DATA 624 Homework 8 - Non-Linear Regression

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Overview

This is homework eight of the Fall 2024 edition of DATA 624. The assignment covers questions 7.2 and 7.5 from the exercise section of chapter 7 in Applied Predictive Modeling by Max Kuhn and Kjell Johnson

First, most of the requried libraries

```
library(tidyverse)
library(ggplot2)
library(gridExtra)
library(AppliedPredictiveModeling)
library(mlbench)
library(caret)
library(earth)
library(kernlab)
library(RANN)
```

7.2 Tuning models on benchmmark datasets:

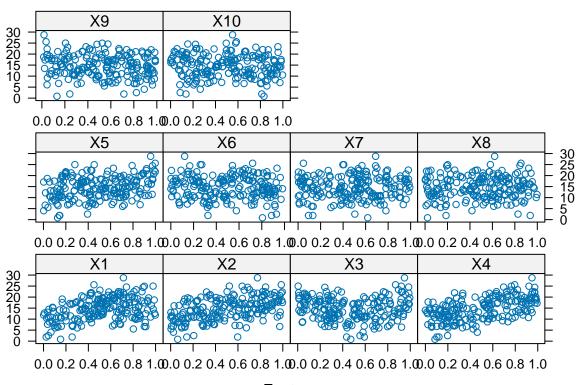
The exercise states: "Friedman (1991) introduced several benchmark data sets create by simulation. One of these simulations used the following nonlinear equation to create data:

$$y = 10\sin(\pi x_1 x_2) + 20(x_3 - 0.5)^2 + 10x_4 + 5x_5 + N(0, \sigma^2)$$

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"

The following code snippet was also provided:

```
trainingData <- mlbench.friedman1(200, sd = 1)
trainingData$x <- data.frame(trainingData$x)
featurePlot(trainingData$x, trainingData$y)</pre>
```



Feature

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

knnModel <- train(x = trainingData$x,
    y = trainingData$y,
    method = "knn",
    preProc = c("center", "scale"),
    tuneLength = 10)
    knnModel</pre>
```

```
## 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 3.719126 0.4938384
##
                             2.959920
        3.596913 0.5402103
                             2.837807
##
##
     9 3.604542 0.5501806
                              2.850472
##
     11 3.612526 0.5576494
                              2.867785
##
     13 3.606714 0.5717275
                              2.882308
##
     15 3.625217 0.5791756
                             2.909228
##
     17 3.610499 0.5969979
                              2.901709
     19 3.606544 0.6127054 2.903831
##
```

```
## 21 3.611499 0.6263947 2.912113 
## 23 3.629909 0.6367596 2.934772 
## 
## RMSE was used to select the optimal model using the smallest value. 
## The final value used for the model was k = 7.
```

I must now tune "several models on these data," and then provide comentary. I ave chosen the following models:

- Multivariate Adaptive Regression Splines (MARS)
- Neural Networks
- Support Vector Machines

7.2 - Multivariate Adaptive Regression Splines

I'm starting with because it's what I'm presenting on during my team's presentation. MARS is a nonparametric regression technique that allows you to model relationships without assuming a particular shape of relationship at the start It's a piecewise model with defined linear relationships called "splines" what map different segments of the data. The boundaries of the segments can overlap and are tied together with "knots.'

```
mc <- trainControl(method = "repeatedcv", number = 3)</pre>
mexpand_g <- expand.grid(.degree = 2:3, .nprune = 4:45)</pre>
life_on_mars <- train(trainingData$x, trainingData$y,</pre>
                       method = "earth",
                       tuneGrid = mexpand_g,
                       preProcess = c("center", "scale", "knnImpute"),
                       tuneLength = 15,
                       trControl = mc)
life on mars
## Multivariate Adaptive Regression Spline
##
## 200 samples
   10 predictor
##
## Pre-processing: centered (10), scaled (10), nearest neighbor imputation (10)
## Resampling: Cross-Validated (3 fold, repeated 1 times)
## Summary of sample sizes: 134, 133, 133
  Resampling results across tuning parameters:
##
##
##
     degree
             nprune
                     RMSE
                                Rsquared
                                            MAE
##
     2
              4
                      3.311659
                                0.6019001
                                           2.719880
##
     2
              5
                      3.132180
                                0.6448154
                                            2.545251
##
     2
              6
                      2.912083
                                0.6896125
                                            2.360018
     2
              7
##
                      2.444828
                               0.7788718
                                           1.902028
     2
              8
##
                      2.272775
                                0.8110137
                                            1.744256
     2
##
              9
                      1.944770
                                0.8591212
                                            1.464891
##
     2
             10
                      1.665242
                                0.8985534
                                            1.324536
##
     2
             11
                      1.635008 0.9012180
                                            1.314050
     2
##
             12
                      1.427742 0.9253497
                                            1.153250
##
     2
             13
                                0.9154320
                      1.522163
                                            1.216036
     2
             14
##
                      1.562438 0.9109944
                                           1.238524
##
     2
             15
                      1.552673 0.9114834
                                           1.250201
##
     2
             16
                      1.535044 0.9133345 1.235728
```

##	2	17	1.535044	0.9133345	1.235728
##	2	18	1.535044	0.9133345	1.235728
##	2	19	1.535044	0.9133345	1.235728
##	2	20	1.535044	0.9133345	1.235728
##	2	21	1.535044	0.9133345	1.235728
##	2	22	1.535044	0.9133345	1.235728
##	2	23	1.535044	0.9133345	1.235728
##	2	24	1.535044	0.9133345	1.235728
##	2	25	1.535044	0.9133345	1.235728
##	2	26	1.535044	0.9133345	1.235728
##	2	27	1.535044	0.9133345	1.235728
##	2	28	1.535044	0.9133345	1.235728
##	2	29	1.535044	0.9133345	1.235728
##	2	30	1.535044	0.9133345	1.235728
##	2	31	1.535044	0.9133345	1.235728
##	2	32	1.535044	0.9133345	1.235728
##	2	33	1.535044	0.9133345	1.235728
##	2	34	1.535044	0.9133345	1.235728
##	2	35	1.535044	0.9133345	1.235728
##	2	36	1.535044	0.9133345	1.235728
##	2	37	1.535044	0.9133345	1.235728
##	2	38	1.535044	0.9133345	1.235728
##	2	39	1.535044	0.9133345	1.235728
##	2	40	1.535044	0.9133345	1.235728
##	2	41	1.535044	0.9133345	1.235728
##	2	42	1.535044	0.9133345	1.235728
##	2	43	1.535044	0.9133345	1.235728
##	2	44	1.535044	0.9133345	1.235728
##	2	45	1.535044	0.9133345	1.235728
##	3	4	3.311659	0.6019001	2.719880
##	3	5	3.132180	0.6448154	2.545251
##	3	6	2.912083	0.6896125	2.360018
##	3	7	2.444828	0.7788718	1.902028
##	3	8	2.272775	0.8110137	1.744256
##	3	9	1.944770	0.8591212	1.464891
##	3	10	1.665242	0.8985534	1.324536
##	3	11	1.635008	0.9012180	1.314050
##	3	12	1.427742	0.9253497	1.153250
##	3	13	1.522163	0.9154320	1.216036
##	3	14	1.562438	0.9109944	1.238524
##	3	15	1.552673	0.9114834	1.250201
##	3	16	1.535044	0.9133345	1.235728
##	3	17	1.535044	0.9133345	1.235728
##	3	18	1.535044	0.9133345	1.235728
##	3	19	1.535044	0.9133345	1.235728
##	3	20	1.535044	0.9133345	1.235728
##	3	21	1.535044	0.9133345	1.235728
##	3	22	1.535044	0.9133345	1.235728
##	3	23	1.535044	0.9133345	1.235728
##	3	23 24	1.535044	0.9133345	1.235728
##	3	25 25	1.535044	0.9133345	1.235728
##	3	26	1.535044	0.9133345	1.235728
##	3	26 27	1.535044	0.9133345	1.235728
##	3	28	1.535044	0.9133345	1.235728
##	S	20	1.000044	0.9133343	1.233120

```
##
     3
             29
                     1.535044 0.9133345 1.235728
##
     3
             30
                     1.535044 0.9133345 1.235728
                     1.535044 0.9133345 1.235728
##
     3
             31
##
     3
             32
                     1.535044 0.9133345 1.235728
##
     3
             33
                     1.535044 0.9133345
                                          1.235728
     3
             34
                     1.535044 0.9133345 1.235728
##
     3
             35
##
                     1.535044 0.9133345 1.235728
##
     3
             36
                     1.535044 0.9133345 1.235728
##
     3
             37
                     1.535044 0.9133345
                                          1.235728
             38
##
     3
                     1.535044 0.9133345 1.235728
##
     3
             39
                     1.535044 0.9133345 1.235728
##
     3
             40
                     1.535044 0.9133345 1.235728
##
     3
             41
                     1.535044 0.9133345 1.235728
##
     3
             42
                     1.535044 0.9133345 1.235728
##
     3
             43
                     1.535044 0.9133345 1.235728
##
     3
             44
                     1.535044 0.9133345 1.235728
##
     3
             45
                     1.535044 0.9133345 1.235728
##
## RMSE was used to select the optimal model using the smallest value.
## The final values used for the model were nprune = 12 and degree = 2.
m_predict <- predict(life_on_mars, newdata = testData$x)</pre>
predict_track <- data.frame(matrix(vector(), 0, 4, # Increased to 4 for the model name
                dimnames = list(NULL, c("RMSE", "r2", "MAE", "model"))),
                stringsAsFactors = FALSE)
m_metrics <- as.data.frame(t(postResample(pred = m_predict, obs = testData$y)))</pre>
m metrics$model <- "MARS"
predict_track <- rbind(predict_track, m_metrics)</pre>
```

7.2 - Support Vector Machines

Support Vector Machines finds an optimal hyperplane to separate data points by maximizing the margin between different targets values. A radial basis function can be used for non-linear data as well.

```
## Support Vector Machines with Radial Basis Function Kernel
##
## 200 samples
## 10 predictor
##
## Pre-processing: centered (10), scaled (10)
```

```
## Resampling: Cross-Validated (5 fold, repeated 3 times)
  Summary of sample sizes: 160, 160, 160, 160, 160, 160, ...
   Resampling results across tuning parameters:
##
##
     С
          sigma
                 RMSE
                            Rsquared
                                        MAE
                                        3.026526
##
         0.05
                            0.7106557
     0.1
                  3.723903
##
     0.1
          0.10
                  3.917585
                            0.7009434
                                        3.174456
##
     0.1
         0.15
                  4.250298
                            0.6803521
                                        3.453626
##
     0.1 0.20
                  4.530993
                            0.6483326
                                        3.702109
##
     0.2 0.05
                  3.094990
                            0.7290384
                                        2.453913
##
     0.2 0.10
                  3.232816
                            0.7272018
                                        2.559308
##
     0.2 0.15
                  3.630465
                            0.7016895
                                        2.899013
##
     0.2 0.20
                  4.035662
                            0.6664100
                                        3.248765
##
     0.3 0.05
                  2.850083
                            0.7420247
                                        2.197422
##
     0.3 0.10
                  2.956281
                            0.7441759
                                        2.276565
##
     0.3
          0.15
                  3.288211
                            0.7165915
                                        2.572111
##
     0.3 0.20
                  3.683004
                            0.6820470
                                        2.921419
##
     0.4 0.05
                  2.735546
                            0.7503461
                                        2.082240
     0.4 0.10
##
                  2.819071
                            0.7504706
                                        2.136744
##
     0.4 0.15
                 3.121262
                            0.7226468
                                        2.400362
##
     0.4 0.20
                 3.481744
                            0.6898263
                                        2.726998
     0.5 0.05
##
                  2.655809
                            0.7570843
                                        2.006147
##
     0.5 0.10
                  2.723461
                            0.7574490
                                        2.048870
##
     0.5 0.15
                  3.017949
                            0.7254601
                                        2.301119
##
     0.5 0.20
                  3.368566
                            0.6912825
                                        2.610398
##
     0.6 0.05
                  2.598904
                            0.7623278
                                        1.959341
##
     0.6 0.10
                  2.661616
                            0.7623015
                                        2.000087
##
     0.6 0.15
                  2.946295
                            0.7281582
                                        2.238830
##
     0.6 0.20
                  3.288601
                            0.6911002
                                        2.527406
##
     0.7 0.05
                  2.549073
                            0.7682990
                                        1.920879
##
     0.7
         0.10
                  2.618822
                            0.7654494
                                        1.968101
##
     0.7
          0.15
                  2.893491
                            0.7306077
                                        2.198658
##
     0.7
          0.20
                  3.227760
                            0.6925924
                                        2.473100
                  2.507235
##
     0.8
         0.05
                            0.7738224
                                        1.891699
##
     0.8
         0.10
                  2.586948
                            0.7678633
                                        1.945064
##
     0.8 0.15
                 2.855315
                            0.7331353
                                        2.169950
##
     0.8 0.20
                 3.182047
                            0.6940005
                                        2.435306
##
     0.9
         0.05
                  2.475813
                            0.7780461
                                        1.870435
     0.9
          0.10
                            0.7701869
##
                  2.561451
                                        1.923824
##
     0.9 0.15
                  2.825430
                            0.7358589
                                        2.145652
##
     0.9 0.20
                  3.148122
                            0.6953027
                                        2.409639
##
     1.0 0.05
                  2.449445
                            0.7815835
                                       1.850789
##
     1.0
          0.10
                  2.541630
                            0.7724449
                                        1.907116
##
     1.0 0.15
                  2.799129
                            0.7386363
                                        2.124024
##
     1.0
          0.20
                  3.120230
                            0.6971721
                                        2.386707
##
## RMSE was used to select the optimal model using the smallest value.
## The final values used for the model were sigma = 0.05 and C = 1.
svm_p<- predict(svm_m, newdata = testData$x)</pre>
svm_metrics <- as.data.frame(t(postResample(pred = svm_p, obs = testData$y)))</pre>
svm_metrics$model <- "SVMs"</pre>
predict_track <- rbind(predict_track, svm_metrics)</pre>
```

Thus far, the The MARS model is ahead of the SVM, with a higher RMSE of 1.34 and R-squared of ~0.938.

For the SVM, the increasing C improved results, but gains leveled off after C = 1. Both models are strong, but MARS might be the better pick here for capturing data variance.

7.2 Neural Networks

This code trains an averaged neural network model using the avNNet method, applying preprocessing steps to center and scale the data. It customizes the model with a tuning grid, cross-validation controls, and specific parameters for network size, weights, and iteration limits.

```
nnet_grid <- expand.grid(.decay = c(0, 0.001, 0.01, 0.05, 0.1), .size = 1:15, .bag = FALSE)
control <- trainControl(method = "repeatedcv", number = 10, repeats = 3)</pre>
nnet maxnwts <- 150
nnet_model <- train(x = trainingData$x,</pre>
                    y = trainingData$y,
                    method = "avNNet",
                    preProcess = c("center", "scale"),
                    tuneGrid = nnet_grid,
                    trControl = control,
                    linout = TRUE,
                    trace = FALSE,
                    MaxNWts = nnet_maxnwts,
                    maxit = 300)
nnet_model
## Model Averaged Neural Network
##
## 200 samples
   10 predictor
##
##
## Pre-processing: centered (10), scaled (10)
## Resampling: Cross-Validated (10 fold, repeated 3 times)
## Summary of sample sizes: 180, 180, 180, 180, 180, 180, ...
## Resampling results across tuning parameters:
##
##
     decay
           size RMSE
                             Rsquared
                                        MAE
                            0.7190798 2.204010
##
     0.000
             1
                  2.802094
##
     0.000
             2
                  2.523775
                            0.7718422 2.000498
     0.000
                  2.121372
                            0.8332285
##
             3
                                        1.695636
##
     0.000
             4
                  2.013886
                            0.8546191
                                        1.567829
##
     0.000
                  2.367556 0.8071777
             5
                                        1.787363
##
     0.000
                  3.162169
                            0.7048747
                                        2.247950
             6
##
     0.000
             7
                  4.834655
                            0.5205897
                                        3.024356
##
     0.000
             8
                  5.474489
                            0.5289465
                                        3.301518
##
     0.000
             9
                  4.923984 0.5868559
                                        2.905196
##
     0.000
                  3.849287
                            0.6118177
            10
                                        2.563422
##
     0.000
            11
                  3.334532
                             0.6533816
                                        2.500506
##
                  3.461783
                            0.6910991
                                        2.596698
     0.000
            12
##
     0.000
           13
                       NaN
                                   NaN
                                             NaN
##
     0.000
            14
                       NaN
                                   NaN
                                             NaN
##
     0.000
                                   NaN
            15
                       NaN
                                             NaN
                  2.778055 0.7207142 2.177187
##
     0.001
             1
     0.001
             2
                  2.539277 0.7694598 2.012517
##
```

2.201545 0.8238616 1.732125

##

0.001

3

```
##
     0.001
              4
                   2.038469 0.8522219
                                          1.612823
##
     0.001
                   2.222230
                              0.8204783
                                          1.728492
              5
                                          1.910654
##
     0.001
                   2.461068
                              0.7799747
##
     0.001
                   2.766955
              7
                              0.7389167
                                          2.167112
##
     0.001
              8
                   3.009032
                              0.7142539
                                          2.245309
##
     0.001
              9
                   3.368694
                              0.6685557
                                          2.542988
##
     0.001
                   2.924293
                              0.7198047
            10
                                          2.257227
     0.001
                              0.7230730
##
            11
                   2.878914
                                          2.244031
##
     0.001
             12
                   2.859150
                              0.7165688
                                          2.268190
##
     0.001
             13
                        NaN
                                    NaN
                                               NaN
##
     0.001
            14
                        NaN
                                    NaN
                                               NaN
##
     0.001
                        NaN
                                    NaN
                                               NaN
            15
     0.010
                   2.756020 0.7256414
##
             1
                                         2.160956
##
     0.010
              2
                   2.532561
                              0.7679450
                                          2.032686
##
     0.010
                   2.219390
                              0.8185134
                                          1.753755
              3
##
     0.010
              4
                   2.098196
                              0.8435576
                                          1.643065
##
     0.010
                   2.165545
                              0.8311878
                                          1.676269
              5
##
     0.010
                   2.367029
                              0.7981274
                                          1.837282
##
     0.010
                   2.526360
                              0.7748758
                                          1.962880
              7
##
     0.010
              8
                   2.743666
                              0.7396926
                                          2.116238
##
     0.010
              9
                   2.838719
                              0.7198539
                                          2.190079
##
     0.010
             10
                   2.751071
                              0.7282082
                                          2.156551
##
     0.010
                   2.867661
                              0.7150112
                                          2.305827
             11
##
     0.010
            12
                   2.946496
                              0.6983125
                                          2.324035
##
                      NaN
                                               NaN
     0.010
             13
                                    NaN
##
     0.010
             14
                       NaN
                                    NaN
                                               NaN
                      NaN
##
     0.010
            15
                                    NaN
                                               NaN
     0.050
                   2.728565
                              0.7295766
                                          2.136572
##
             1
     0.050
                   2.550234
##
              2
                              0.7664020
                                         2.020062
     0.050
                   2.243660
##
              3
                              0.8151612
                                         1.767740
##
     0.050
              4
                   2.066508
                              0.8456286
                                          1.623204
##
     0.050
              5
                   2.195013
                              0.8246665
                                          1.705472
     0.050
                   2.385456
##
                              0.7988194
                                          1.871967
##
     0.050
                   2.516904
                              0.7742450
                                          1.939992
              7
##
     0.050
              8
                   2.612743
                              0.7627249
                                          2.030529
##
     0.050
             9
                   2.704107
                              0.7438953
                                          2.113998
##
     0.050
             10
                   2.621658
                              0.7584304
                                          2.045466
##
     0.050
                   2.730381
                              0.7400997
                                          2.144502
             11
##
     0.050
             12
                   2.788834
                              0.7317214
                                          2.178176
##
     0.050
                                               NaN
             13
                        {\tt NaN}
                                    {\tt NaN}
##
     0.050
                        NaN
                                               NaN
             14
                                    \mathtt{NaN}
##
     0.050
                        \mathtt{NaN}
                                    NaN
                                               NaN
            15
     0.100
                   2.736295
                              0.7278178
                                          2.142121
##
              1
##
     0.100
                              0.7711798
                                         2.028058
              2
                   2.527389
##
     0.100
                   2.168856
                              0.8232641
                                          1.733253
              3
##
     0.100
                   2.155233
                              0.8333829
                                          1.701868
              4
                   2.172664
##
     0.100
              5
                              0.8277510
                                          1.698866
##
     0.100
                   2.291981
                              0.8124337
                                          1.796571
##
     0.100
              7
                   2.508576
                              0.7766792
                                          1.973119
##
     0.100
              8
                   2.534458
                              0.7659478
                                          1.964556
     0.100
##
              9
                   2.573739
                              0.7640563
                                          2.003362
##
     0.100
             10
                   2.610022
                              0.7561825
                                         2.029116
                   2.522858
##
     0.100
             11
                              0.7767753
                                         1.991092
##
     0.100
            12
                   2.674768 0.7477552 2.086116
```

```
##
     0.100 13
                        NaN
                                    NaN
                                              NaN
     0.100 14
                        NaN
                                    NaN
                                              NaN
##
##
     0.100 15
                        NaN
                                    NaN
                                              NaN
##
## Tuning parameter 'bag' was held constant at a value of FALSE
## RMSE was used to select the optimal model using the smallest value.
## The final values used for the model were size = 4, decay = 0 and bag = FALSE.
nn p <- predict(nnet model, newdata = testData$x)</pre>
nn_metrics <- as.data.frame(t(postResample(pred = nn_p, obs = testData$y)))</pre>
nn_metrics$model <- "Neural Networks"</pre>
predict_track <- rbind(predict_track, nn_metrics)</pre>
predict_track
##
         RMSE Rsquared
                                              model
                               MAE
## 1 1.233097 0.9382421 0.9869724
                                               MARS
## 2 2.296046 0.7887541 1.7584783
                                               SVMc
## 3 1.931904 0.8493991 1.4735077 Neural Networks
```

The final part of the question states: "Which models appear to give the best performance? Does MARS select the informative predictors (those named X1–X5)?"

${ m Answer}:$

Based on the above, the mars model came out ahead. It did a better job of capturing the underlying patterns in the data. While SVMs and Neural Networks showed decent performance, their higher RMSE values suggest that they may not predict as accurately as MARS for this particular dataset.

7.5 training several non-linear models

The exercise states: "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.

I'll first bring in the data from 6.3.

Now I can run amm the models again, using the same order as earlier.

```
nnet_g <- expand.grid(.decay = c(0, 0.001, 0.01), .size = 1:1, .bag = FALSE)</pre>
nnet_mw \leftarrow 5 * (ncol(ctr) + 1) + 5 + 1
nnmt <- train(Yield ~ ., data = ctr,</pre>
               method = "avNNet",
               tuneGrid = nnet_g,
               trControl = chem_ct,
               linout = TRUE,
               trace = FALSE,
               MaxNWts = nnet_mw,
               maxit = 130)
nnpt <- predict(nnmt, newdata = ctt)</pre>
marst <- train(Yield ~ ., data = ctr,</pre>
                method = "earth",
                tuneGrid = mexpand_gt,
                trControl = chem_ct)
marspt <- predict(marst, newdata = ctt)</pre>
svmtt <- train(Yield ~ ., data = ctr,</pre>
                method = "svmRadial",
                tuneLength = 8,
                trControl = chem ct)
svmpt <- predict(svmtt, newdata = ctt)</pre>
chem_r <- data.frame(Model = character(),</pre>
                      RMSE = numeric(),
                      R_squared = numeric(),
                      MAE = numeric(),
                      stringsAsFactors = FALSE)
knn_r <- postResample(pred = knnpt, obs = ctt$Yield)
chem_r <- rbind(chem_r, data.frame(Model = "KNN",</pre>
                                       RMSE = knn_r[1],
                                       R_{squared} = knn_r[2],
                                       MAE = knn_r[3])
nn r <- postResample(pred = nnpt, obs = ctt$Yield)
chem_r <- rbind(chem_r, data.frame(Model = "Averaged Neural Network",</pre>
                                       RMSE = nn_r[1],
                                       R_{squared} = nn_r[2],
                                       MAE = nn_r[3])
mars_r <- postResample(pred = marspt, obs = ctt$Yield)</pre>
chem_r <- rbind(chem_r, data.frame(Model = "MARS",</pre>
                                       RMSE = mars_r[1],
                                       R_squared = mars_r[2],
                                       MAE = mars_r[3])
svm_results <- postResample(pred = svmpt, obs = ctt$Yield)</pre>
chem_r <- rbind(chem_r, data.frame(Model = "SVM",</pre>
                                       RMSE = svm_results[1],
                                       R_squared = svm_results[2],
```

7.5.a - Which nonlinear regression model gives the optimal resampling and test set performance?

Answer: SVM has the lowest RMSE at 0.7649 and the highest R-squared at 0.8526684 among all models. This shows it has best predictive accuracy and also accounts for a lot of the variance in the data. It also has the lowest MAE at 0.6, which means its making the smallest average prediction errors as well.

Based on the above, I would say SVM provided the optimal resampling and test set performance based.

```
perfs <- as.data.frame(rbind(
    "KNN" = postResample(pred = knnpt, obs = ctt $Yield),
    "MARS" = postResample(pred = marspt, obs = ctt $Yield),
    "SVM" = postResample(pred = svmpt, obs = ctt $Yield),
    "Averaged Neural Network" = postResample(pred = nnpt, obs = ctt $Yield)
))

perfs <- cbind(Model = rownames(perfs), perfs)
rownames(perfs) <- NULL

perfs <- perfs %>% arrange(RMSE)
```

```
## Model RMSE Rsquared MAE
## 1 SVM 1.159326 0.4430202 0.9447833
## 2 Averaged Neural Network 1.204325 0.3933972 0.9887849
## 3 KNN 1.222443 0.4035379 0.9609687
## 4 MARS 1.247842 0.3866294 0.9904590
```

7.5.b - Determining the most important predictors

The next component question states:

"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?"

Answer: As with the last time we worked with this same dataset, there's pretty much an even split between biological and process variables at the top.

```
varImp(svmtt, 10)
```

```
## loess r-squared variable importance
##
## only 20 most important variables shown (out of 57)
##
## Overall
## ManufacturingProcess32 100.00
## ManufacturingProcess13 89.95
```

```
## BiologicalMaterial06
                             82.97
## BiologicalMaterial03
                             78.17
## ManufacturingProcess17
                             75.61
## ManufacturingProcess36
                             69.03
## ManufacturingProcess09
                             66.81
## BiologicalMaterial12
                             66.17
## ManufacturingProcess31
                             65.78
## ManufacturingProcess06
                             63.53
## BiologicalMaterial02
                             61.89
## ManufacturingProcess33
                             52.91
## ManufacturingProcess29
                             49.55
## BiologicalMaterial01
                             47.04
## BiologicalMaterial04
                             46.91
## BiologicalMaterial11
                             43.99
## ManufacturingProcess11
                             42.92
## BiologicalMaterial08
                             42.42
## BiologicalMaterial09
                             40.69
## ManufacturingProcess12
                             37.30
```

7.5.c Exploring relationships in the data

The final component question states:

"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?"

Answer:

A lot of random patterns here but also strong ones. Maufacturing Process 36 has a very specific style of distribution against yield. I would be curious to know what's driving that. My intuition would now say there will always be some sort of meaningful relationship but it does breakdown along biological/processing lines.

```
top_vars <- varImp(svmtt)$importance %>%
    arrange(desc(Overall)) %>%
    head(10) %>%
    rownames()
besties <- top_vars

plotter <- lapply(besties, function(predictor) {
    ggplot(ctt, aes(x = .data[[predictor]], y = Yield)) +
        geom_point() +
        labs(x = predictor, y = "Yield", title = paste(predictor, "vs Yield")) +
        theme(plot.title = element_text(size = 10))
})
grid.arrange(grobs = plotter)</pre>
```

