Team 2 - Homework Two

Assignment 2: KJ 7.2; KJ 7.5

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Dependencies

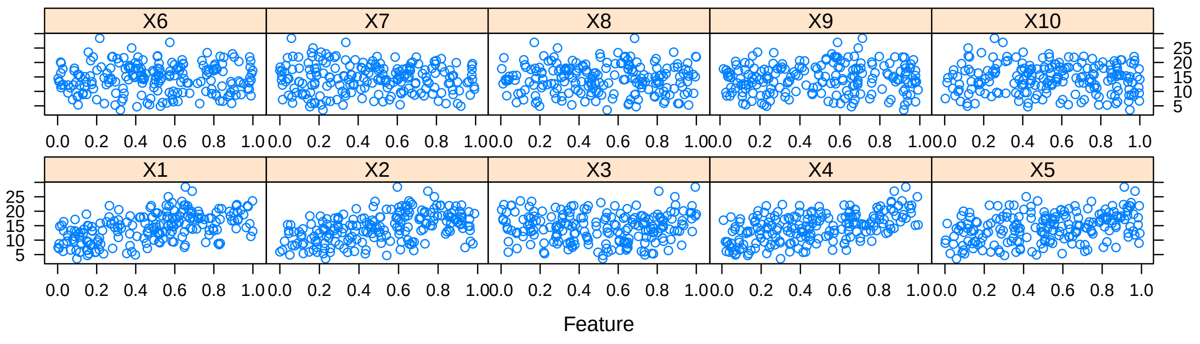
```r
# predictive modeling
libraries("mlbench", "caret", "mice", "AppliedPredictiveModeling",
    "recipes", "tibble", "tidyverse")

# Formatting Libraries
libraries("default", "knitr", "kableExtra")

# Plotting Libraries
libraries("ggplot2", "grid", "ggfortify")
```

(1) Kuhn & Johnson 7.2

Friedman (1991) introduced several benchmark data sets create by simulation. One of these simulations used the following nonlinear equation to create data: $y = 10\sin(\pi x_1 x_2) + 20(x_3 - 0.5)^2 + 10x_4 + 5x_5 + N(0, \sigma^2)$; where the x values are random variables uniformly distributed between $[0, 1]$ (there are also 5 other non-informative variables also created in the simulation).

The package `mlbench` contains a function called `mlbench.friedman1` that simulates these data:

```r
set.seed(200)
trainingData <- mlbench.friedman1(200, sd = 1)
trainingData$x <- data.frame(trainingData$x)
featurePlot(trainingData$x, trainingData$y)
```



```r
testData <- mlbench.friedman1(5000, sd = 1)
testData$x <- data.frame(testData$x)
```

(a) Tune several models on these data.

For example:

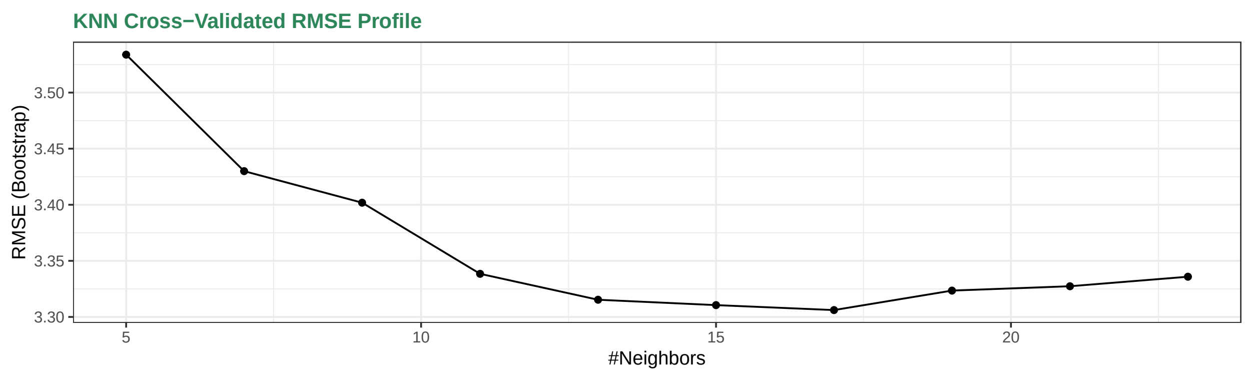
Train set model & performance:

```
k-Nearest Neighbors

200 samples
 10 predictor

Pre-processing: centered (10), scaled (10)
Resampling: Bootstrapped (25 reps)
Summary of sample sizes: 200, 200, 200, 200, 200, 200, ...
Resampling results across tuning parameters:

  k   RMSE      Rsquared   MAE
   5  3.533813  0.5130609  2.910827
   7  3.429971  0.5461330  2.818732
   9  3.401852  0.5637178  2.775645
  11  3.338443  0.5938918  2.728206
  13  3.315336  0.6142508  2.700334
  15  3.310544  0.6284303  2.697967
  17  3.306122  0.6423117  2.698210
  19  3.323482  0.6487590  2.718881
  21  3.327365  0.6585681  2.718610
  23  3.335849  0.6635003  2.725054

RMSE was used to select the optimal model using the smallest value.
The final value used for the model was k = 17.
```

Test set performance values:

```
     RMSE  Rsquared       MAE
3.2040595 0.6819919 2.5683461
```

RMSE Plot:



Model 1:

Train set model & performance:

```
Linear Regression

200 samples
 10 predictor

Pre-processing: principal component signal extraction (10), centered
 (10), scaled (10)
Resampling: Cross-Validated (10 fold, repeated 5 times)
Summary of sample sizes: 180, 180, 180, 180, 180, 180, ...
Resampling results:

  RMSE      Rsquared   MAE
  2.432147  0.7653831  1.951699

Tuning parameter 'intercept' was held constant at a value of TRUE
```

Test set performance values:

```
     RMSE  Rsquared       MAE
2.6970680 0.7084666 2.0600540
```

This method has no tuning parameters to view in a cross validation plot.

Model 2:

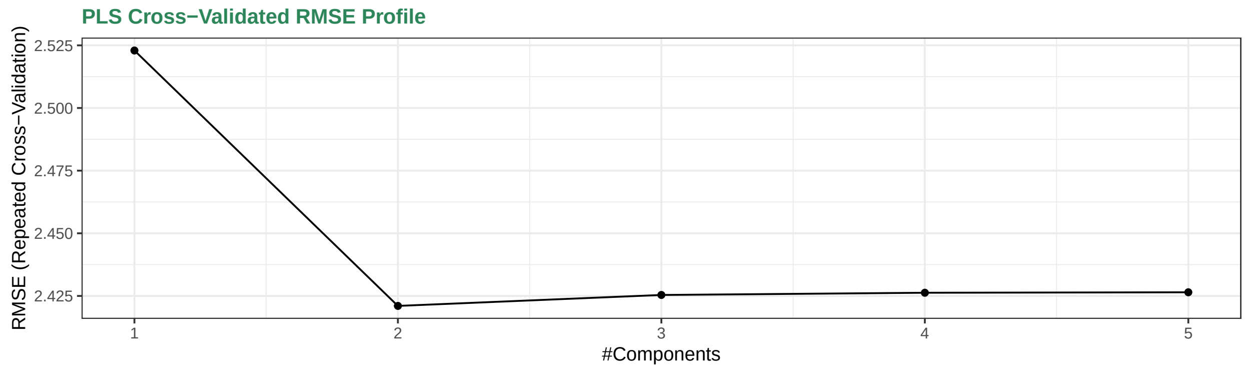
Train set model & performance:

```
Partial Least Squares

200 samples
 10 predictor

Pre-processing: principal component signal extraction (10), centered
 (10), scaled (10)
Resampling: Cross-Validated (10 fold, repeated 5 times)
Summary of sample sizes: 180, 180, 180, 180, 180, 180, ...
Resampling results across tuning parameters:

  ncomp  RMSE      Rsquared   MAE
  1      2.522945  0.7537245  2.006956
  2      2.421026  0.7743143  1.930347
  3      2.425394  0.7738312  1.934872
  4      2.426279  0.7735851  1.936843
  5      2.426467  0.7736047  1.937165

RMSE was used to select the optimal model using the smallest value.
The final value used for the model was ncomp = 2.
```

Test set performance values:

```
    RMSE Rsquared      MAE
2.685591 0.710292 2.052676
```

RMSE Plot:



Model 3:

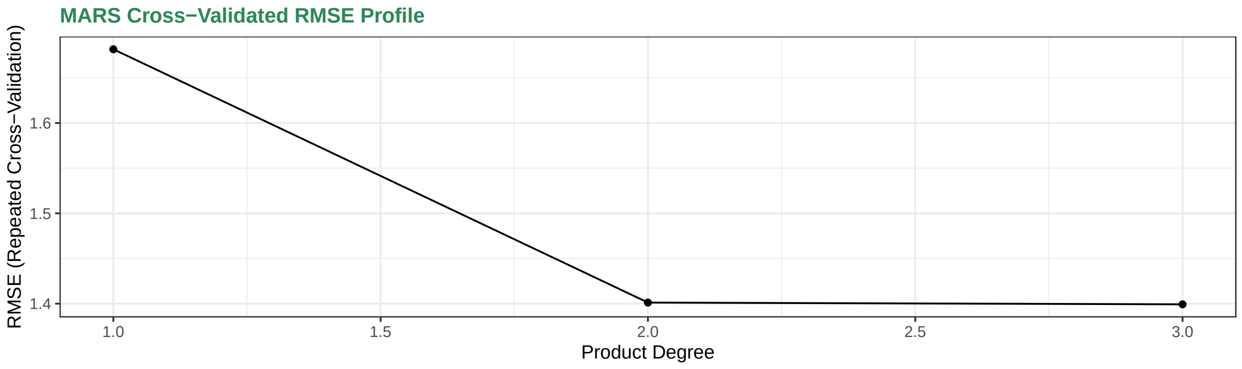
Train set model & performance:

```
Multivariate Adaptive Regression Spline

200 samples
 10 predictor

No pre-processing
Resampling: Cross-Validated (10 fold, repeated 5 times)
Summary of sample sizes: 180, 180, 180, 180, 180, 180, ...
Resampling results across tuning parameters:

  degree  RMSE      Rsquared   MAE
  1       1.681637  0.8915313  1.318973
  2       1.401175  0.9240245  1.108177
  3       1.399221  0.9243424  1.108727

Tuning parameter 'nprune' was held constant at a value of 10
RMSE was used to select the optimal model using the smallest value.
The final values used for the model were nprune = 10 and degree = 3.
```

Test set performance values:

```
     RMSE  Rsquared       MAE
1.4064480 0.9197345 1.1230234
```

RMSE Plot:



(b) Which models appear to give the best performance? Does MARS select the informative predictors (those named X1-X5)?

The MARS model has the lowest RMSE accuracy scores for both our training and test sets. This model appeared to give the best performance.

Table 1: Model Performance

	RMSE	**RSquared**	**MAE**
knnTrain	3.3061	3.3061	3.3061
knnTest	3.2041	0.6820	2.5683
lmTrain	2.4321	0.7654	1.9517
lmTest	2.6971	0.7085	2.0601
plsTrain	2.4210	0.7743	1.9303
plsTest	2.6856	0.7103	2.0527
marsTrain	**1.3992**	**0.9243**	**1.1087**
marsTest	**1.4064**	**0.9197**	**1.1230**

In addition, the MARS model selected the important indicator variables: X1-X5.

Table 2: MARS Model - Variable Importance

	Overall
X1	100.00
X4	84.82
X2	68.49
X5	47.76
X3	37.85
X6	0.00
X7	0.00
X8	0.00
X9	0.00
X10	0.00

(2) Kuhn & Johnson 7.5

Exercise 6.3 describes data for a chemical manufacturing process. Use the same data imputation, data splitting, and pre-processing steps as before and train several nonlinear regression models.

Model 1:

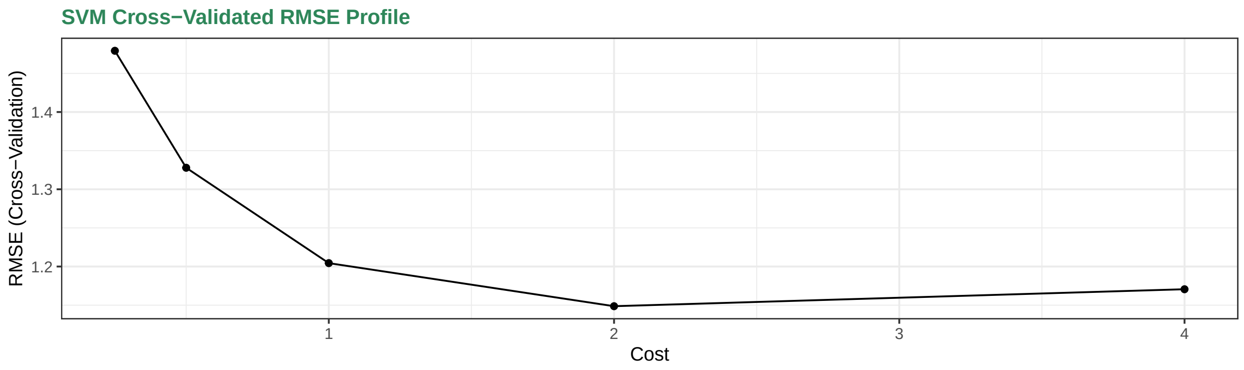
Train set model & performance:

```
Support Vector Machines with Radial Basis Function Kernel

144 samples
 56 predictor

Pre-processing: principal component signal extraction (56), centered
 (56), scaled (56)
Resampling: Cross-Validated (10 fold)
Summary of sample sizes: 128, 130, 128, 129, 130, 130, ...
Resampling results across tuning parameters:

  C     RMSE      Rsquared   MAE
  0.25  1.479290  0.5318113  1.2199718
  0.50  1.327842  0.5575704  1.0858449
  1.00  1.204413  0.6047723  0.9644347
  2.00  1.148657  0.6279010  0.9052238
  4.00  1.170610  0.6115252  0.9054392

Tuning parameter 'sigma' was held constant at a value of 0.02499863
RMSE was used to select the optimal model using the smallest value.
The final values used for the model were sigma = 0.02499863 and C = 2.
```

Test set performance values:

```
     RMSE  Rsquared       MAE
1.1827222 0.6923342 0.9625217
```

RMSE Plot:



Model 2:

Train set model & performance:

```
Bayesian Ridge Regression (Model Averaged)

144 samples
```

```
 56 predictor

No pre-processing
Resampling: Cross-Validated (10 fold)
Summary of sample sizes: 128, 129, 132, 131, 130, 128, ...
Resampling results:

  RMSE      Rsquared   MAE
  1.273043  0.5922451  0.9631175
```

Test set performance values:

```
     RMSE  Rsquared       MAE
1.1507908 0.6643818 0.9519415
```

This method has no tuning parameters to view in a cross validation plot.

Model 3:

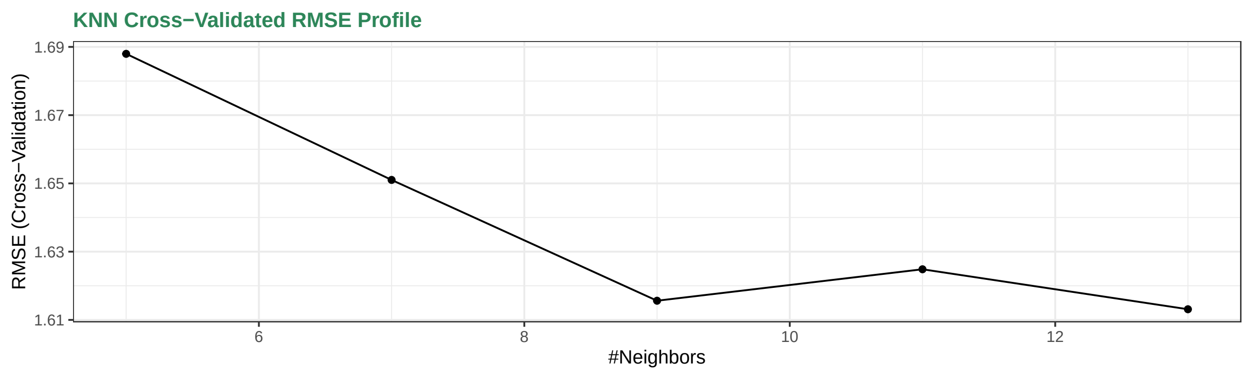
Train set model & performance:

```
k-Nearest Neighbors

144 samples
 56 predictor

No pre-processing
Resampling: Cross-Validated (10 fold)
Summary of sample sizes: 129, 129, 129, 130, 129, 130, ...
Resampling results across tuning parameters:

  k   RMSE      Rsquared   MAE
   5  1.687968  0.2163019  1.383713
   7  1.651019  0.2294142  1.336691
   9  1.615617  0.2496203  1.300205
  11  1.624835  0.2353595  1.297321
  13  1.613121  0.2430771  1.288989

RMSE was used to select the optimal model using the smallest value.
The final value used for the model was k = 13.
```

Test set performance values:

```
     RMSE  Rsquared       MAE
1.6339912 0.3535211 1.2331010
```

RMSE Plot:



Model 4:

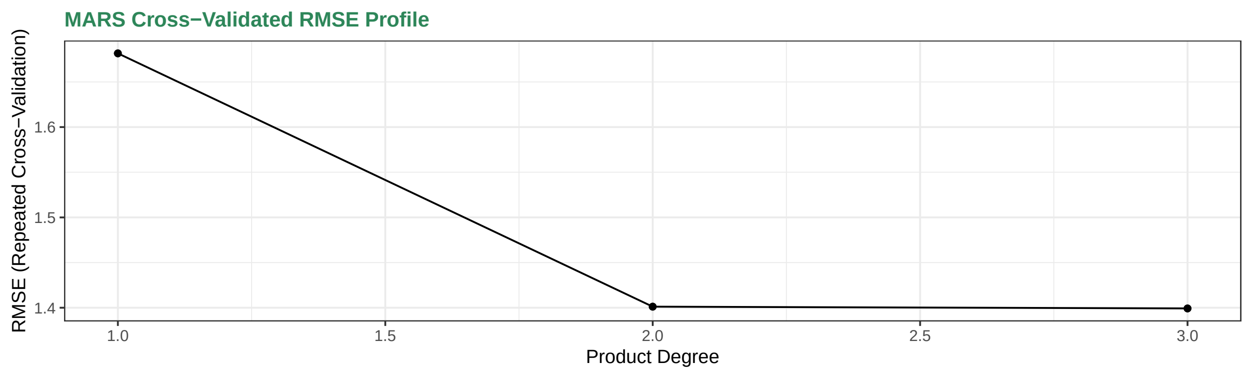
Train set model & performance:

```
Multivariate Adaptive Regression Spline

144 samples
 56 predictor

No pre-processing
Resampling: Cross-Validated (10 fold)
Summary of sample sizes: 131, 130, 129, 129, 129, 130, ...
Resampling results across tuning parameters:

  degree  RMSE      Rsquared   MAE
  1       1.191434  0.5999031  0.9678534
  2       1.179800  0.5975469  0.9527528
  3       1.295966  0.5590689  1.0728564

Tuning parameter 'nprune' was held constant at a value of 10
RMSE was used to select the optimal model using the smallest value.
The final values used for the model were nprune = 10 and degree = 2.
```

Test set performance values:

```
     RMSE  Rsquared       MAE
1.0218879 0.7391895 0.8412308
```

RMSE Plot:



(a) Which nonlinear regression model gives the optimal resampling and test set performance?

We trained four models on the chemical manufacturing process data: Support Vector Machines with Radial Basis Function Kernel (SVM), Bayesian Ridge Regression (Model Averaged), k-Nearest Neighbors (KNN), and Multivariate Adaptive Regression Spline (MARS).

We found that the SVM and Bayesian Ridge approach produced the lowest test accuracy score. However, the train accuracy for the Baysian Ridge was much higher than the test accuracy, indicating that model may have been overfitted to the training data. MARS also produced similiarly low accuracy scores with a slight degree of overfitting. While the MARS test RMSE was lower than SVM's test accuracy measures, SVM outperformed MARS with the training accuracy. There was a smaller difference between the train and test accuracy with the SVM method. As a result, we choose this as our optimal model for resampling and test set performance.

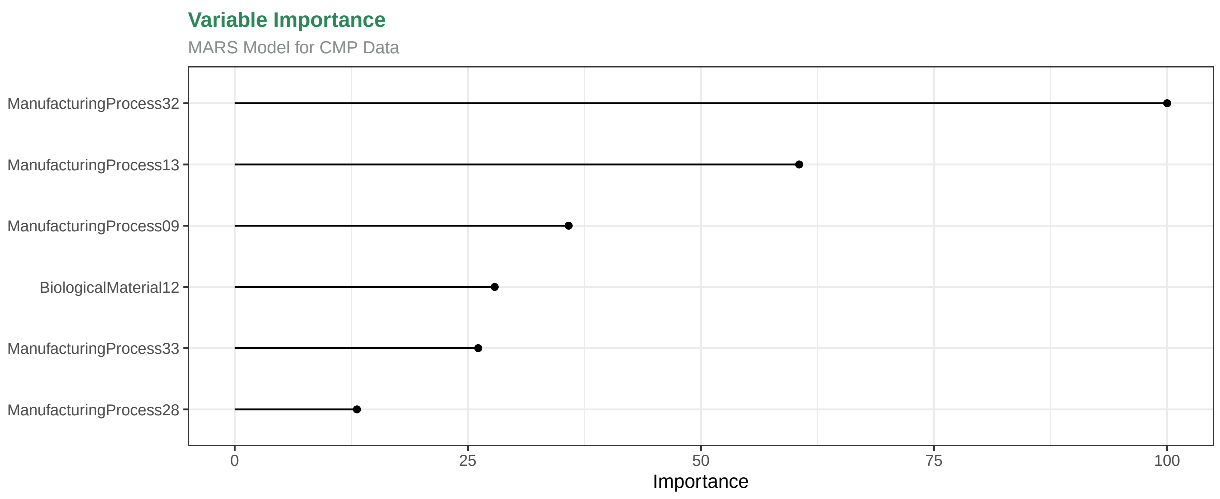
Table 3: Model Performance

	RMSE	Rsquared	MAE
svmTrain	**1.1706**	**0.6115**	**0.9054**
svmTest	**1.1827**	**0.6923**	**0.9625**
knnTrain	1.6248	1.6248	1.6248
knnTest	1.6340	0.3535	1.2331
bma_rrTrain	1.2730	0.5922	0.9631
bma_rrTest	1.1508	0.6644	0.9519
marsTrain	1.1914	0.5999	0.9679
marsTest	1.0219	0.7392	0.8412

(b) Which predictors are most important in the optimal nonlinear regression model? Do either the biological or process variables dominate the list? How do the top ten important predictors compare to the top ten predictors from the optimal linear model?

The `caret` package does not allow the `varImp` function to work on SVM models, so we instead used MARS to evaluate predictor importance of our optimal nonlinear regression models. We found this to be a suitable replacement because the MARS and SVM had similiar accuracy performance, albiet the MARS model may be slightly overfitted to the train data.

In our homework from Chapter 6, our PLS linear model identified mostly biological process variables as the important predictors. This differs from the non-linear important predictors identified in our MARS model. Conversely, the MARS method calculated variable importance for 7 indicators, of which 5 were manufacturing variables.



(c) Explore the relationships between the top predictors and the response for the predictors that are unique to the optimal nonlinear regression model. Do these plots reveal intuition about the biological or process predictors and their relationship with yield?

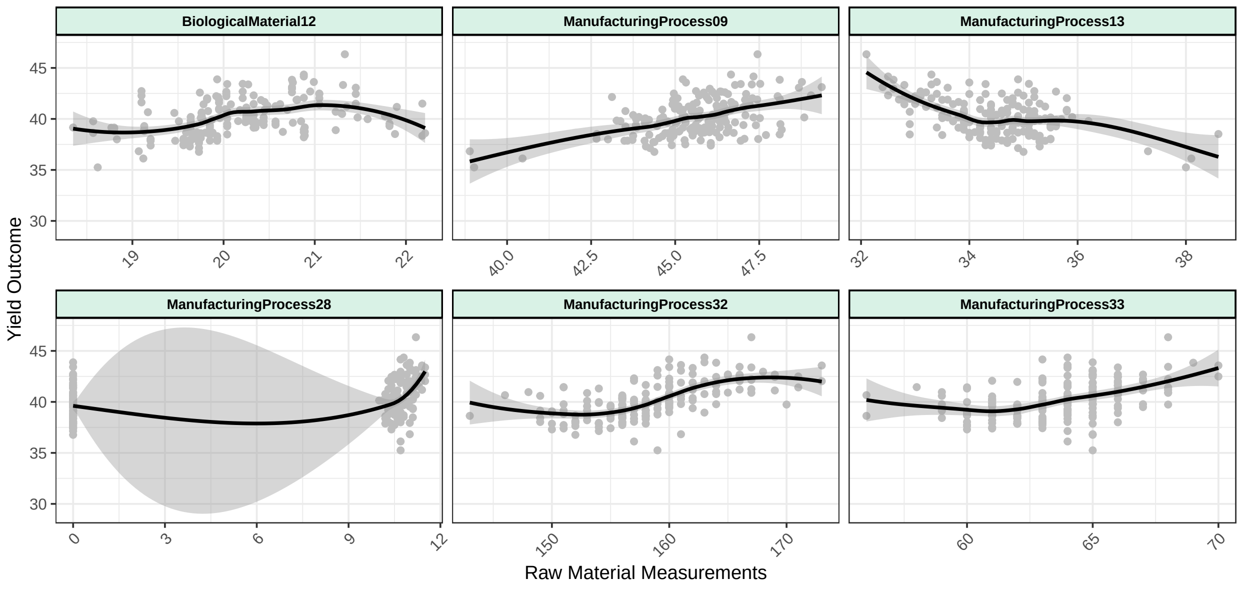
The following shows correlation between our top predictor and response variables using our MARS model.

Table 4: Correlation

Variable	Correlation
ManufacturingProcess32	0.6122974
ManufacturingProcess09	0.4276381
ManufacturingProcess33	0.4204690
BiologicalMaterial12	0.3262966
ManufacturingProcess28	0.2617653
ManufacturingProcess13	-0.4552924

We can use a scatterplot to further look at their relationship. With the exception of `ManufacturingProcess09`, none of the variables exibit a strong linear pattern when examined against yield. This depiction could help explain why variable importance results from our selected linear model varied greatly from our non-linear model.

Variable Importance Scatterplot



R Code

```
# (7.2 example)
set.seed(200)
trainingData <- mlbench.friedman1(200, sd = 1)
trainingData$x <- data.frame(trainingData$x)
featurePlot(trainingData$x, trainingData$y)
testData <- mlbench.friedman1(5000, sd = 1)
testData$x <- data.frame(testData$x)
# Example
knnModel <- train(x = trainingData$x, y = trainingData$y,
    method = "knn", preProc = c("center", "scale"),
    tuneLength = 10)
knnPred <- predict(knnModel, newdata = testData$x)
knnPerf <- postResample(pred = knnPred, obs = testData$y)
knnPlot <- ggplot(knnModel) + theme_bw() + theme() +
    labs(title = "KNN Cross-Validated RMSE Profile")

# Model 1
lmModel <- train(x = trainingData$x, y = trainingData$y,
    method = "lm", preProc = "pca", trControl = trainControl(method = "repeatedcv",
        repeats = 5))
lmPred <- predict(lmModel, newdata = testData$x)
lmPerf <- postResample(pred = lmPred, obs = testData$y)

# Model 2
plsModel <- train(x = trainingData$x, y = trainingData$y,
    method = "pls", preProc = "pca", tuneLength = 5,
    trControl = trainControl(method = "repeatedcv",
        repeats = 5))
plsPred <- predict(plsModel, newdata = testData$x)
```

```r
plsPerf <- postResample(pred = plsPred, obs = testData$y)
plsplot <- ggplot(plsModel) + theme_bw() + theme() +
    labs(title = "PLS Cross-Validated RMSE Profile")

# Model 3
marsModel <- train(x = trainingData$x, y = trainingData$y,
    method = "earth", metric = "RMSE", tuneGrid = expand.grid(degree = 1:3,
        nprune = 10), trControl = trainControl(method = "repeatedcv",
        repeats = 5))
marsPred <- predict(marsModel, newdata = testData$x)
marsPerf <- postResample(pred = marsPred, obs = testData$y)
marsplot <- ggplot(marsModel) + theme_bw() + theme() +
    labs(title = "MARS Cross-Validated RMSE Profile")

# (7.2b)
performance_table <- rbind(knnTrain = c(RMSE = knnModel$results$RMSE[6],
    RSquared = knnModel$results$RMSE[6], MAE = knnModel$results$RMSE[6]),
    knnTest = knnPerf, lmTrain = c(RMSE = lmModel$results$RMSE,
        RSquared = lmModel$results$Rsquared, MAE = lmModel$results$MAE),
    lmTest = lmPerf, plsTrain = c(plsModel$results$RMSE[2],
        plsModel$results$Rsquared[2], plsModel$results$MAE[2]),
    plsTest = plsPerf, marsTrain = c(marsModel$results$RMSE,
        marsModel$results$Rsquared, marsModel$results$MAE),
    marsTest = marsPerf) %>% kable(caption = "Model Performance",
    digits = 4) %>% kable_styling() %>% row_spec() %>%
    row_spec(row = 7:8, background = "#d9f2e6")

marsImp <- varImp(marsModel)

marsImptbl <- marsImp$importance %>% kable(caption = "MARS Model - Variable Importance",
    digits = 2) %>% kable_styling()


# (7.5a) Models FOR FINAL HW SUBMISSION, DO NOT
# REPEAT STEPS: JUST CALL VARIABLES FROM PRIOR
# ASSIGNMENT.
data(ChemicalManufacturingProcess)
CMP_Impute <- mice(ChemicalManufacturingProcess, m = 5,
    printFlag = F)
CMP_DF <- mice::complete(CMP_Impute, 2)

# Set random seed
set.seed(5)

# Create Partition for Train/Test Splits
trainingRows <- createDataPartition(CMP_DF$Yield, p = 0.8,
    list = FALSE)

# Split Train/Test Data
train <- CMP_DF[trainingRows, ]
test <- CMP_DF[-trainingRows, ]

# Pre-Process Recipe
```

```r
rec <- recipes::recipe(CMP_DF, Yield ~ .)
rec <- rec %>% step_nzv(all_predictors(), options = list(freq_cut = 95/5,
    unique_cut = 10))
prep_rec = prep(rec, training = CMP_DF)
CMP_DF_TF = bake(prep_rec, CMP_DF)

# Create Partition for Train/Test Splits
trainingRows <- createDataPartition(CMP_DF_TF$Yield,
    p = 0.8, list = FALSE)

# Split Train/Test Data
train <- CMP_DF_TF[trainingRows, ]
test <- CMP_DF_TF[-trainingRows, ]

# Non-Linear Model 1: Support Vector Machines with
# Radial Basis Function Kernel
svmModel <- train(Yield ~ ., data = train, method = "svmRadial",
    preProcess = "pca", trControl = trainControl(method = "cv",
        number = 10), tuneLength = 5)
svmPred <- predict(svmModel, newdata = test)
svmPerf <- postResample(pred = svmPred, obs = test$Yield)
svmPlot <- ggplot(svmModel) + theme_bw() + theme() +
    labs(title = "SVM Cross-Validated RMSE Profile")

# Non-Linear Model 2: Bayesian Ridge Regression
# (Model Averaged)
bma_rrModel <- train(Yield ~ ., data = train, method = "blassoAveraged",
    trControl = trainControl(method = "cv", number = 10),
    tuneLength = 5)
bma_rrPred <- predict(bma_rrModel, newdata = test)
bma_rrPerf <- postResample(pred = bma_rrPred, obs = test$Yield)

# Non-Linear Model 3: k-Nearest Neighbors (KNN)
knnModel <- train(Yield ~ ., data = train, method = "knn",
    trControl = trainControl(method = "cv", number = 10),
    tuneLength = 5)
knnPred <- predict(knnModel, newdata = test)
knnPerf <- postResample(pred = knnPred, obs = test$Yield)
knnPlot <- ggplot(knnModel) + theme_bw() + theme() +
    labs(title = "KNN Cross-Validated RMSE Profile")

# Non-Linear Model 4: Multivariate Adaptive
# Regression Spline (MARS)
marsModel <- train(Yield ~ ., data = train, method = "earth",
    tuneGrid = expand.grid(degree = 1:3, nprune = 10),
    trControl = trainControl(method = "cv", number = 10),
    tuneLength = 5)
marsPred <- predict(marsModel, newdata = test)
marsPerf <- postResample(pred = marsPred, obs = test$Yield)
marsPlot <- ggplot(marsModel) + theme_bw() + theme() +
    labs(title = "MARS Cross-Validated RMSE Profile")

# Performance
```

```r
performance_table2 <- rbind(svmTrain = c(svmModel$results$RMSE[5],
    svmModel$results$Rsquared[5], svmModel$results$MAE[5]),
    svmTest = svmPerf, knnTrain = c(RMSE = knnModel$results$RMSE[2],
        RSquared = knnModel$results$RMSE[2], MAE = knnModel$results$RMSE[2]),
    knnTest = knnPerf, bma_rrTrain = c(RMSE = bma_rrModel$results$RMSE,
        RSquared = bma_rrModel$results$Rsquared, MAE = bma_rrModel$results$MAE),
    bma_rrTest = bma_rrPerf, marsTrain = c(marsModel$results$RMSE,
        marsModel$results$Rsquared, marsModel$results$MAE),
    marsTest = marsPerf) %>% kable(caption = "Model Performance",
    digits = 4) %>% kable_styling() %>% row_spec() %>%
    row_spec(row = 1:2, background = "#d9f2e6")


# (7.5b)
marsImp <- varImp(marsModel)

mars_most_important <- as.data.frame(marsImp$importance) %>%
    rownames_to_column("Variable") %>% filter(Overall >
    0)

plot2 <- ggplot(mars_most_important, aes(x = reorder(Variable,
    Overall), y = Overall)) + geom_point() + geom_segment(aes(x = Variable,
    xend = Variable, y = 0, yend = Overall)) + labs(title = "Variable Importance",
    subtitle = "MARS Model for CMP Data", x = "", y = "Importance") +
    coord_flip() + theme_bw() + theme()

# (7.5c)
top <- mars_most_important$Variable
cor <- cor(train[, top], train$Yield, method = "pearson")
cor_tbl <- cor %>% as.data.frame() %>% rownames_to_column("Variable") %>%
    rename(Correlation = V1) %>% arrange(desc(Correlation)) %>%
    kable(caption = "Correlation") %>% kable_styling()
plot3 <- CMP_DF[, top] %>% cbind(Yield = CMP_DF$Yield) %>%
    gather(key = "Variable", value = "Value", -Yield) %>%
    ggplot(aes(Value, Yield, color = Variable)) + geom_point(color = "grey") +
    geom_smooth(stat = "smooth", color = "black", method = "loess") +
    facet_wrap(~Variable, scales = "free_x", nrow = 2) +
    labs(title = "Variable Importance Scatterplot",
        y = "Yield Outcome", x = "Raw Material Measurements") +
    theme_bw() + theme(legend.position = "none", axis.text.x = element_text(angle = 45,
    hjust = 1))
```