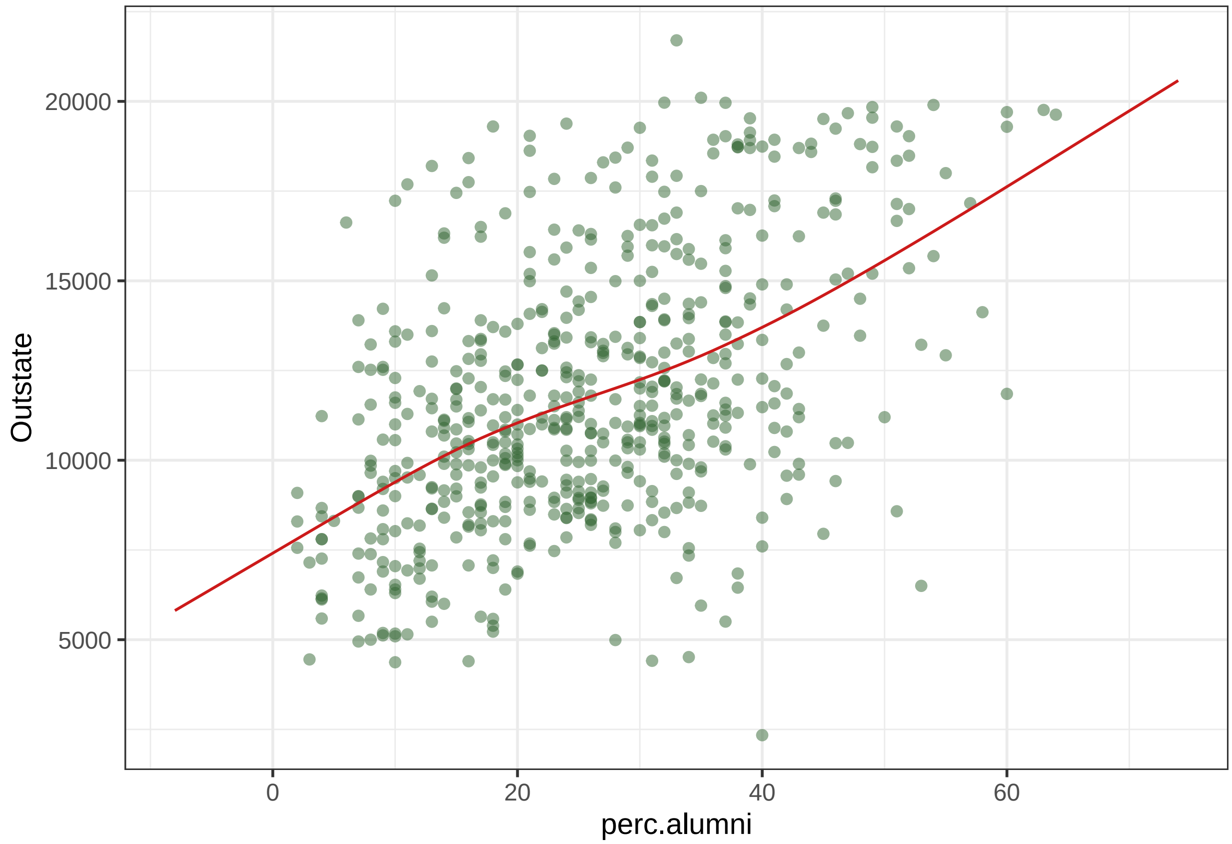
Plot for df = 8

```
p +
  geom_line(aes(x = perc.alumni, y = pred), data = pred.ss.df_8,
            color = rgb(.8, .1, .1, 1)) + theme_bw()
```



Plot for df obtained by generalized cross-validation

```
p +
  geom_line(aes(x = perc.alumni, y = pred), data = pred.ss.df,
            color = rgb(.8, .1, .1, 1)) + theme_bw()
```



Description of the results

For df = 5:

The plot of the smoothing spline fit for df = 5 has a bit of a curve in the first half of the line (near the lower values of `perc.alomni``(x)` and `Outstate`), making it non-linear. A positive (i.e., upward) relationship between `perc.alomni`(x) and `Outstate` (y) can be observed from the plot. The plot is non-linear because the specified df is 5, which greater than 2 and makes the plot non-linear and slightly curvy.

For df = 2:

The plot of the smoothing spline fit for df = 2 appears linear, with a p positive (i.e., upward) relationship between `perc.alomni`(x) and `Outstate` (y). The plot is linear because the specified df is 2, making it similar to a second degree polynomial resulting in a linear plot.

For df = 8:

The plot of the smoothing spline fit for df = 8 is the curviest (most non-linear) yet because it has the highest value specified for the df. Distinct curves in the line are present, with a larger curve in the first half of the line (near the lower values of `perc.alomni``(x)` and `Outstate`). A positive (i.e., upward) relationship between `perc.alomni`(x) and `Outstate` (y) can be observed from the plot. The plot is non-linear because the specified df is 8, which quite a bit larger than 2 and makes the plot non-linear and curvy.

For df obtained by generalized cross-validation:

The plot of the smoothing spline fit for the df obtained by generalized cross-validation (3.779231) is slightly curvy, with a positive (i.e., upward) relationship between `perc.alomni`(x) and `Outstate` (y). There is a slight curve present in the first half of the line (near the lower values of `perc.alomni``(x)` and `Outstate`), while the rest of the line appears fairly linear. The plot is slighly curvy because the df obtained by generalized cross-validation is a bit larger than 2, making the plot non-linear and slightly curvy.

(b) Fit a generalized additive model (GAM) using all the predictors.

Using the caret package and the training dataset:

```
set.seed(1)

# 10-fold cross-validation repeated 5 times
ctrl1 <- trainControl(method = "cv", number = 10)

# fit GAM using all predictors
gam.fit_all <- train(x, y, # test dataset
                 method = "gam",
                 trControl = ctrl1, # 10-fold CV
                 control = gam.control(maxit = 200)) # Adjusted due to failure to converge at default s
```

```
## Warning: model fit failed for Fold08: select= TRUE, method=GCV.Cp Error in magic(G$y, G$X, msp, G$S,
##   magic, the gcv/ubre optimizer, failed to converge after 400 iterations.

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

```
gam.fit_all$bestTune
```

```
##   select method
## 1  FALSE GCV.Cp
```

```
# fit GAM using selection specification
gam.fit_select <- train(x, y, # test dataset
                 method = "gam",
                 tuneGrid = data.frame(method = "GCV.Cp", select = c(TRUE)),
                 trControl = ctrl1, # 10-fold CV
                 control = gam.control(maxit = 200))  # Adjusted due to failure to converge at default
```

```
## Warning: model fit failed for Fold01: method=GCV.Cp, select=TRUE Error in magic(G$y, G$X, msp, G$S, 
##   magic, the gcv/ubre optimizer, failed to converge after 400 iterations.

## Warning: There were missing values in resampled performance measures.
```

```
gam.fit_select$bestTune
```

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

Predictors included in GAM model

The final GAM model for all predictors is as follows:

```
# GAM using all predictors
gam.fit_all$finalModel
```

```
##
## Family: gaussian
## Link function: identity
##
## Formula:
## .outcome ~ s(perc.alumni) + s(Terminal) + s(Books) + s(Grad.Rate) +
##     s(PhD) + s(Top10perc) + s(Top25perc) + s(S.F.Ratio) + s(Personal) +
##     s(P.Undergrad) + s(Room.Board) + s(Enroll) + s(Accept) +
##     s(F.Undergrad) + s(Apps) + s(Expend)
##
## Estimated degrees of freedom:
## 6.05 1.00 2.17 3.56 1.81 1.00 1.00
## 3.69 1.00 1.00 2.47 1.00 4.19 5.51
## 4.45 6.87  total = 47.75
##
## GCV score: 2824207
```

Outstate ~ s(perc.alumni) + s(Terminal) + s(Books) + s(Grad.Rate) + s(PhD) + s(Top10perc) + s(Top25perc) + s(S.F.Ratio) + s(Personal) + s(P.Undergrad) + s(Room.Board) + s(Enroll) + s(Accept) + s(F.Undergrad) + s(Apps) + s(Expend)

Estimated degrees of freedom (for each predictor and total sum): 6.05 1.00 2.17 3.56 1.81 1.00 1.00 3.69 1.00 1.00 2.47 1.00 4.19 5.51 4.45 6.87 total = 47.75

GCV score: 2824207

The final GAM model for the selection specification:

GAM using selection specification

```
gam.fit_select$finalModel
```

```
##
## Family: gaussian
## Link function: identity
##
## Formula:
## .outcome ~ s(perc.alumni) + s(Terminal) + s(Books) + s(Grad.Rate) +
##     s(PhD) + s(Top10perc) + s(Top25perc) + s(S.F.Ratio) + s(Personal) +
##     s(P.Undergrad) + s(Room.Board) + s(Enroll) + s(Accept) +
##     s(F.Undergrad) + s(Apps) + s(Expend)
##
## Estimated degrees of freedom:
## 6.077 0.198 1.095 1.437 0.000 0.832 0.000
```

```
## 3.853 0.638 0.796 3.770 1.000 4.625 5.917
## 4.603 5.930  total = 41.77
##
## GCV score: 2766492
```

The estimated degrees of freedom (for each predictor and total sum): 6.077 0.198 1.095 1.437 **0.000** 0.832 **0.000** 3.853 0.638 0.796 3.770 1.000 4.625 5.917 4.603 5.930 total = 41.77

GCV score: 2766492

Since the df for the 5th predictor (`PhD`) and 7th predictor (`Top25perc`) are 0, these two variables were removed from the final mode. Therefore, the final model using the selection specification is as follows:

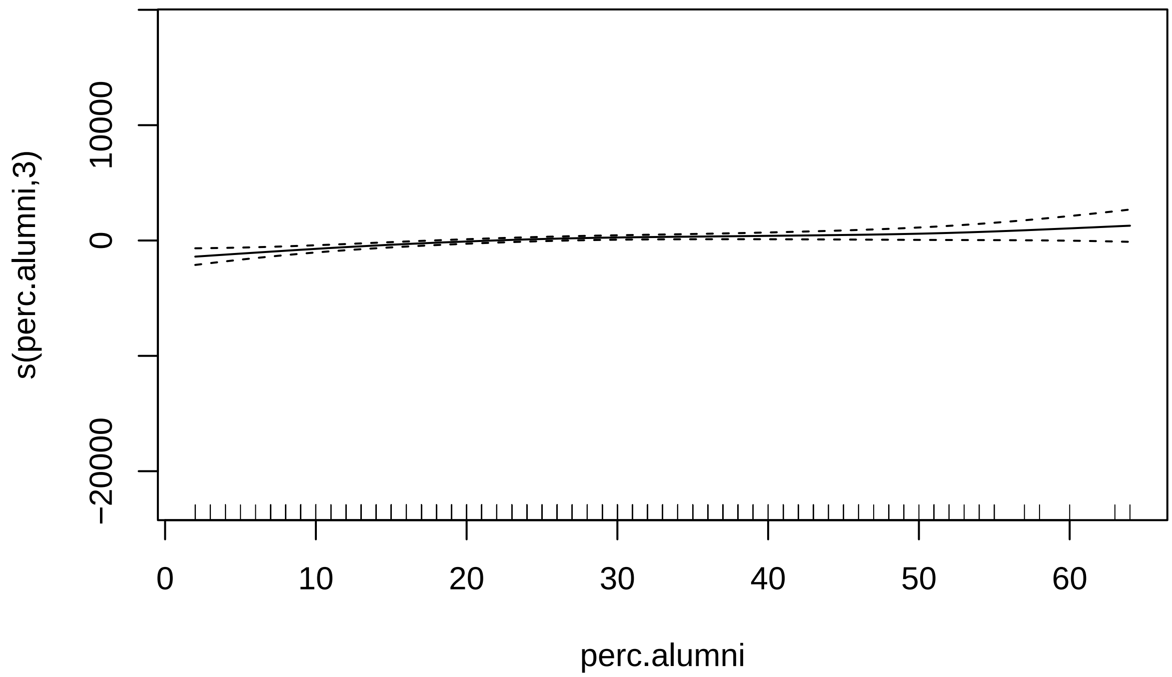
Outstate ~ s(perc.alumni) + s(Terminal) + s(Books) + s(Grad.Rate) + s(Top10perc) + s(S.F.Ratio) + s(Personal) + s(P.Undergrad) + s(Room.Board) + s(Enroll) + s(Accept) + s(F.Undergrad) + s(Apps) + s(Expend)

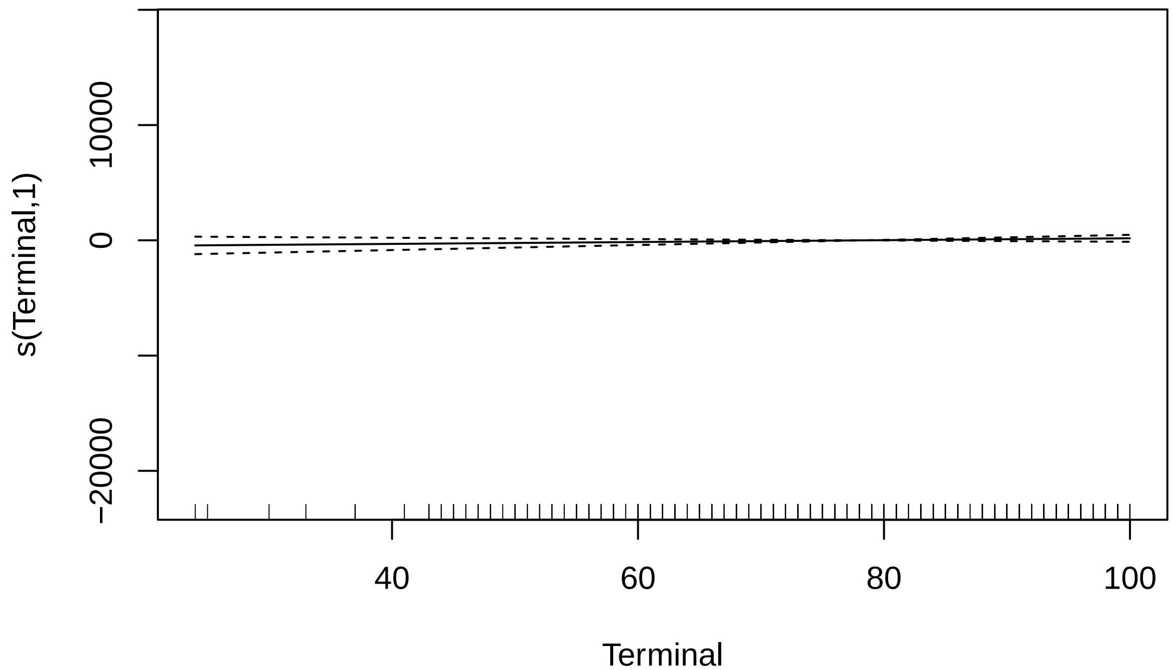
The full model contains all 16 predictors, while the model using the selection specification only has 14 predictors, with PhD and Top25perc removed from the final model. All predictors have the s operator added.

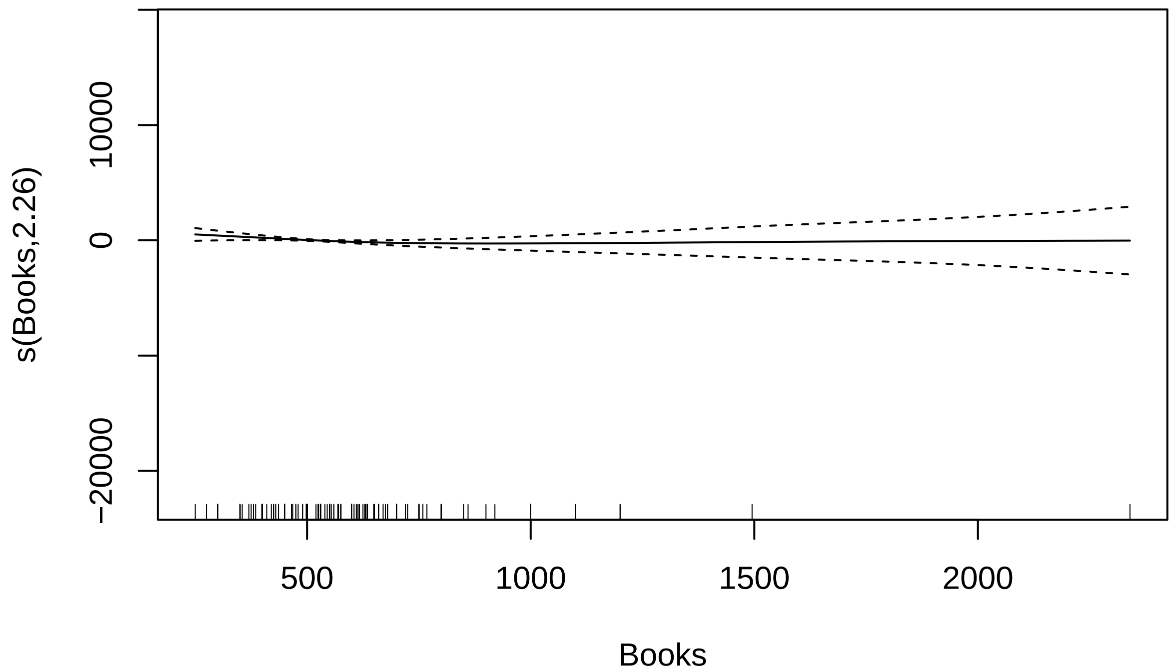
Plot of the results

Predictor plots:

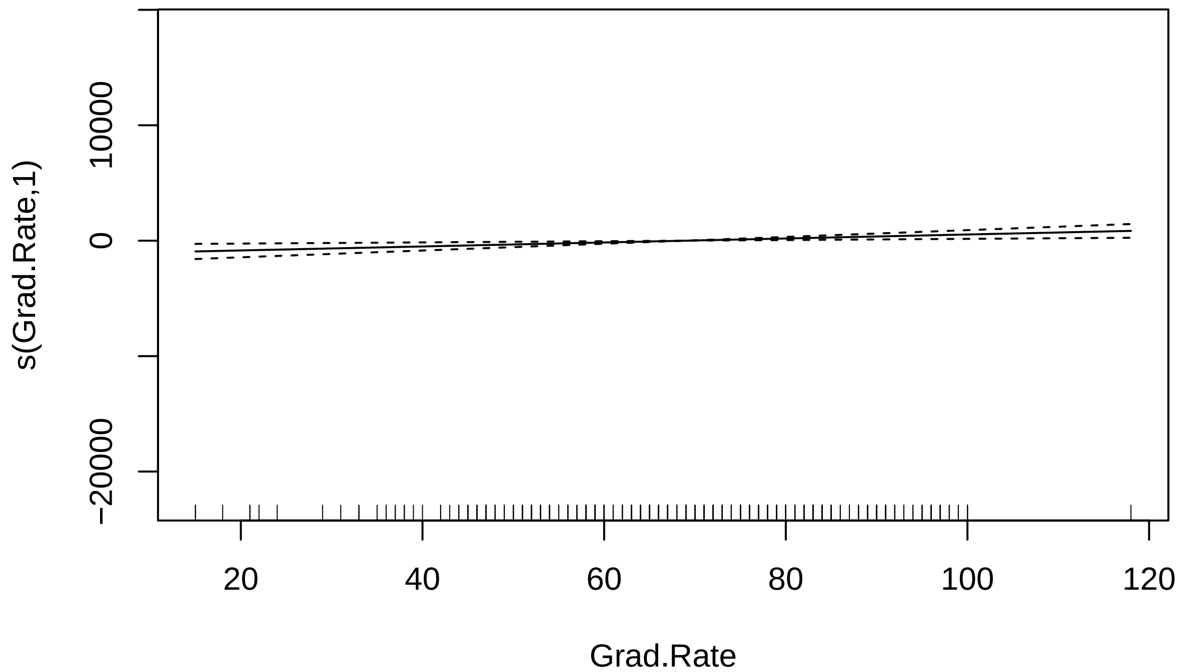
```
set.seed(1)

# Formula based on final GAM model with 14 predictors (gam.fit_select)
gam.m1 <- gam(Outstate ~ s(perc.alumni) + s(Terminal) + s(Books) +
                s(Grad.Rate)+ s(Top10perc) + s(S.F.Ratio) + s(Personal) +
                s(P.Undergrad) + s(Room.Board) + s(Enroll) + s(Accept) +
                s(F.Undergrad) + s(Apps) + s(Expend),
              data = College_train) # training dataset

plot(gam.m1)
```

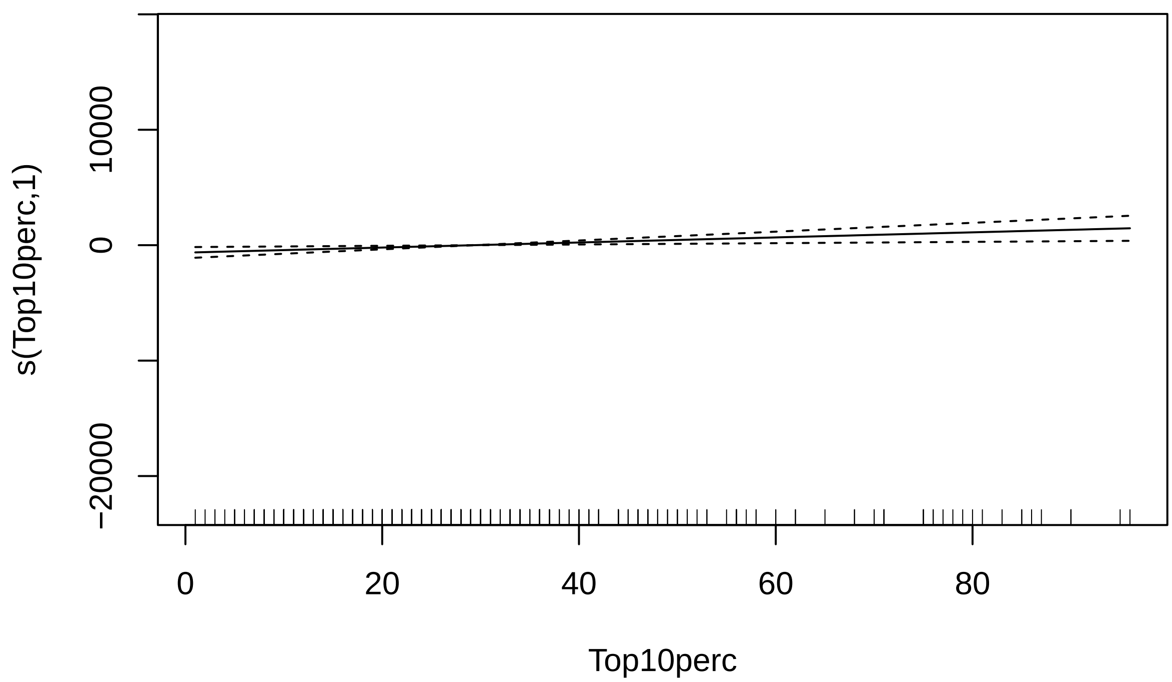

s(perc.alumni,3)
10000
0
−20000
0
10
20
30
40
50
60
perc.alumni

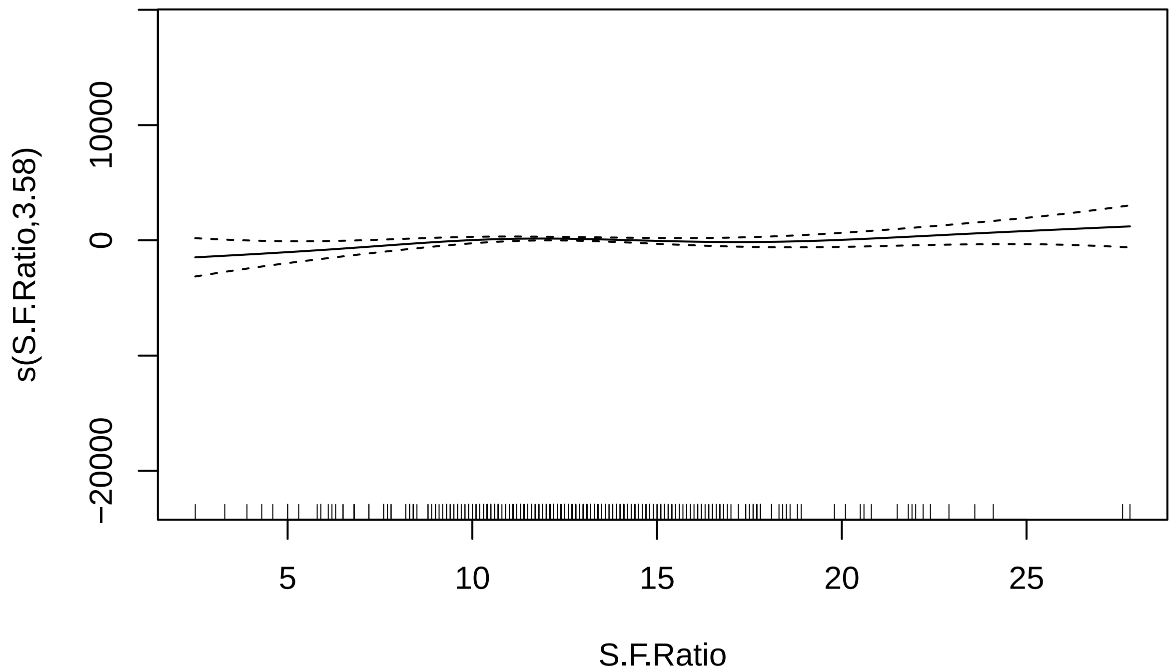

s(Terminal,1)
−20000
0
10000
40
60
80
100
Terminal

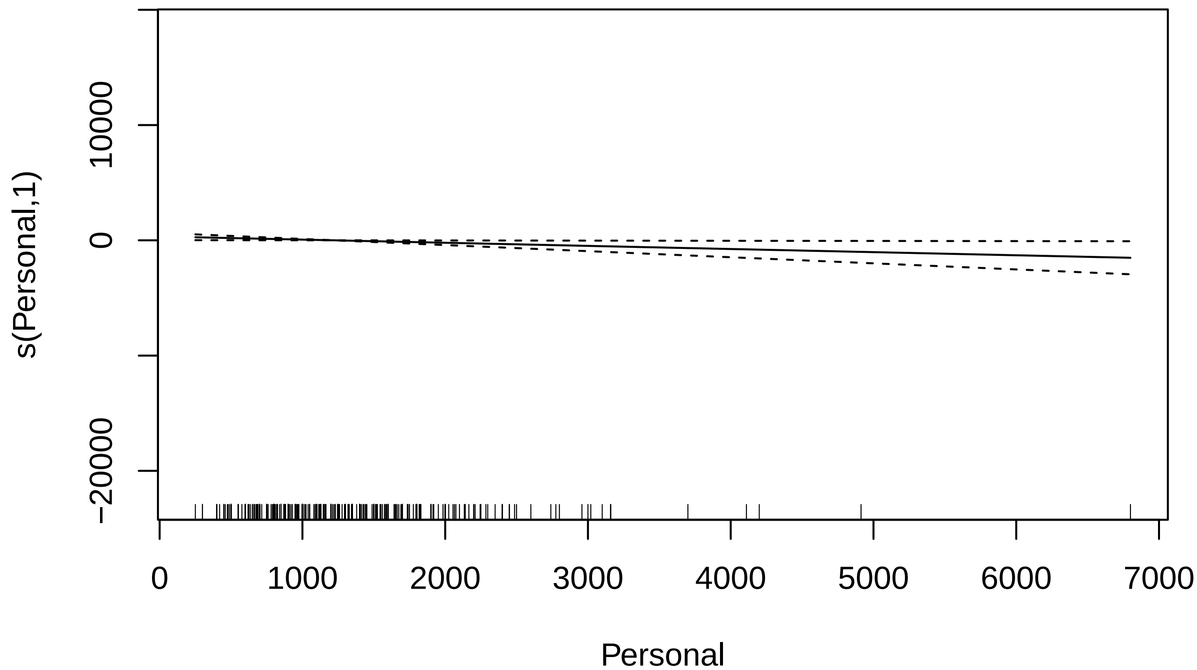


s(Books,2.26)
10000
0
−20000
500
1000
1500
2000
Books

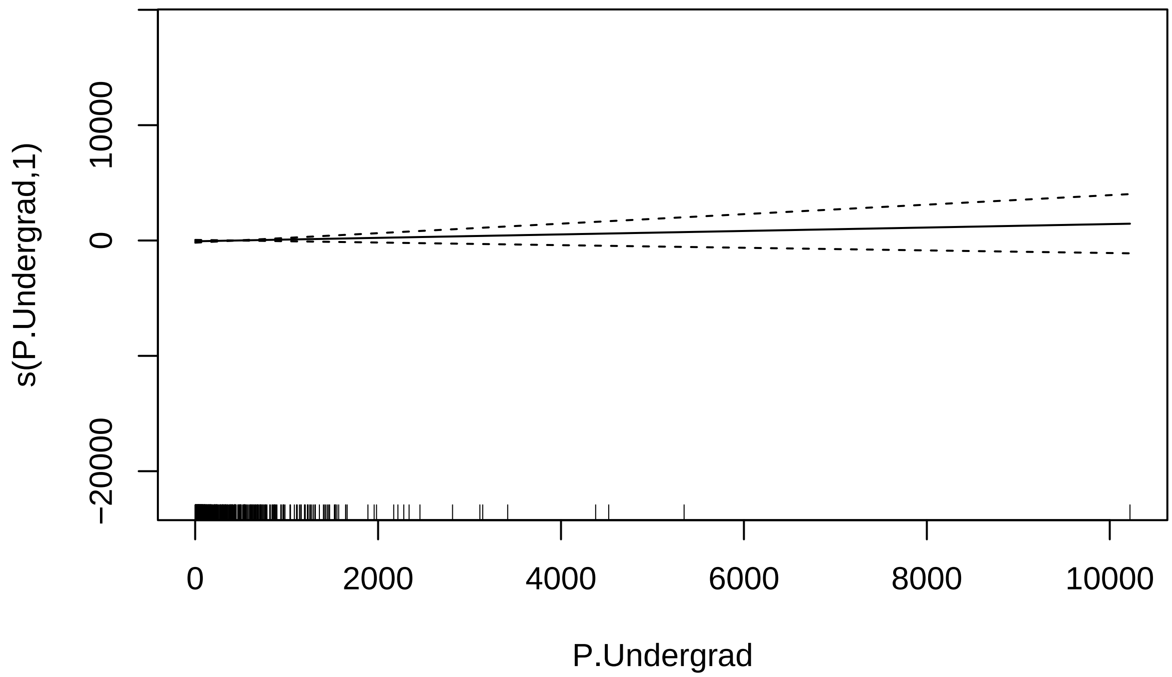

s(Grad.Rate,1)
10000
0
−20000
20
40
60
80
100
120
Grad.Rate

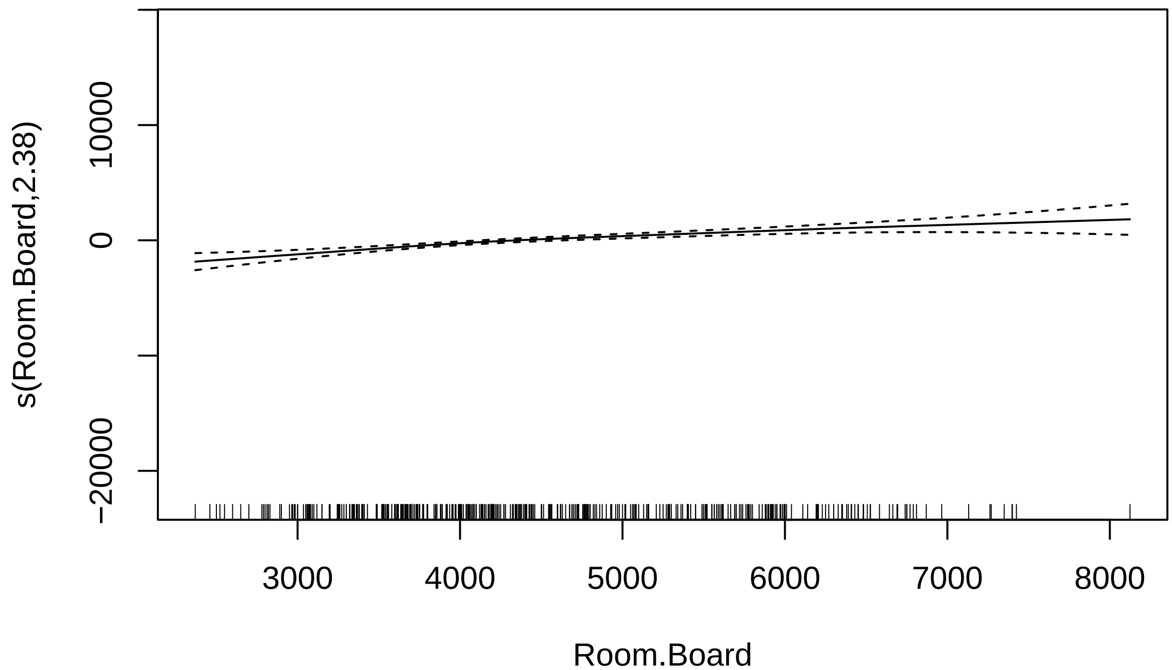

s(Top10perc,1)
10000
0
−20000
0
20
40
60
80
Top10perc

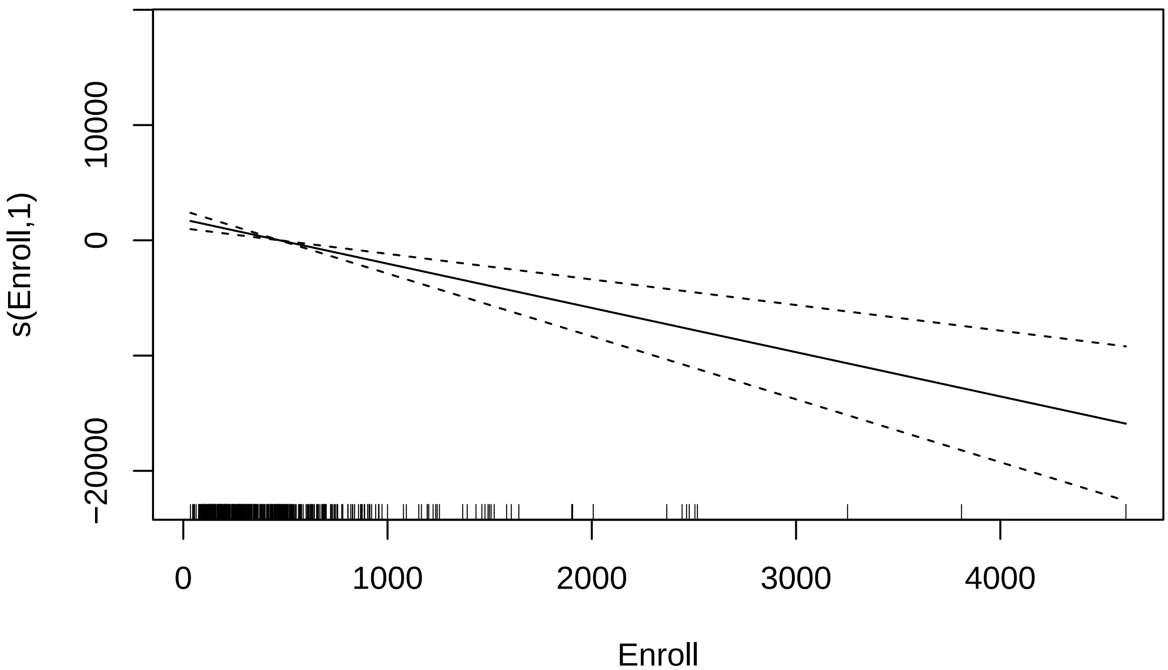

s(S.F.Ratio,3.58)
−20000
0
10000
5
10
15
20
25
S.F.Ratio

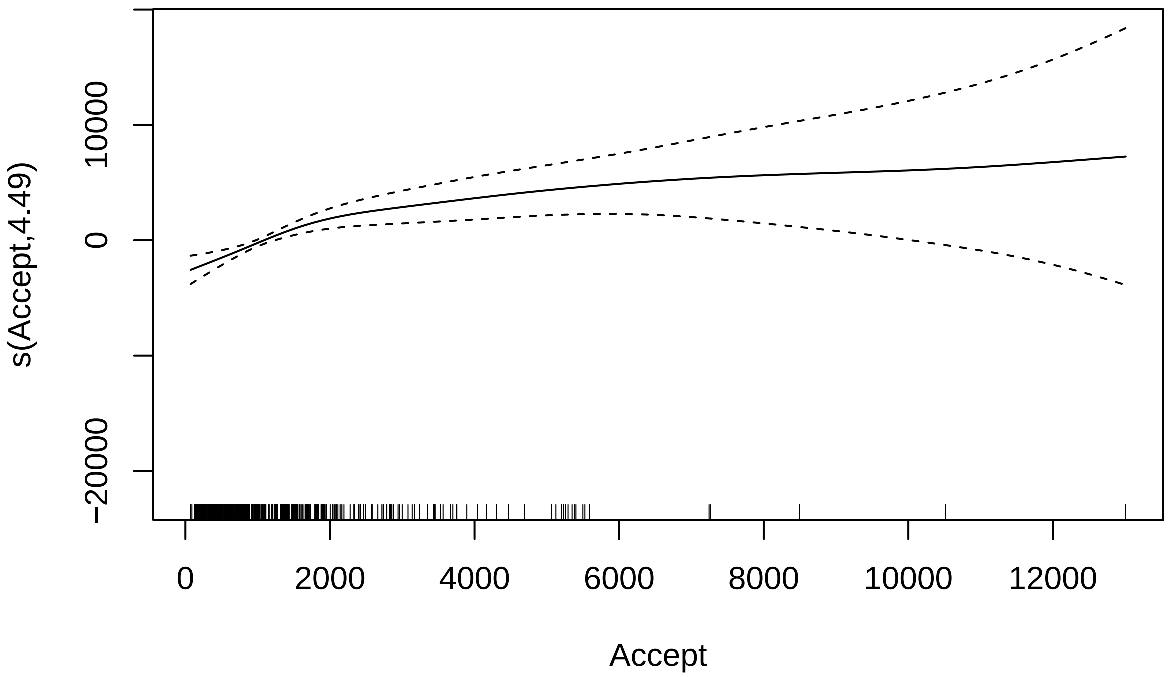


s(Personal,1)
10000
0
−20000
0
1000
2000
3000
4000
5000
6000
7000
Personal

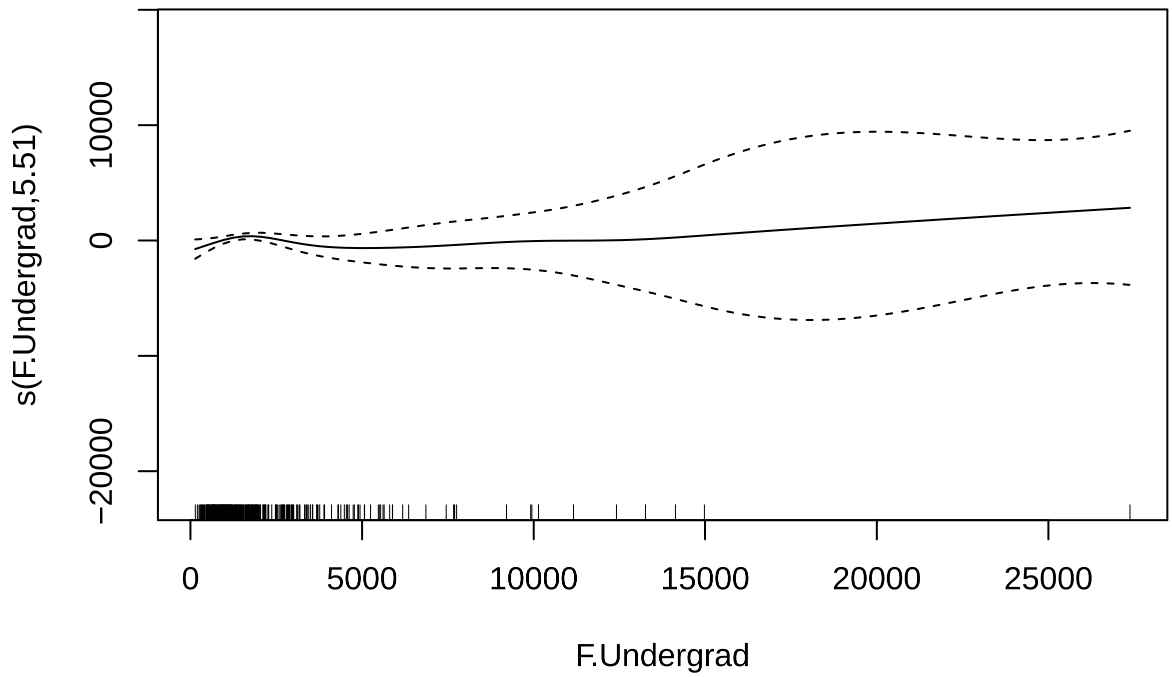

s(P.Undergrad,1)
−20000
0
10000
0
2000
4000
6000
8000
10000
P.Undergrad

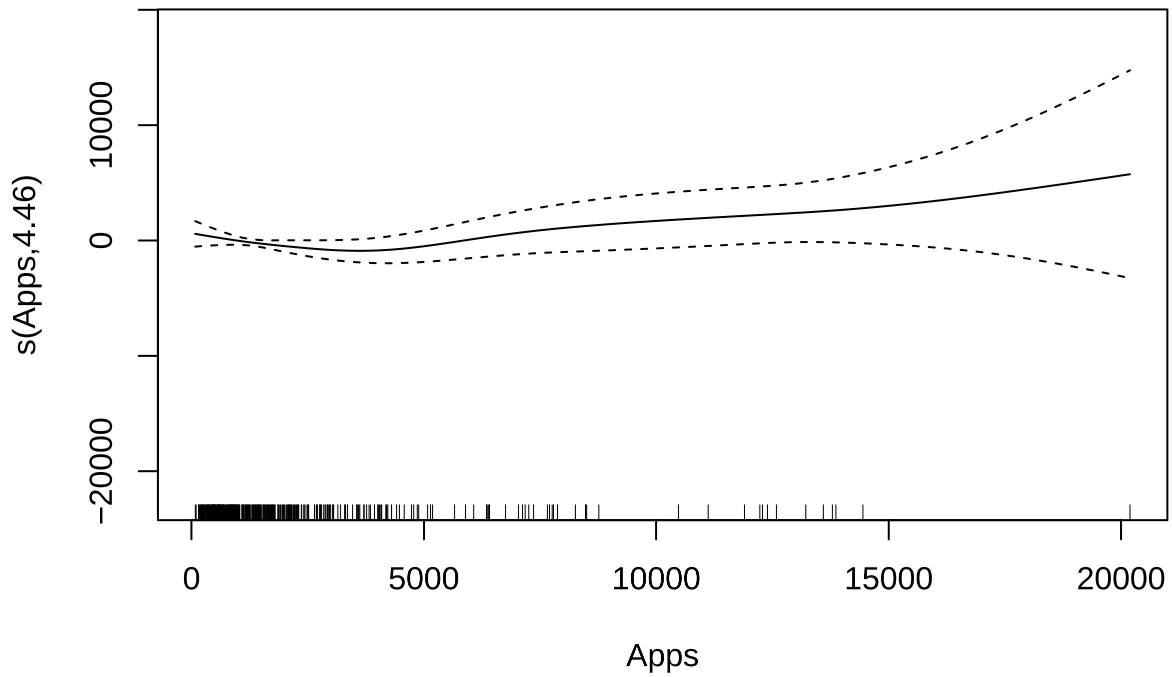

s(Room.Board,2.38)
10000
0
−20000
3000
4000
5000
6000
7000
8000
Room.Board

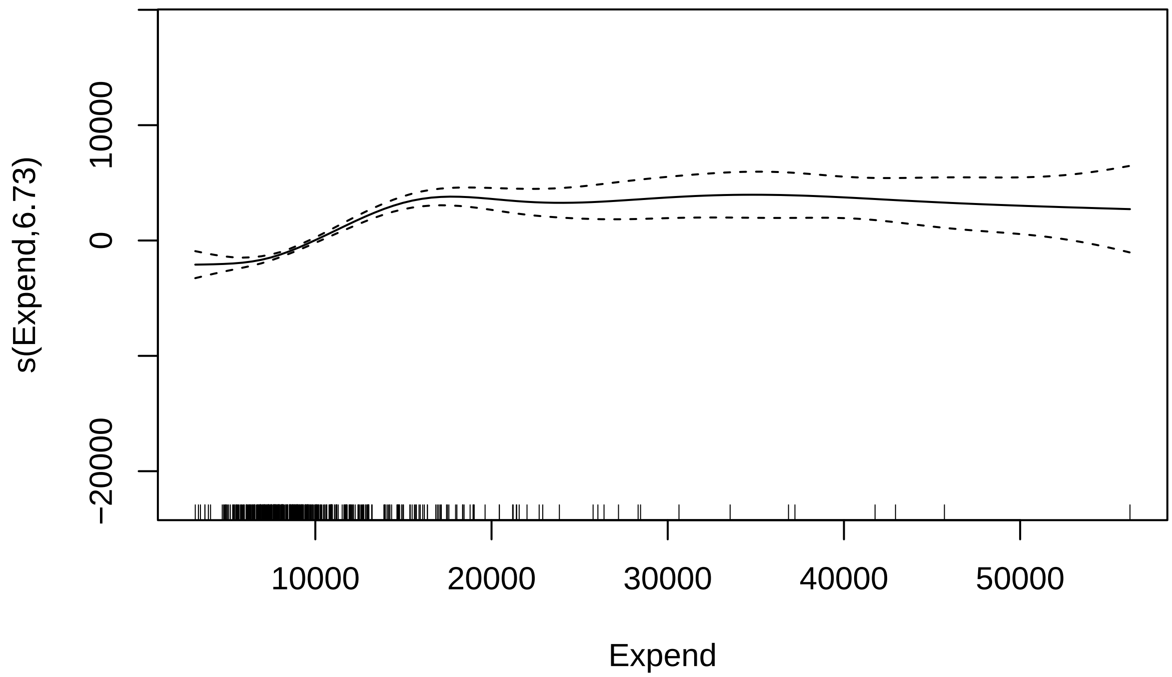

s(Enroll,1)
10000
0
−20000
0
1000
2000
3000
4000
Enroll



s(Accept,4.49)
10000
0
−20000
0
2000
4000
6000
8000
10000
12000
Accept

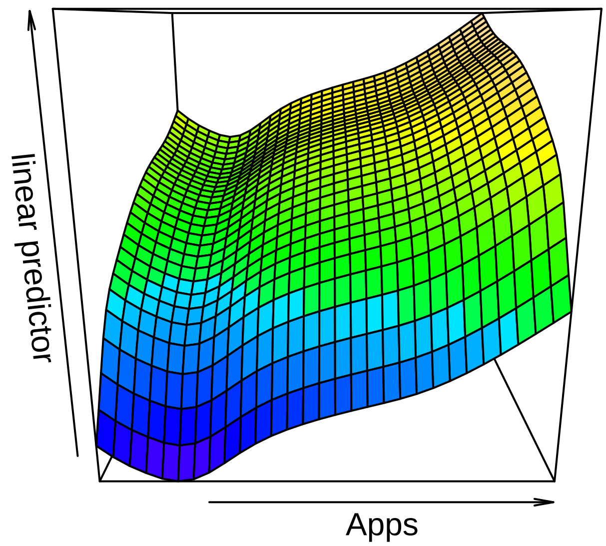

s(F.Undergrad,5.51)
10000
0
−20000
0
5000
10000
15000
20000
25000
F.Undergrad


s(Apps,4.46)
10000
0
−20000
0
5000
10000
15000
20000
Apps



Bivariate plot for the arbitrarily chosen `Apps` and `Accept` predictor variables:

```
vis.gam(gam.m1, view = c("Apps", "Accept"),
color = "topo")
```



Explanation of findings

From the plot, it can be observed that most of the predictors have a fairly small credible interval window, which may be used as an approximation of the 95% confidence interval. A small credible interval window for predictors means that the uncertainty of the estimate is small and variability is small, indicating the the curve can be "trusted" for these predictors. However, it's also worth noting that a few predictors have a larger credible interval window at higher values of the predictor. For example, the plots for the `Accept` and `F.Undergrad` predictors show a credible interval window that is small at smaller values for the variables, and lets larger for larger values of the variables. This indicates that the the uncertainty of the estimate increases for larger values of the predictors and perhaps the curve shouldn't be "trusted" as easily for data points that fall within these larger values.

Test error

The test error should be retrieved by first fitting the GAM model using the test dataset and then using it to calculate the test error. However, I has running into difficulty with my code not running when I fit the model using the test dataset. I'm curious if there are not enough data points for it to run properly using the specifications. I emailed the teaching team about this issue on 3/9. For purposes of this timely submission of my homework, I am calculating the error for the model fit using the training dataset here. However, I acknowledge that this is not alligned with best practices.

```
set.seed(1)

# test error using GAM fit for all predictors
```

```r
# gam.fit_test_all <- train(x2, y2, # test dataset
                 # method = "gam",
                 # trControl = ctrl1, # 10-fold CV
                 # control = gam.control(maxit = 200)) # Adjusted due to failure to converge at default

# gam.fit_test_all$results$RMSE

gam.fit_all$results$RMSE # Using previous model because the code woudln't run with test data
```

```
## [1] 1785.113 1833.612
```

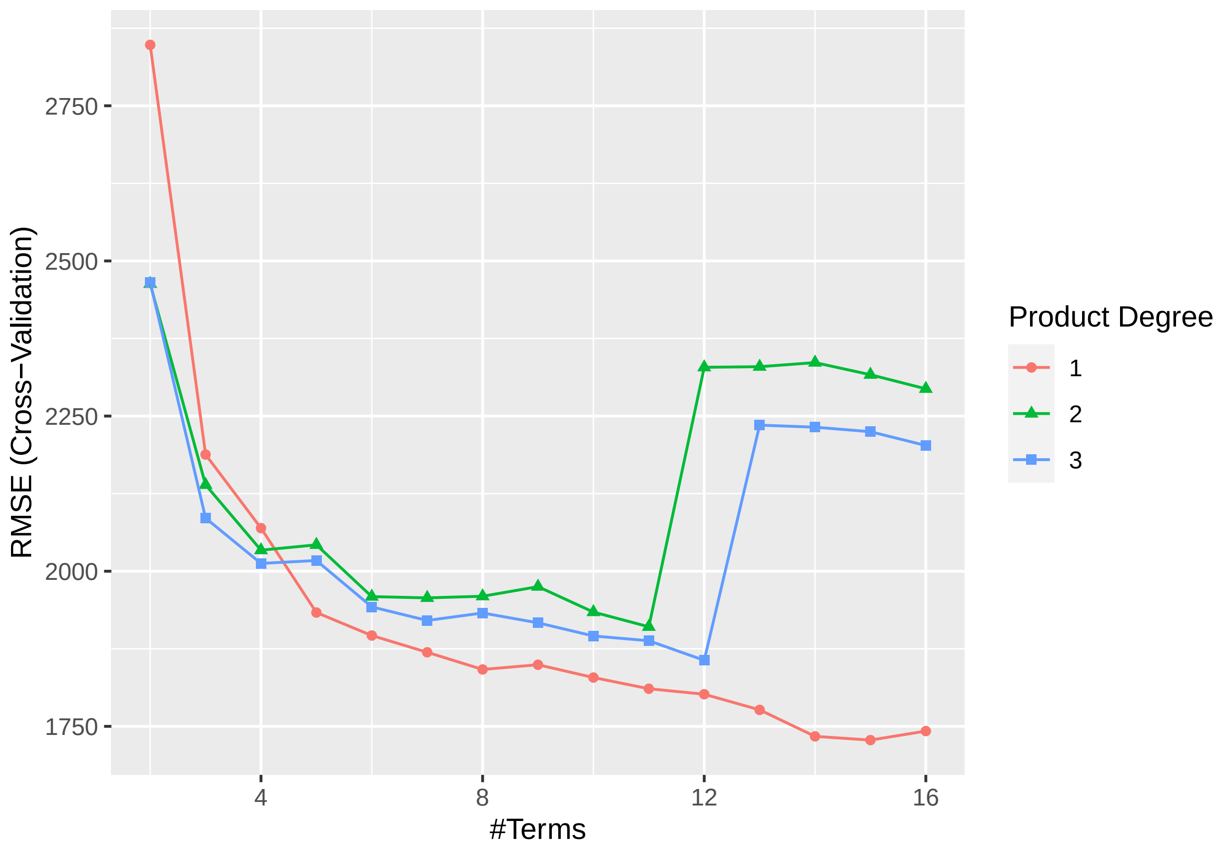
```r
# test error using GAM fit for selection specification
# gam.fit_test_select <- train(x2, y2, # test dataset
                 # method = "gam",
                 # tuneGrid = data.frame(method = "GCV.Cp", select = c(TRUE)),
                 # trControl = ctrl1, # 10-fold CV
                 # control = gam.control(maxit = 200)) # Adjusted due to failure to converge at default

# gam.fit_test_select$results$RMSE
```

The error is for the GAM model fit for all predictors is using the model fit with the training data is 1759.699 1848.859.

(c) Multivariate adaptive regression spline (MARS) model using all the predictors.

Fit MARS model using the caret package and training dataset:

```r
set.seed(1)

# create grid of all possible pairs that can take degree and nprune values
mars_grid <- expand.grid(degree = 1:3, # number of possible product hinge functions in 1 term
                         nprune = 2:16) # Upper bound of number of terms in model

mars.fit <- train(x, y, # training dataset
                  method = "earth",
                  tuneGrid = mars_grid,
                  trControl = ctrl1) # 10-fold CV

ggplot(mars.fit)
```




```
mars.fit$bestTune
```

```
##    nprune degree
## 14     15      1
```

The upper bound of the number of terms in the MARS model is 15 based on the minimum value for RMSE in the plot. Also, the model that appears to be the best in terms of the cross validation error is the model with a product degree of 1.

The final MARS model contains the following predictors, coefficients, and hinge functions:

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

```
##                 (Intercept)            h(Expend-15736)
##               11990.4787273                 -0.7057251
##              h(79-Grad.Rate)          h(Room.Board-4250)
##                 -33.9331530                  0.4027510
##           h(4250-Room.Board)         h(F.Undergrad-1411)
##                  -1.2922196                 -1.2632483
##            h(22-perc.alumni)              h(Expend-6874)
##                 -88.2417155                  0.6963456
##    CollegeBennington College      CollegeSpelman College
##                6674.2643400              -6243.6619045
##              h(1656-Accept) CollegeCreighton University
##                  -1.5964172              -5804.7888985
```

```
##  CollegeLivingstone College                  h(Apps-946)
##              -5741.1315285                    0.2744830
##         h(F.Undergrad-3128)
##                  0.9641141
```

The final MARS model includes 10 hinge functions for the following predictors: `Expend` (pair), `Grad.Rate`, `Room.Board` (reflective pair), `F.Undergrad`, `perc.alumni`, `Accept`, `Apps`, and `F.Undergrad`.

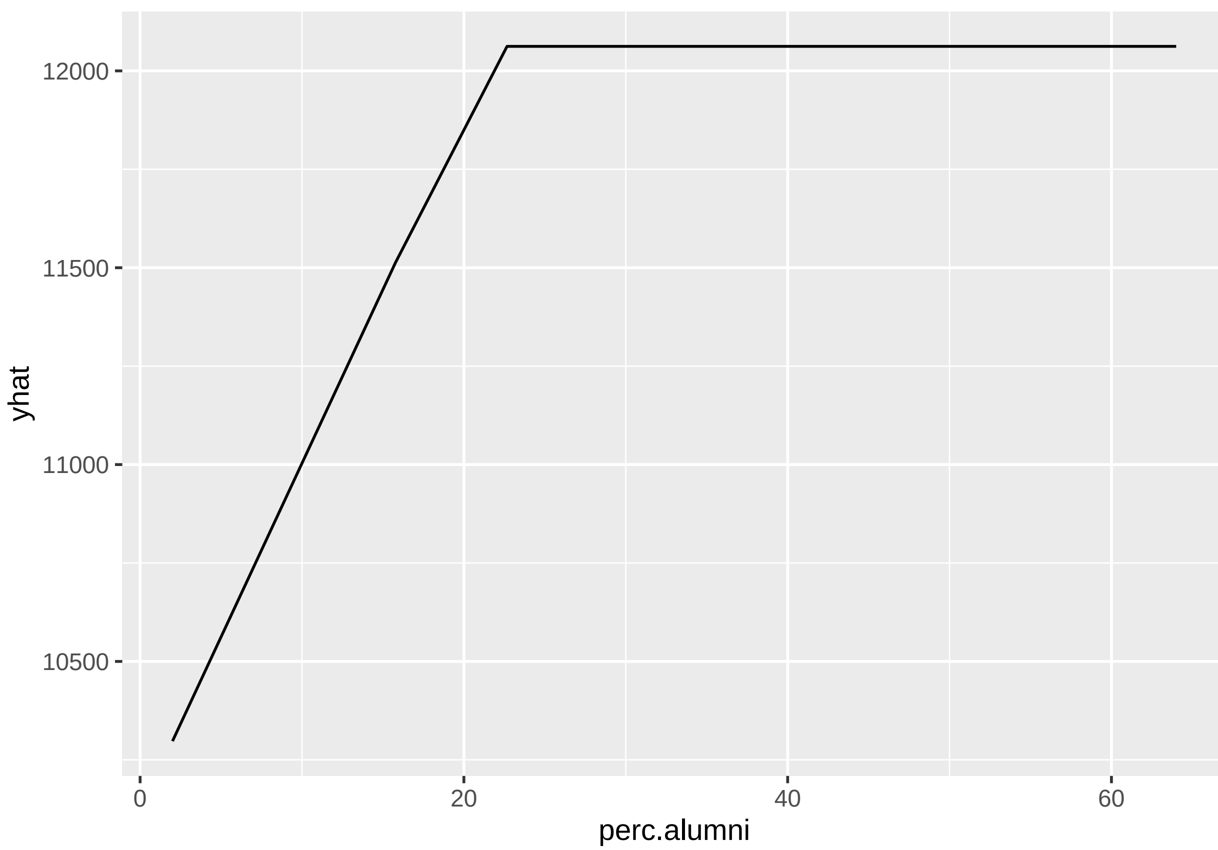
The final model is as follows:

Outstate ~ 11990.478727 - 0.7057251(h(Expend-15736)) - 33.9331530(h(79-Grad.Rate)) + 0.4027510(h(Room.Board-4250)) - 1.2922196(h(4250-Room.Board)) - 1.2632483(h(F.Undergrad-1411)) - 88.2417155(h(22-perc.alumni)) + 0.6963456(h(Expend-6874)) + 6674.2643400(CollegeBennington College) - 243.6619045(CollegeSpelman College) - 1.5964172(h(1656-Accept)) - 5804.7888985(CollegeCreighton University) - 5741.1315285(CollegeLivingstone College) + 0.2744830 (h(Apps-946)) + 0.9641141(h(F.Undergrad-3128))

Partial dependence plots

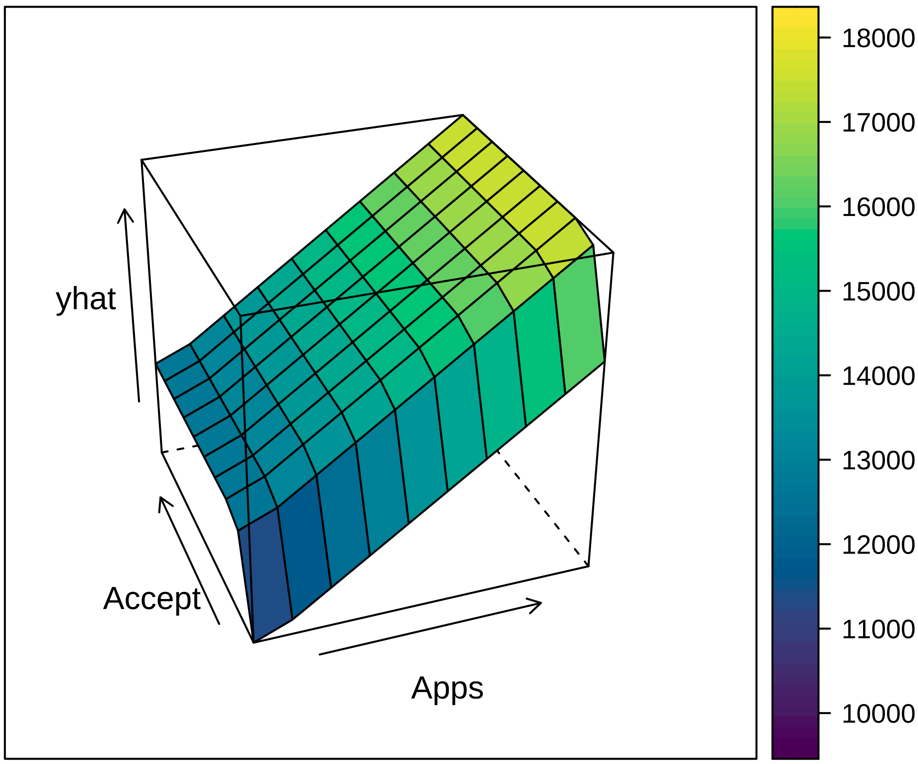
Plot of a single arbitrary predictor in the final model `perc.alumni`:

```
p1 <- pdp::partial(mars.fit,
                   pred.var = c("perc.alumni"),
                   grid.resolution = 10) %>%
  autoplot()

p1
```



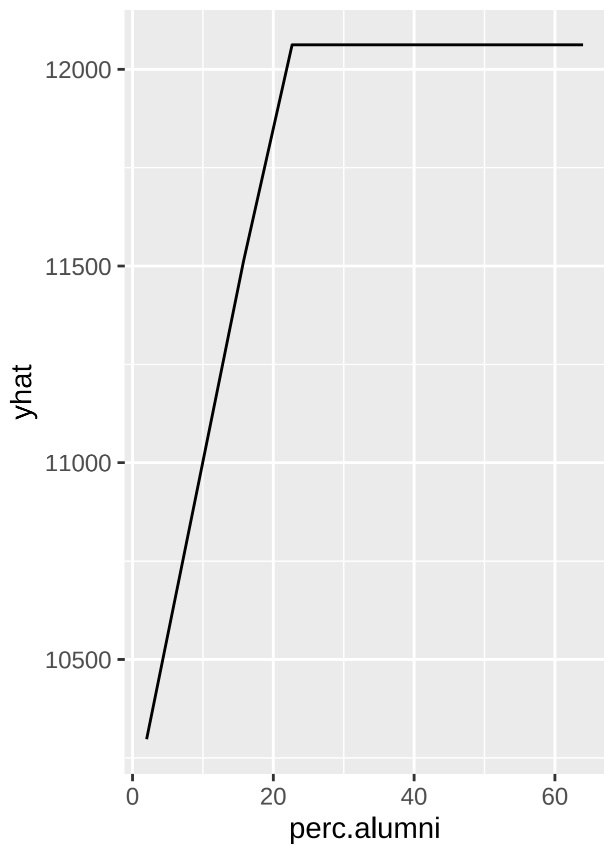
Plot of an interaction partial dependence plot between arbitrary predictors in the final model `Apps` and `Accept`:

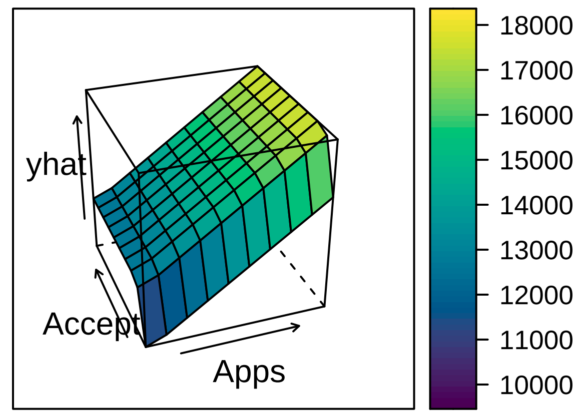
```
p2 <- pdp::partial(mars.fit,
                   pred.var = c("Apps", "Accept"),
                   grid.resolution = 10) %>%
  pdp::plotPartial(levelplot = FALSE,
                   zlab = "yhat",
                   drape = TRUE,
                   screen = list(z = 20, x = -60))

p2
```



Both partial dependence plots combined:

```
grid.arrange(p1, p2, ncol = 2)
```





The partial dependence plots above allow for better understanding of the relationship between the `perc.alumni`, `Apps`, and `Accept` features and the outcome `Outstate` and the marginal effects of these predictors.

Test error

Fit model using the test dataset and calculate the test error:

```r
set.seed(1)

mars.fit_test <- train(x2, y2, # test dataset
                 method = "earth",
                 tuneGrid = mars_grid,
                 trControl = ctrl1) # 10-fold CV

mars.fit_test$results$RMSE
```

```
##  [1] 2204.917 2122.136 2159.673 2041.297 2215.930 2166.897 2059.312 2206.141
##  [9] 2262.332 1912.192 1997.782 2075.348 1919.975 2198.623 2372.489 1885.352
## [17] 2228.544 2174.672 1913.535 2174.585 2109.206 1904.036 2194.783 2105.128
## [25] 1916.521 2207.314 2384.038 1971.612 2265.302 2379.313 1982.716 2305.072
## [33] 2374.530 2021.322 2258.392 2524.099 2027.059 2300.720 2516.018 1999.069
## [41] 2287.392 2483.779 1978.073 2510.076 2689.759
```

(d) Preference for the use of MARS model over a linear model when predicting the out-of-state tuition.

The choice between a MARS model and a linear model for calculating out-of-state tuition costs from a set of predictors would depend on the nature of the data and predictors desired, as well as the degree of complexity that the researcher is comfortable with in their model.

If the relationship between the predictors and the outcome (i.e., the out-of-state tuition costs) is expected to be linear or relatively straightforward, a linear model is appropriate and may be preferred because it is a simple model. Linear models assume a linear relationship between the predictors and the outcome, and are well-suited for general application situations where the predictor variables have a clear and direct impact on the outcome.

However, if there is reason to believe that the relationship between the predictors and the outcome is non-linear or more complex, a MARS model may be more appropriate, even though it is a much more complex model. MARS models are able to capture non-linear relationships by creating piecewise linear regression functions, and can be useful for handling interactions between predictors.

All of this said, for general applications, I only think that the MARS is a better approach compared to a linear model if the relationship between the predictors and the outcome is non-linear. If the relationship is somewhat linear, then a linear model is preferred in general applications because it is much simpler.