DATA624 Homework 1 - Week 4

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# Libraries

Loading in the libraries referenced in Sect. 6.5.

library(elasticnet)  
library(caret)  
library(MASS)  
library(lars)  
library(stats)  
library(pls)  
library(tidyverse)  
library(dplyr)  
library(RANN)  
library(GGally)  
library(naniar)

# Week 4

## KJ 6.3

*A chemical manufacturing process for a pharmaceutical product was discussed in Sec. 1.4. In this problem, the objective is to understand the relationship between biological measurements of the raw materials (predictors), measurements of the manufacturing process (predictors), and the response of product yield. Biological predictors cannot be changed but can be used to assess the quality of the raw material before processing. On the other hand, manufacturing process predictors can be changed in the manufacturing process. Improving product yield by 1% will boost revenue by approximately one hundred thousand dollars per batch ($100,000/batch):*

### (a)

*Start R and use these commands to load the data:*

*The matrix processPredictors contains the 57 predictors (12 describing the input of biological material and 45 describing the process predictors) for the 176 manufacturing runs. yield contains the percent yield for each run.*

library(AppliedPredictiveModeling)  
data(ChemicalManufacturingProcess)  
df\_raw <- ChemicalManufacturingProcess

### b.

*A small percentage of cells in the predictor set contain missing values. Use the imputation function to fill in these missing values (e.g., see Sec. 3.8).*

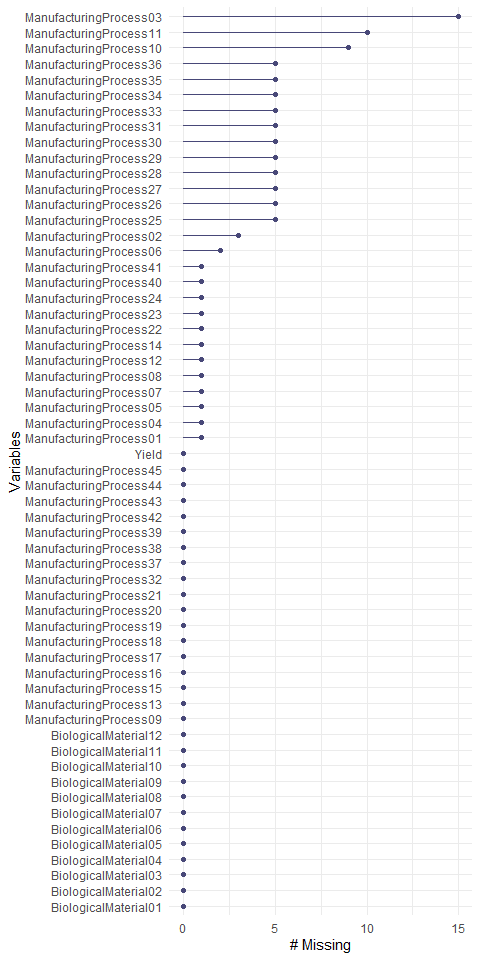
summary(df\_raw)

#> Yield BiologicalMaterial01 BiologicalMaterial02 BiologicalMaterial03  
#> Min. :35.25 Min. :4.580 Min. :46.87 Min. :56.97   
#> 1st Qu.:38.75 1st Qu.:5.978 1st Qu.:52.68 1st Qu.:64.98   
#> Median :39.97 Median :6.305 Median :55.09 Median :67.22   
#> Mean :40.18 Mean :6.411 Mean :55.69 Mean :67.70   
#> 3rd Qu.:41.48 3rd Qu.:6.870 3rd Qu.:58.74 3rd Qu.:70.43   
#> Max. :46.34 Max. :8.810 Max. :64.75 Max. :78.25   
#>   
#> BiologicalMaterial04 BiologicalMaterial05 BiologicalMaterial06  
#> Min. : 9.38 Min. :13.24 Min. :40.60   
#> 1st Qu.:11.24 1st Qu.:17.23 1st Qu.:46.05   
#> Median :12.10 Median :18.49 Median :48.46   
#> Mean :12.35 Mean :18.60 Mean :48.91   
#> 3rd Qu.:13.22 3rd Qu.:19.90 3rd Qu.:51.34   
#> Max. :23.09 Max. :24.85 Max. :59.38   
#>   
#> BiologicalMaterial07 BiologicalMaterial08 BiologicalMaterial09  
#> Min. :100.0 Min. :15.88 Min. :11.44   
#> 1st Qu.:100.0 1st Qu.:17.06 1st Qu.:12.60   
#> Median :100.0 Median :17.51 Median :12.84   
#> Mean :100.0 Mean :17.49 Mean :12.85   
#> 3rd Qu.:100.0 3rd Qu.:17.88 3rd Qu.:13.13   
#> Max. :100.8 Max. :19.14 Max. :14.08   
#>   
#> BiologicalMaterial10 BiologicalMaterial11 BiologicalMaterial12  
#> Min. :1.770 Min. :135.8 Min. :18.35   
#> 1st Qu.:2.460 1st Qu.:143.8 1st Qu.:19.73   
#> Median :2.710 Median :146.1 Median :20.12   
#> Mean :2.801 Mean :147.0 Mean :20.20   
#> 3rd Qu.:2.990 3rd Qu.:149.6 3rd Qu.:20.75   
#> Max. :6.870 Max. :158.7 Max. :22.21   
#>   
#> ManufacturingProcess01 ManufacturingProcess02 ManufacturingProcess03  
#> Min. : 0.00 Min. : 0.00 Min. :1.47   
#> 1st Qu.:10.80 1st Qu.:19.30 1st Qu.:1.53   
#> Median :11.40 Median :21.00 Median :1.54   
#> Mean :11.21 Mean :16.68 Mean :1.54   
#> 3rd Qu.:12.15 3rd Qu.:21.50 3rd Qu.:1.55   
#> Max. :14.10 Max. :22.50 Max. :1.60   
#> NA's :1 NA's :3 NA's :15   
#> ManufacturingProcess04 ManufacturingProcess05 ManufacturingProcess06  
#> Min. :911.0 Min. : 923.0 Min. :203.0   
#> 1st Qu.:928.0 1st Qu.: 986.8 1st Qu.:205.7   
#> Median :934.0 Median : 999.2 Median :206.8   
#> Mean :931.9 Mean :1001.7 Mean :207.4   
#> 3rd Qu.:936.0 3rd Qu.:1008.9 3rd Qu.:208.7   
#> Max. :946.0 Max. :1175.3 Max. :227.4   
#> NA's :1 NA's :1 NA's :2   
#> ManufacturingProcess07 ManufacturingProcess08 ManufacturingProcess09  
#> Min. :177.0 Min. :177.0 Min. :38.89   
#> 1st Qu.:177.0 1st Qu.:177.0 1st Qu.:44.89   
#> Median :177.0 Median :178.0 Median :45.73   
#> Mean :177.5 Mean :177.6 Mean :45.66   
#> 3rd Qu.:178.0 3rd Qu.:178.0 3rd Qu.:46.52   
#> Max. :178.0 Max. :178.0 Max. :49.36   
#> NA's :1 NA's :1   
#> ManufacturingProcess10 ManufacturingProcess11 ManufacturingProcess12  
#> Min. : 7.500 Min. : 7.500 Min. : 0.0   
#> 1st Qu.: 8.700 1st Qu.: 9.000 1st Qu.: 0.0   
#> Median : 9.100 Median : 9.400 Median : 0.0   
#> Mean : 9.179 Mean : 9.386 Mean : 857.8   
#> 3rd Qu.: 9.550 3rd Qu.: 9.900 3rd Qu.: 0.0   
#> Max. :11.600 Max. :11.500 Max. :4549.0   
#> NA's :9 NA's :10 NA's :1   
#> ManufacturingProcess13 ManufacturingProcess14 ManufacturingProcess15  
#> Min. :32.10 Min. :4701 Min. :5904   
#> 1st Qu.:33.90 1st Qu.:4828 1st Qu.:6010   
#> Median :34.60 Median :4856 Median :6032   
#> Mean :34.51 Mean :4854 Mean :6039   
#> 3rd Qu.:35.20 3rd Qu.:4882 3rd Qu.:6061   
#> Max. :38.60 Max. :5055 Max. :6233   
#> NA's :1   
#> ManufacturingProcess16 ManufacturingProcess17 ManufacturingProcess18  
#> Min. : 0 Min. :31.30 Min. : 0   
#> 1st Qu.:4561 1st Qu.:33.50 1st Qu.:4813   
#> Median :4588 Median :34.40 Median :4835   
#> Mean :4566 Mean :34.34 Mean :4810   
#> 3rd Qu.:4619 3rd Qu.:35.10 3rd Qu.:4862   
#> Max. :4852 Max. :40.00 Max. :4971   
#>   
#> ManufacturingProcess19 ManufacturingProcess20 ManufacturingProcess21  
#> Min. :5890 Min. : 0 Min. :-1.8000   
#> 1st Qu.:6001 1st Qu.:4553 1st Qu.:-0.6000   
#> Median :6022 Median :4582 Median :-0.3000   
#> Mean :6028 Mean :4556 Mean :-0.1642   
#> 3rd Qu.:6050 3rd Qu.:4610 3rd Qu.: 0.0000   
#> Max. :6146 Max. :4759 Max. : 3.6000   
#>   
#> ManufacturingProcess22 ManufacturingProcess23 ManufacturingProcess24  
#> Min. : 0.000 Min. :0.000 Min. : 0.000   
#> 1st Qu.: 3.000 1st Qu.:2.000 1st Qu.: 4.000   
#> Median : 5.000 Median :3.000 Median : 8.000   
#> Mean : 5.406 Mean :3.017 Mean : 8.834   
#> 3rd Qu.: 8.000 3rd Qu.:4.000 3rd Qu.:14.000   
#> Max. :12.000 Max. :6.000 Max. :23.000   
#> NA's :1 NA's :1 NA's :1   
#> ManufacturingProcess25 ManufacturingProcess26 ManufacturingProcess27  
#> Min. : 0 Min. : 0 Min. : 0   
#> 1st Qu.:4832 1st Qu.:6020 1st Qu.:4560   
#> Median :4855 Median :6047 Median :4587   
#> Mean :4828 Mean :6016 Mean :4563   
#> 3rd Qu.:4877 3rd Qu.:6070 3rd Qu.:4609   
#> Max. :4990 Max. :6161 Max. :4710   
#> NA's :5 NA's :5 NA's :5   
#> ManufacturingProcess28 ManufacturingProcess29 ManufacturingProcess30  
#> Min. : 0.000 Min. : 0.00 Min. : 0.000   
#> 1st Qu.: 0.000 1st Qu.:19.70 1st Qu.: 8.800   
#> Median :10.400 Median :19.90 Median : 9.100   
#> Mean : 6.592 Mean :20.01 Mean : 9.161   
#> 3rd Qu.:10.750 3rd Qu.:20.40 3rd Qu.: 9.700   
#> Max. :11.500 Max. :22.00 Max. :11.200   
#> NA's :5 NA's :5 NA's :5   
#> ManufacturingProcess31 ManufacturingProcess32 ManufacturingProcess33  
#> Min. : 0.00 Min. :143.0 Min. :56.00   
#> 1st Qu.:70.10 1st Qu.:155.0 1st Qu.:62.00   
#> Median :70.80 Median :158.0 Median :64.00   
#> Mean :70.18 Mean :158.5 Mean :63.54   
#> 3rd Qu.:71.40 3rd Qu.:162.0 3rd Qu.:65.00   
#> Max. :72.50 Max. :173.0 Max. :70.00   
#> NA's :5 NA's :5   
#> ManufacturingProcess34 ManufacturingProcess35 ManufacturingProcess36  
#> Min. :2.300 Min. :463.0 Min. :0.01700   
#> 1st Qu.:2.500 1st Qu.:490.0 1st Qu.:0.01900   
#> Median :2.500 Median :495.0 Median :0.02000   
#> Mean :2.494 Mean :495.6 Mean :0.01957   
#> 3rd Qu.:2.500 3rd Qu.:501.5 3rd Qu.:0.02000   
#> Max. :2.600 Max. :522.0 Max. :0.02200   
#> NA's :5 NA's :5 NA's :5   
#> ManufacturingProcess37 ManufacturingProcess38 ManufacturingProcess39  
#> Min. :0.000 Min. :0.000 Min. :0.000   
#> 1st Qu.:0.700 1st Qu.:2.000 1st Qu.:7.100   
#> Median :1.000 Median :3.000 Median :7.200   
#> Mean :1.014 Mean :2.534 Mean :6.851   
#> 3rd Qu.:1.300 3rd Qu.:3.000 3rd Qu.:7.300   
#> Max. :2.300 Max. :3.000 Max. :7.500   
#>   
#> ManufacturingProcess40 ManufacturingProcess41 ManufacturingProcess42  
#> Min. :0.00000 Min. :0.00000 Min. : 0.00   
#> 1st Qu.:0.00000 1st Qu.:0.00000 1st Qu.:11.40   
#> Median :0.00000 Median :0.00000 Median :11.60   
#> Mean :0.01771 Mean :0.02371 Mean :11.21   
#> 3rd Qu.:0.00000 3rd Qu.:0.00000 3rd Qu.:11.70   
#> Max. :0.10000 Max. :0.20000 Max. :12.10   
#> NA's :1 NA's :1   
#> ManufacturingProcess43 ManufacturingProcess44 ManufacturingProcess45  
#> Min. : 0.0000 Min. :0.000 Min. :0.000   
#> 1st Qu.: 0.6000 1st Qu.:1.800 1st Qu.:2.100   
#> Median : 0.8000 Median :1.900 Median :2.200   
#> Mean : 0.9119 Mean :1.805 Mean :2.138   
#> 3rd Qu.: 1.0250 3rd Qu.:1.900 3rd Qu.:2.300   
#> Max. :11.0000 Max. :2.100 Max. :2.600   
#>

paste0("Missing Values: ",sum(is.na(ChemicalManufacturingProcess)))

#> [1] "Missing Values: 106"

gg\_miss\_var(df\_raw)



preProcess\_NAdata\_model <- preProcess(df\_raw, method ="medianImpute")  
df <- predict(preProcess\_NAdata\_model, newdata = df\_raw)

paste0(sum(is.na(df))," values missing after imputation")

#> [1] "0 values missing after imputation"

### c.

*Split the data into a training and test set, pre-process the data, and tune a model of your choice from this chapter. What is the optimal value of the performance metric?*

**Code References:** [**https://topepo.github.io/caret/pre-processing.html#the-preprocess-function**](https://topepo.github.io/caret/pre-processing.html#the-preprocess-function)

#### Splitting data in to training and test set

# Create the training and test datasets  
set.seed(100)  
  
# Step 1: Get row numbers for the training data  
trainRowNumbers <- createDataPartition(df$Yield, p=0.8, list=FALSE)  
  
# Step 2: Create the training dataset  
trainData <- df[trainRowNumbers,]  
  
# Step 3: Create the test dataset  
testData <- df[-trainRowNumbers,]

#### Data preprocess

preProcValues <- preProcess(trainData, method = c("center", "scale"))  
  
trainTransformed <- predict(preProcValues, trainData)  
testTransformed <- predict(preProcValues, testData)  
  
trainTransformed

#> Yield BiologicalMaterial01 BiologicalMaterial02 BiologicalMaterial03  
#> 1 -1.139159835 -0.155287245 -1.443390150 -2.608532178  
#> 2 1.214401957 2.377273855 1.380310695 0.004938767  
#> 3 0.997068548 2.377273855 1.380310695 0.004938767  
#> 6 1.813394034 -0.342351418 0.733264233 -0.534664654  
#> 7 1.574857366 1.614627614 2.247997522 1.230858059  
#> 9 0.710824546 0.837591822 2.032315368 1.143825249  
#> 10 1.219702772 0.837591822 2.032315368 1.143825249  
#> 11 1.002369363 1.168551511 1.444767431 0.634061649  
#> 12 1.341621513 1.168551511 1.444767431 0.634061649  
#> 13 1.744483441 1.168551511 1.444767431 0.634061649  
#> 14 0.069425950 1.830470890 1.266271855 0.442589467  
#> 15 0.716125361 -0.184066349 1.866215318 0.566922053  
#> 16 0.562401731 1.110993305 1.214210645 0.179004386  
#> 18 -0.004785458 1.844860442 1.001007596 -0.059714178  
#> 19 -0.450053905 1.657796269 1.075380753 -0.044794268  
#> 21 0.037621061 1.657796269 1.075380753 -0.044794268  
#> 23 0.292060174 0.319567961 0.738222443 -0.072147436  
#> 25 1.712678552 2.607506682 2.047189999 1.486983185  
#> 26 -1.759355172 0.348347064 0.083738665 -0.300919393  
#> 27 -2.596883918 0.780033615 -0.283168907 -1.608898192  
#> 28 -2.135713026 0.722475409 0.063905823 -1.002155175  
#> 30 -0.953631315 0.247620202 1.556327165 2.409530968  
#> 31 -0.089598495 0.765644064 1.521619692 2.140972584  
#> 33 1.839898109 0.693696305 1.501786851 1.603855815  
#> 34 -0.821110944 -1.709358830 1.429892799 2.220545438  
#> 35 -0.264525385 0.938318684 1.462121167 1.305457610  
#> 36 0.382174026 -0.083339487 0.406022344 0.639034952  
#> 37 1.225003586 -1.493515554 0.926634440 0.892673426  
#> 38 1.331019883 -1.493515554 0.926634440 0.892673426  
#> 39 1.103084845 -1.493515554 0.926634440 0.892673426  
#> 40 0.679019657 -0.932323038 0.564685078 0.474915939  
#> 41 0.700222917 0.348347064 0.842344862 0.922513247  
#> 43 2.226857592 0.578579892 0.004407298 0.581841963  
#> 44 2.126142110 0.578579892 0.004407298 0.581841963  
#> 46 1.304515809 0.851981374 1.216689750 1.618775725  
#> 47 1.490044329 0.851981374 1.216689750 1.618775725  
#> 48 1.956516035 0.851981374 1.216689750 1.618775725  
#> 49 3.281719747 2.319715648 2.317412468 1.651102197  
#> 50 -0.216818052 0.837591822 0.401064133 0.509729063  
#> 51 0.514694397 0.837591822 0.401064133 0.509729063  
#> 52 -0.004785458 0.837591822 0.401064133 0.509729063  
#> 53 1.346922328 1.729744028 1.541452534 1.171178418  
#> 54 0.000515357 0.736864960 0.477916395 1.009546057  
#> 55 -0.200915607 0.736864960 0.477916395 1.009546057  
#> 57 -0.534866942 0.420294823 0.051510297 0.365503264  
#> 58 0.111832469 0.420294823 0.051510297 0.365503264  
#> 60 0.180743062 0.521021685 0.455604448 0.947379764  
#> 61 0.223149581 0.305178409 0.130841664 0.502269108  
#> 62 -1.033143538 -0.284793211 -0.181525593 -0.126853774  
#> 63 -0.768102796 -0.284793211 -0.181525593 -0.126853774  
#> 65 0.928157955 0.017387375 -0.677346637 -0.775869870  
#> 66 0.997068548 0.017387375 -0.677346637 -0.775869870  
#> 67 0.959962844 0.017387375 -0.677346637 -0.775869870  
#> 68 0.901653881 -0.068949935 -0.243503224 -0.330759214  
#> 69 -0.232720496 -0.126508142 -0.469101799 -0.233779797  
#> 70 -0.407647386 -0.126508142 -0.469101799 -0.233779797  
#> 72 -0.407647386 0.319567961 -0.719491426 -1.036968299  
#> 73 -0.036590347 0.132503789 -0.550912271 -0.616724160  
#> 75 -0.943029686 0.046166478 0.854740388 1.489469836  
#> 76 -0.736297907 0.046166478 0.854740388 1.489469836  
#> 77 -0.752200351 -0.011391728 0.378752186 0.847913696  
#> 78 -0.635582425 -0.270403659 -0.397207747 -0.479958316  
#> 79 0.138336543 0.880760477 0.688640339 1.091605563  
#> 80 -0.132005014 0.880760477 0.688640339 1.091605563  
#> 83 0.451084619 0.636138098 0.448167132 0.716121155  
#> 84 0.763832695 0.636138098 0.448167132 0.716121155  
#> 85 0.403377285 0.636138098 0.448167132 0.716121155  
#> 86 -0.614379165 -0.083339487 -0.853363108 -0.843009466  
#> 87 -0.709793832 -0.083339487 -0.853363108 -0.843009466  
#> 88 -0.450053905 -0.083339487 -0.853363108 -0.843009466  
#> 89 0.329165877 0.132503789 -0.077403174 0.427669557  
#> 90 -0.465956349 0.132503789 -0.077403174 0.427669557  
#> 92 -0.518964498 -0.112118590 -0.265815171 0.208844207  
#> 93 -0.089598495 1.398784339 0.363877555 0.673848076  
#> 94 -0.126704199 1.240499270 0.475437290 0.885213471  
#> 95 0.329165877 -0.241624556 -0.449268957 -0.263619618  
#> 96 -0.153208274 -0.543805142 -0.322834591 -0.238753101  
#> 98 0.350369137 -0.543805142 -0.322834591 -0.238753101  
#> 99 -1.170964724 -0.730869314 -0.905424317 -0.855442724  
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#> 103 -1.112655761 -0.673311107 -1.021942263 -0.850469421  
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#> 106 -0.905923982 -0.658921555 -0.982276579 -0.957395444  
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#> 108 -0.211517237 -0.817206624 -0.357542064 -0.231293146  
#> 109 -0.338736793 -0.817206624 -0.357542064 -0.231293146  
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#> 111 0.122434098 0.060556030 0.824991126 1.007059405  
#> 112 0.021718616 0.060556030 0.824991126 1.007059405  
#> 113 -0.100200125 0.060556030 0.824991126 1.007059405  
#> 114 -0.190313977 -0.371130521 0.237443189 0.512215715  
#> 115 0.906954696 -0.831596176 -0.421998800 -0.059714178  
#> 116 1.060678326 -0.299182763 -0.580661534 0.703687897  
#> 117 1.977719295 0.060556030 -0.689742163 1.225884755  
#> 118 -0.301631089 -1.090608106 -0.979797474 -0.999668523  
#> 119 0.021718616 -1.090608106 -0.979797474 -0.999668523  
#> 120 -0.163809903 -1.090608106 -0.979797474 -0.999668523  
#> 121 0.233751210 -1.335230485 -1.562387200 -1.337853156  
#> 122 0.270856914 -0.486246935 -1.336788625 -1.651171271  
#> 123 1.288613365 -0.471857383 -0.699658584 -0.599317598  
#> 125 0.689621287 -0.860375279 -0.662472006 -0.890255848  
#> 127 1.129588919 -0.184066349 -0.607931691 -0.186533415  
#> 128 0.779735139 -0.184066349 -0.607931691 -0.186533415  
#> 129 1.368125587 -0.184066349 -0.607931691 -0.186533415  
#> 130 0.800938399 -0.140897694 0.133320770 0.437616164  
#> 131 0.392775656 -0.140897694 0.133320770 0.437616164  
#> 132 0.355669952 -0.140897694 0.133320770 0.437616164  
#> 133 -0.200915607 0.002997823 -0.550912271 -0.221346539  
#> 134 -1.112655761 0.521021685 -0.384812221 -0.089553998  
#> 135 -1.213371243 -1.694969278 -1.686342461 -1.596464933  
#> 136 -1.123257390 -1.694969278 -1.686342461 -1.596464933  
#> 137 -1.462509540 -1.694969278 -1.686342461 -1.596464933  
#> 138 -0.524265313 -0.097729039 -1.180604997 -0.880309241  
#> 139 -1.329989169 -0.371130521 -1.190521418 -1.017075085  
#> 140 -0.200915607 -1.522294658 -2.115227664 -2.461819728  
#> 141 -0.789306055 -0.759648417 -1.297122942 -1.081728030  
#> 142 0.085328395 -0.155287245 -0.206316645 0.024831980  
#> 143 0.207247136 -0.155287245 -0.206316645 0.024831980  
#> 144 0.260255284 -0.155287245 -0.206316645 0.024831980  
#> 147 -0.025988717 -0.515026038 -0.523642114 -0.487418272  
#> 148 -0.534866942 -1.248893175 -1.827651459 -2.106228533  
#> 149 -0.805208500 -1.522294658 -2.115227664 -2.461819728  
#> 150 0.679019657 -1.176945417 -0.724449636 -0.616724160  
#> 152 -1.197468798 -0.155287245 -0.674867532 -0.581911036  
#> 153 -1.446607096 -0.155287245 -0.674867532 -0.581911036  
#> 154 -1.398899762 -0.155287245 -0.674867532 -0.581911036  
#> 155 -1.181566354 -0.198455901 -0.655034690 -0.579424385  
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#> 28 -0.456755 -0.4369878 0.176065846  
#> 30 -0.456755 -0.4369878 0.176065846  
#> 31 -0.456755 -0.4369878 0.235721097  
#> 33 2.174154 1.3869613 0.176065846  
#> 34 2.174154 1.3869613 0.176065846  
#> 35 -0.456755 -0.4369878 0.235721097  
#> 36 2.174154 3.2109104 -0.181865662  
#> 37 -0.456755 -0.4369878 -0.062555159  
#> 38 -0.456755 -0.4369878 -0.122210410  
#> 39 2.174154 3.2109104 -0.181865662  
#> 40 -0.456755 -0.4369878 0.056755343  
#> 41 -0.456755 -0.4369878 -0.241520913  
#> 43 2.174154 1.3869613 0.056755343  
#> 44 -0.456755 -0.4369878 -0.181865662  
#> 46 -0.456755 -0.4369878 -0.360831415  
#> 47 -0.456755 -0.4369878 -0.122210410  
#> 48 2.174154 1.3869613 0.176065846  
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#> 50 -0.456755 -0.4369878 0.176065846  
#> 51 -0.456755 -0.4369878 0.056755343  
#> 52 2.174154 3.2109104 0.056755343  
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#> 58 -0.456755 -0.4369878 -0.002899908  
#> 60 -0.456755 -0.4369878 0.116410594  
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#> 62 -0.456755 -0.4369878 0.235721097  
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#> 66 -0.456755 -0.4369878 0.235721097  
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#> 68 -0.456755 -0.4369878 -0.062555159  
#> 69 -0.456755 -0.4369878 0.355031599  
#> 70 2.174154 1.3869613 0.355031599  
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#> 73 -0.456755 -0.4369878 0.116410594  
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#> 76 -0.456755 -0.4369878 0.176065846  
#> 77 -0.456755 -0.4369878 0.176065846  
#> 78 -0.456755 -0.4369878 0.056755343  
#> 79 -0.456755 -0.4369878 0.056755343  
#> 80 -0.456755 -0.4369878 -0.002899908  
#> 83 -0.456755 -0.4369878 0.116410594  
#> 84 -0.456755 -0.4369878 0.116410594  
#> 85 -0.456755 -0.4369878 0.176065846  
#> 86 -0.456755 -0.4369878 0.116410594  
#> 87 2.174154 1.3869613 0.235721097  
#> 88 -0.456755 -0.4369878 0.235721097  
#> 89 -0.456755 -0.4369878 0.116410594  
#> 90 -0.456755 -0.4369878 -0.002899908  
#> 92 -0.456755 -0.4369878 0.176065846  
#> 93 -0.456755 -0.4369878 0.116410594  
#> 94 -0.456755 -0.4369878 0.355031599  
#> 95 2.174154 1.3869613 0.295376348  
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#> 98 -0.456755 -0.4369878 0.116410594  
#> 99 2.174154 1.3869613 0.235721097  
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#> 101 -0.456755 -0.4369878 0.116410594  
#> 103 -0.456755 -0.4369878 0.056755343  
#> 105 -0.456755 -0.4369878 0.235721097  
#> 106 -0.456755 -0.4369878 0.355031599  
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#> 108 -0.456755 -0.4369878 0.176065846  
#> 109 -0.456755 1.3869613 0.235721097  
#> 110 -0.456755 -0.4369878 0.116410594  
#> 111 -0.456755 -0.4369878 0.176065846  
#> 112 -0.456755 -0.4369878 -0.002899908  
#> 113 2.174154 1.3869613 -0.002899908  
#> 114 -0.456755 -0.4369878 0.056755343  
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#> 118 2.174154 1.3869613 0.235721097  
#> 119 -0.456755 -0.4369878 0.176065846  
#> 120 -0.456755 -0.4369878 0.355031599  
#> 121 -0.456755 -0.4369878 0.176065846  
#> 122 -0.456755 -0.4369878 0.295376348  
#> 123 2.174154 3.2109104 0.116410594  
#> 125 -0.456755 -0.4369878 0.116410594  
#> 127 -0.456755 -0.4369878 0.056755343  
#> 128 2.174154 1.3869613 0.056755343  
#> 129 -0.456755 -0.4369878 0.235721097  
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#> 133 -0.456755 -0.4369878 0.355031599  
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#> 135 -0.456755 -0.4369878 0.295376348  
#> 136 -0.456755 -0.4369878 0.235721097  
#> 137 2.174154 1.3869613 0.235721097  
#> 138 -0.456755 -0.4369878 0.295376348  
#> 139 -0.456755 -0.4369878 0.235721097  
#> 140 -0.456755 -0.4369878 0.295376348  
#> 141 2.174154 1.3869613 0.235721097  
#> 142 -0.456755 -0.4369878 0.235721097  
#> 143 -0.456755 -0.4369878 0.235721097  
#> 144 -0.456755 -0.4369878 0.295376348  
#> 147 -0.456755 -0.4369878 0.235721097  
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#> 149 2.174154 1.3869613 0.355031599  
#> 150 -0.456755 -0.4369878 0.414686850  
#> 152 -0.456755 -0.4369878 0.176065846  
#> 153 -0.456755 -0.4369878 -0.002899908  
#> 154 2.174154 1.3869613 -0.360831415  
#> 155 -0.456755 -0.4369878 -0.002899908  
#> 156 -0.456755 -0.4369878 -0.181865662  
#> 157 2.174154 3.2109104 -0.241520913  
#> 158 -0.456755 -0.4369878 0.414686850  
#> 159 -0.456755 -0.4369878 0.474342102  
#> 160 -0.456755 -0.4369878 0.474342102  
#> 161 -0.456755 -0.4369878 0.414686850  
#> 162 -0.456755 -0.4369878 0.235721097  
#> 165 -0.456755 -0.4369878 0.176065846  
#> 166 -0.456755 -0.4369878 0.056755343  
#> 167 -0.456755 -0.4369878 0.056755343  
#> 168 -0.456755 -0.4369878 -0.002899908  
#> 169 -0.456755 -0.4369878 0.295376348  
#> 171 -0.456755 -0.4369878 0.235721097  
#> 172 -0.456755 -0.4369878 -6.743943295  
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#> 176 -0.456755 -0.4369878 -6.743943295  
#> ManufacturingProcess43 ManufacturingProcess44 ManufacturingProcess45  
#> 1 4.96373382 -0.06482661 0.6679796  
#> 2 0.09341225 0.29421306 0.1183278  
#> 3 0.32533233 -0.06482661 0.3931537  
#> 6 3.10837322 -0.06482661 -0.4313240  
#> 7 -0.37042790 0.65325272 0.1183278  
#> 9 0.09341225 0.29421306 -0.1564981  
#> 10 -0.13850782 0.29421306 0.6679796  
#> 11 0.32533233 0.29421306 -0.9809758  
#> 12 -0.13850782 0.65325272 -0.9809758  
#> 13 -0.13850782 0.29421306 0.6679796  
#> 14 -0.60234797 -0.42386627 -0.7061499  
#> 15 -0.13850782 0.29421306 -0.4313240  
#> 16 0.32533233 0.29421306 0.9428055  
#> 18 1.94877285 -0.06482661 0.1183278  
#> 19 2.18069292 -0.42386627 0.3931537  
#> 21 2.64453307 -0.78290593 -0.4313240  
#> 23 -0.13850782 0.29421306 0.6679796  
#> 25 -0.37042790 -0.42386627 0.6679796  
#> 26 -0.13850782 -0.42386627 0.1183278  
#> 27 -0.37042790 -0.42386627 -0.4313240  
#> 28 1.02109255 -0.42386627 0.1183278  
#> 30 -0.83426805 0.29421306 0.1183278  
#> 31 -0.60234797 0.65325272 0.6679796  
#> 33 -0.37042790 0.29421306 0.6679796  
#> 34 -0.83426805 -0.06482661 0.3931537  
#> 35 -0.60234797 0.29421306 1.2176314  
#> 36 0.09341225 0.65325272 -0.1564981  
#> 37 0.55725240 0.29421306 0.6679796  
#> 38 0.78917248 -0.06482661 0.6679796  
#> 39 1.48493270 -0.06482661 0.6679796  
#> 40 0.32533233 0.29421306 0.3931537  
#> 41 0.32533233 0.29421306 0.1183278  
#> 43 -0.37042790 0.65325272 0.6679796  
#> 44 -0.37042790 -0.06482661 0.6679796  
#> 46 -0.37042790 -0.06482661 0.3931537  
#> 47 0.55725240 -0.06482661 -0.1564981  
#> 48 1.25301263 -0.06482661 0.6679796  
#> 49 1.02109255 -0.06482661 -0.1564981  
#> 50 0.09341225 -0.06482661 -0.4313240  
#> 51 3.80413345 -0.06482661 -0.1564981  
#> 52 0.32533233 -0.06482661 0.1183278  
#> 53 0.55725240 0.65325272 0.3931537  
#> 54 0.78917248 0.29421306 0.1183278  
#> 55 0.09341225 0.29421306 -0.1564981  
#> 57 0.32533233 0.29421306 0.1183278  
#> 58 -1.99386842 0.65325272 0.1183278  
#> 60 -0.37042790 -0.06482661 0.3931537  
#> 61 0.09341225 -0.06482661 0.1183278  
#> 62 -0.13850782 -0.06482661 -0.1564981  
#> 63 -0.13850782 -0.06482661 -0.4313240  
#> 65 0.09341225 0.65325272 0.3931537  
#> 66 1.25301263 0.29421306 -0.9809758  
#> 67 1.25301263 0.29421306 -0.9809758  
#> 68 0.78917248 0.29421306 -0.9809758  
#> 69 0.78917248 -0.06482661 0.9428055  
#> 70 1.94877285 -0.06482661 0.3931537  
#> 72 0.78917248 -0.06482661 -0.7061499  
#> 73 0.78917248 -0.06482661 -0.9809758  
#> 75 -0.13850782 0.65325272 -0.1564981  
#> 76 1.02109255 0.29421306 0.6679796  
#> 77 -0.60234797 0.65325272 0.3931537  
#> 78 1.02109255 0.29421306 0.1183278  
#> 79 -0.13850782 0.65325272 0.9428055  
#> 80 0.09341225 1.01229238 0.1183278  
#> 83 1.71685278 0.29421306 0.6679796  
#> 84 1.48493270 0.29421306 0.6679796  
#> 85 1.71685278 0.65325272 0.6679796  
#> 86 0.32533233 0.29421306 0.6679796  
#> 87 0.55725240 -0.06482661 -0.1564981  
#> 88 0.55725240 0.29421306 0.3931537  
#> 89 0.55725240 0.29421306 0.3931537  
#> 90 -0.13850782 0.29421306 -0.1564981  
#> 92 0.55725240 -0.06482661 0.1183278  
#> 93 0.09341225 -0.06482661 -0.4313240  
#> 94 0.09341225 0.29421306 0.9428055  
#> 95 -0.13850782 0.29421306 0.3931537  
#> 96 -0.13850782 0.29421306 0.1183278  
#> 98 0.09341225 0.29421306 -0.1564981  
#> 99 0.55725240 0.29421306 0.1183278  
#> 100 0.09341225 0.29421306 0.3931537  
#> 101 -0.13850782 0.29421306 0.3931537  
#> 103 0.32533233 -0.06482661 0.6679796  
#> 105 -0.13850782 0.29421306 -0.4313240  
#> 106 -0.13850782 0.29421306 0.3931537  
#> 107 -0.13850782 0.29421306 -0.7061499  
#> 108 -0.13850782 0.29421306 0.6679796  
#> 109 -0.13850782 0.29421306 -0.7061499  
#> 110 0.09341225 -0.06482661 0.6679796  
#> 111 1.94877285 -0.06482661 0.1183278  
#> 112 0.78917248 0.29421306 0.3931537  
#> 113 0.09341225 -0.06482661 0.3931537  
#> 114 0.55725240 -0.06482661 0.3931537  
#> 115 -0.83426805 0.29421306 0.3931537  
#> 116 -0.60234797 0.29421306 0.1183278  
#> 117 -0.37042790 0.29421306 0.1183278  
#> 118 -0.13850782 0.29421306 -0.4313240  
#> 119 -0.13850782 -0.42386627 0.6679796  
#> 120 -0.83426805 0.29421306 0.1183278  
#> 121 -0.83426805 -0.42386627 -0.7061499  
#> 122 -0.83426805 -0.06482661 -0.1564981  
#> 123 -0.83426805 0.29421306 0.1183278  
#> 125 -0.60234797 0.29421306 0.1183278  
#> 127 -0.60234797 0.29421306 0.1183278  
#> 128 -0.37042790 0.29421306 -0.4313240  
#> 129 -0.83426805 0.65325272 0.1183278  
#> 130 -0.83426805 0.29421306 0.3931537  
#> 131 -1.06618812 0.29421306 0.1183278  
#> 132 -0.60234797 -0.06482661 -0.1564981  
#> 133 -1.06618812 0.65325272 0.3931537  
#> 134 -1.06618812 0.29421306 0.1183278  
#> 135 -1.06618812 0.29421306 0.6679796  
#> 136 -0.83426805 -0.06482661 0.6679796  
#> 137 -0.83426805 0.29421306 0.6679796  
#> 138 -0.83426805 -0.06482661 -0.1564981  
#> 139 -0.37042790 0.29421306 0.3931537  
#> 140 -1.06618812 -0.06482661 0.6679796  
#> 141 -0.83426805 -0.06482661 0.3931537  
#> 142 -0.60234797 -0.06482661 0.3931537  
#> 143 -0.83426805 -0.06482661 0.3931537  
#> 144 -0.83426805 0.29421306 0.3931537  
#> 147 -0.83426805 -0.06482661 -0.7061499  
#> 148 -0.60234797 -0.06482661 -0.1564981  
#> 149 -1.06618812 -0.42386627 -0.9809758  
#> 150 -0.83426805 -0.06482661 -0.7061499  
#> 152 -0.37042790 0.29421306 -0.7061499  
#> 153 -0.83426805 0.29421306 -0.1564981  
#> 154 -0.37042790 -0.06482661 -0.1564981  
#> 155 -0.83426805 -0.06482661 -0.9809758  
#> 156 -1.06618812 0.29421306 0.3931537  
#> 157 -0.83426805 0.29421306 0.3931537  
#> 158 -0.83426805 -0.06482661 0.3931537  
#> 159 -1.29810820 -0.06482661 0.3931537  
#> 160 -0.37042790 -0.06482661 -0.1564981  
#> 161 -1.29810820 -0.06482661 0.3931537  
#> 162 -1.29810820 0.29421306 -0.9809758  
#> 165 -1.06618812 -0.06482661 0.3931537  
#> 166 -0.13850782 -0.42386627 0.1183278  
#> 167 -0.37042790 -0.06482661 0.6679796  
#> 168 -0.83426805 -0.42386627 -0.1564981  
#> 169 -1.53002827 -0.06482661 0.1183278  
#> 171 -0.83426805 -0.06482661 0.1183278  
#> 172 -0.60234797 -6.52754050 -5.9278421  
#> 174 -0.60234797 -6.52754050 -5.9278421  
#> 176 -0.60234797 -6.52754050 -5.9278421

xTrain <- trainTransformed %>% dplyr::select(-Yield)  
  
yTrain <- trainTransformed %>% dplyr::select(Yield)  
  
xTest <- testTransformed %>% dplyr::select(-Yield)  
  
yTest <- testTransformed %>% dplyr::select(Yield)

#### Tune model

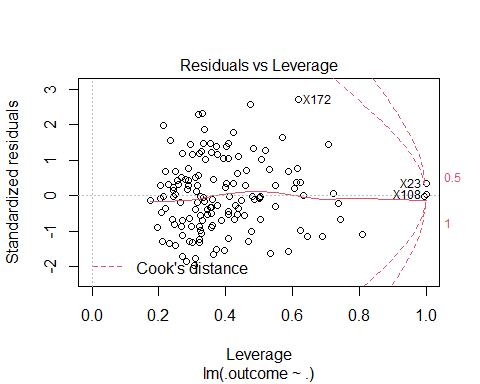
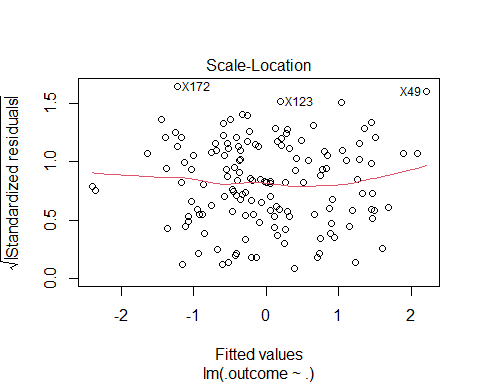
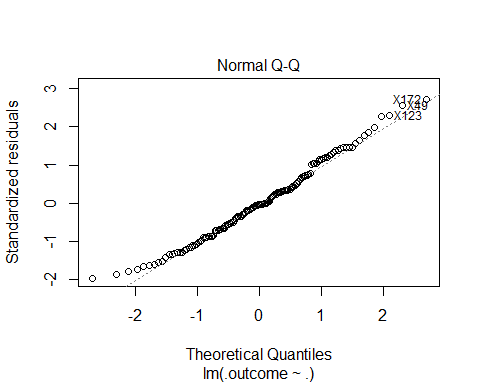
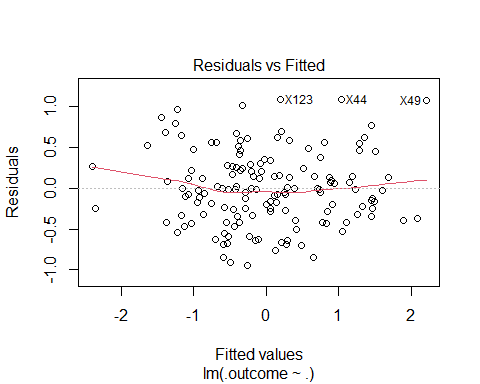
lm\_model <- train(xTrain, yTrain$Yield, method="lm", trControl=trainControl(method="repeatedcv",repeats=5) )  
lm\_model

#> Linear Regression   
#>   
#> 144 samples  
#> 57 predictor  
#>   
#> No pre-processing  
#> Resampling: Cross-Validated (10 fold, repeated 5 times)   
#> Summary of sample sizes: 130, 130, 130, 130, 130, 129, ...   
#> Resampling results:  
#>   
#> RMSE Rsquared MAE   
#> 1.761794 0.4240885 0.9535992  
#>   
#> Tuning parameter 'intercept' was held constant at a value of TRUE

summary(lm\_model)

#>   
#> Call:  
#> lm(formula = .outcome ~ ., data = dat)  
#>   
#> Residuals:  
#> Min 1Q Median 3Q Max   
#> -0.94229 -0.32402 -0.01611 0.27082 1.08863   
#>   
#> Coefficients: (1 not defined because of singularities)  
#> Estimate Std. Error t value Pr(>|t|)   
#> (Intercept) 5.976e-15 4.806e-02 0.000 1.000000   
#> BiologicalMaterial01 -4.427e-02 1.526e-01 -0.290 0.772353   
#> BiologicalMaterial02 -3.308e-01 3.389e-01 -0.976 0.331731   
#> BiologicalMaterial03 4.753e-01 6.692e-01 0.710 0.479458   
#> BiologicalMaterial04 3.532e-01 5.446e-01 0.649 0.518351   
#> BiologicalMaterial05 2.226e-01 1.359e-01 1.638 0.105019   
#> BiologicalMaterial06 -4.333e-01 7.684e-01 -0.564 0.574310   
#> BiologicalMaterial07 -6.008e-02 6.591e-02 -0.912 0.364529   
#> BiologicalMaterial08 3.743e-01 3.249e-01 1.152 0.252400   
#> BiologicalMaterial09 -2.401e-01 4.308e-01 -0.557 0.578744   
#> BiologicalMaterial10 -2.577e-01 4.919e-01 -0.524 0.601723   
#> BiologicalMaterial11 -4.132e-01 2.634e-01 -1.569 0.120324   
#> BiologicalMaterial12 3.514e-01 3.274e-01 1.073 0.286024   
#> ManufacturingProcess01 6.577e-02 1.126e-01 0.584 0.560733   
#> ManufacturingProcess02 -1.436e-01 2.235e-01 -0.642 0.522426   
#> ManufacturingProcess03 -5.261e-02 6.781e-02 -0.776 0.439911   
#> ManufacturingProcess04 2.078e-01 1.272e-01 1.634 0.105899   
#> ManufacturingProcess05 2.950e-02 7.370e-02 0.400 0.689959   
#> ManufacturingProcess06 6.251e-02 6.940e-02 0.901 0.370186   
#> ManufacturingProcess07 -1.235e-01 6.963e-02 -1.773 0.079705 .   
#> ManufacturingProcess08 -3.101e-02 8.605e-02 -0.360 0.719467   
#> ManufacturingProcess09 2.693e-01 2.002e-01 1.345 0.182045   
#> ManufacturingProcess10 -4.858e-01 3.447e-01 -1.410 0.162224   
#> ManufacturingProcess11 1.235e-01 3.918e-01 0.315 0.753313   
#> ManufacturingProcess12 1.037e-01 1.158e-01 0.895 0.373017   
#> ManufacturingProcess13 -6.186e-01 3.041e-01 -2.034 0.044980 \*   
#> ManufacturingProcess14 -1.188e-01 3.556e-01 -0.334 0.739056   
#> ManufacturingProcess15 4.393e-02 3.428e-01 0.128 0.898317   
#> ManufacturingProcess16 1.796e-01 1.131e-01 1.588 0.115923   
#> ManufacturingProcess17 3.498e-01 2.979e-01 1.174 0.243426   
#> ManufacturingProcess18 1.359e-01 4.543e-01 0.299 0.765598   
#> ManufacturingProcess19 -4.053e-02 3.698e-01 -0.110 0.912976   
#> ManufacturingProcess20 -9.016e-02 2.693e-01 -0.335 0.738580   
#> ManufacturingProcess21 NA NA NA NA   
#> ManufacturingProcess22 -3.489e-02 9.213e-02 -0.379 0.705790   
#> ManufacturingProcess23 -5.067e-02 8.900e-02 -0.569 0.570635   
#> ManufacturingProcess24 -6.569e-02 8.834e-02 -0.744 0.459147   
#> ManufacturingProcess25 -1.104e+00 3.925e+00 -0.281 0.779124   
#> ManufacturingProcess26 2.494e+00 4.122e+00 0.605 0.546699   
#> ManufacturingProcess27 -1.853e+00 2.634e+00 -0.704 0.483592   
#> ManufacturingProcess28 -2.508e-01 1.103e-01 -2.273 0.025516 \*   
#> ManufacturingProcess29 7.245e-01 1.024e+00 0.708 0.481071   
#> ManufacturingProcess30 -1.634e-01 3.769e-01 -0.434 0.665622   
#> ManufacturingProcess31 -7.095e-02 4.416e-01 -0.161 0.872739   
#> ManufacturingProcess32 8.601e-01 2.142e-01 4.015 0.000126 \*\*\*  
#> ManufacturingProcess33 -4.972e-01 1.947e-01 -2.553 0.012409 \*   
#> ManufacturingProcess34 -2.865e-02 9.031e-02 -0.317 0.751788   
#> ManufacturingProcess35 -1.008e-01 1.187e-01 -0.849 0.398053   
#> ManufacturingProcess36 1.202e-01 1.611e-01 0.746 0.457671   
#> ManufacturingProcess37 -1.722e-01 7.867e-02 -2.189 0.031260 \*   
#> ManufacturingProcess38 -3.440e-02 9.206e-02 -0.374 0.709540   
#> ManufacturingProcess39 -5.994e-03 1.153e-01 -0.052 0.958678   
#> ManufacturingProcess40 2.272e-01 1.574e-01 1.444 0.152465   
#> ManufacturingProcess41 -1.827e-01 1.663e-01 -1.099 0.274874   
#> ManufacturingProcess42 -1.197e-01 2.447e-01 -0.489 0.626108   
#> ManufacturingProcess43 7.436e-02 9.718e-02 0.765 0.446220   
#> ManufacturingProcess44 1.021e-01 2.436e-01 0.419 0.676172   
#> ManufacturingProcess45 1.261e-01 1.289e-01 0.978 0.330755   
#> ---  
#> Signif. codes: 0 '\*\*\*' 0.001 '\*\*' 0.01 '\*' 0.05 '.' 0.1 ' ' 1  
#>   
#> Residual standard error: 0.5767 on 87 degrees of freedom  
#> Multiple R-squared: 0.7976, Adjusted R-squared: 0.6674   
#> F-statistic: 6.124 on 56 and 87 DF, p-value: 3.995e-14

plot(lm\_model$finalModel)



### d.

**Resampling examples from Sect. 4.9 of the text.**

*Predict the response for the test set. What is the value of the performance metric and how does this compare with the resampled performance metric of the training set?*

Predict using the test data set and get the model’s performance values

finalLMPred <- predict(lm\_model$finalModel, newdata = xTest)  
## The function 'postResample' can be used to get the test set  
## performance values  
postResample(pred = finalLMPred, obs = yTest$Yield)

#> RMSE Rsquared MAE   
#> 1.2731407 0.1443080 0.7636275

As it can be seen in the table below, the resampled performance metrix of the test set is much better than that of the training data set. The RMSE for the test set is smaller than that of the training one.

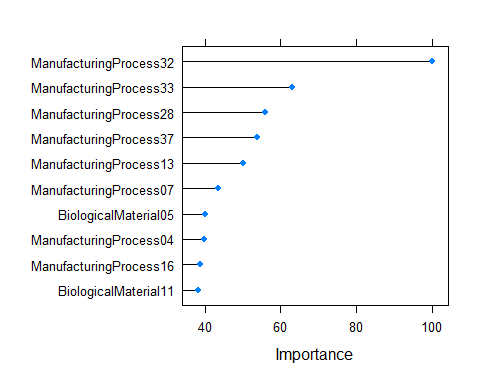
| Model | RMSE | Rsquared | MAE |
| --- | --- | --- | --- |
| Linear Model (Training) | 1.7617940 | 0.4240885 | 0.9535992 |
| Linear Model (Test) | 1.2731407 | 0.1443080 | 0.7636275 |

### e.

*Which predictors are the most important in the model you have trained? Do either the biological or process predictors dominate the list?*

Below is a list of the top 10 most important predictors for the Linear Regression model.

plot(caret::varImp(lm\_model), top = 10)



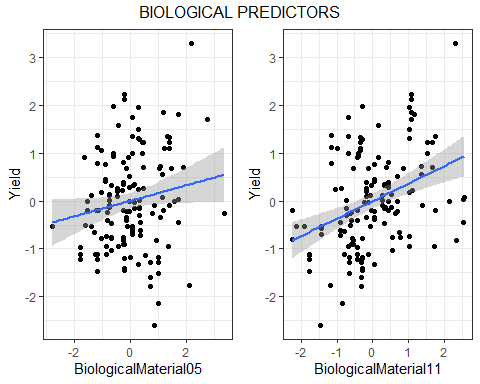
caret::varImp(lm\_model, scale = FALSE)

#> lm variable importance  
#>   
#> only 20 most important variables shown (out of 56)  
#>   
#> Overall  
#> ManufacturingProcess32 4.0149  
#> ManufacturingProcess33 2.5534  
#> ManufacturingProcess28 2.2726  
#> ManufacturingProcess37 2.1892  
#> ManufacturingProcess13 2.0342  
#> ManufacturingProcess07 1.7731  
#> BiologicalMaterial05 1.6381  
#> ManufacturingProcess04 1.6339  
#> ManufacturingProcess16 1.5880  
#> BiologicalMaterial11 1.5688  
#> ManufacturingProcess40 1.4435  
#> ManufacturingProcess10 1.4096  
#> ManufacturingProcess09 1.3452  
#> ManufacturingProcess17 1.1744  
#> BiologicalMaterial08 1.1522  
#> ManufacturingProcess41 1.0988  
#> BiologicalMaterial12 1.0735  
#> ManufacturingProcess45 0.9781  
#> BiologicalMaterial02 0.9761  
#> BiologicalMaterial07 0.9115

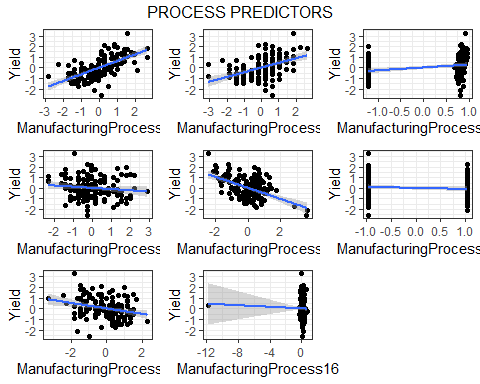
### f.

*Explore the relationships between each of the top predictors and the response. How could this information be helpful in improving yield in the future runs of the manufacturing process?*

library(gridExtra)  
  
top10lmPred <- trainTransformed %>%  
 select(Yield,   
 ManufacturingProcess32,  
 ManufacturingProcess33,  
 ManufacturingProcess28,  
 ManufacturingProcess37,  
 ManufacturingProcess13,  
 ManufacturingProcess07,  
 BiologicalMaterial05,  
 ManufacturingProcess04,  
 ManufacturingProcess16,  
 BiologicalMaterial11)  
  
plt01 <- top10lmPred %>%  
 ggplot(aes(x = ManufacturingProcess32, y = Yield)) +  
 geom\_point() + geom\_smooth(method = "lm") + theme\_bw()  
  
plt02 <- top10lmPred %>%  
 ggplot(aes(x = ManufacturingProcess33, y = Yield)) +  
 geom\_point()+ geom\_smooth(method = "lm") + theme\_bw()  
  
plt03 <- top10lmPred %>%  
 ggplot(aes(x = ManufacturingProcess28, y = Yield)) +  
 geom\_point() + geom\_smooth(method = "lm") + theme\_bw()  
  
plt04 <- top10lmPred %>%  
 ggplot(aes(x = ManufacturingProcess37, y = Yield)) +  
 geom\_point() + geom\_smooth(method = "lm") + theme\_bw()  
  
plt05 <- top10lmPred %>%  
 ggplot(aes(x = ManufacturingProcess13, y = Yield)) +  
 geom\_point() + geom\_smooth(method = "lm") + theme\_bw()  
  
plt06 <- top10lmPred %>%  
 ggplot(aes(x = ManufacturingProcess07, y = Yield)) +  
 geom\_point() + geom\_smooth(method = "lm") + theme\_bw()  
  
plt07 <- top10lmPred %>%  
 ggplot(aes(x = BiologicalMaterial05, y = Yield)) +  
 geom\_point() + geom\_smooth(method = "lm") + theme\_bw()  
  
plt08 <- top10lmPred %>%  
 ggplot(aes(x = ManufacturingProcess04, y = Yield)) +  
 geom\_point() + geom\_smooth(method = "lm") + theme\_bw()  
  
plt09 <- top10lmPred %>%  
 ggplot(aes(x = ManufacturingProcess16, y = Yield)) +  
 geom\_point() + geom\_smooth(method = "lm") + theme\_bw()  
  
plt10 <- top10lmPred %>%  
 ggplot(aes(x = BiologicalMaterial11, y = Yield)) +  
 geom\_point() + geom\_smooth(method = "lm") + theme\_bw()  
  
# Biological Predictors  
grid.arrange(plt07, plt10, nrow = 1, top = "BIOLOGICAL PREDICTORS")



# Process Predictors  
grid.arrange(plt01, plt02, plt03, plt04, plt05, plt06, plt08, plt09,  
 nrow = 3, top = "PROCESS PREDICTORS")



We use scatter plots between the top 10 predictors of the model and the response variable.

The conclusion is:

* The 2 biological predictors BiologicalMaterial05 and BiologicalMaterial11 appear to have a low positive correlation to the response.
* The top 2 predictors appears to be ManufacturingProcess32 and ManufacturingProcess33. Which, appear to have a positive correlation with the response.
* The predictors ManufacturingProcess04 and ManufacturingProcess13 seem to have a negative correlation with the response.
* The predictor ManufacturingProcess37 seems to have a low negative correlation with the response.
* The remaining predictors ManufacturingProcess07, ManufacturingProcess16 and ManufacturingProcess28 seem to have no correlation to the response.

# Week 5

## KJ 7.2

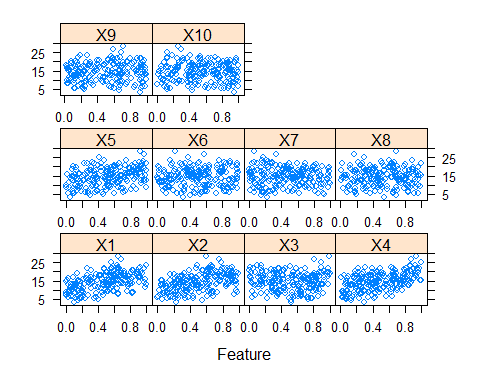
Friedman (1991) introduced several benchmark data sets create by simulation.

One of these simulations used the following nonlinear equation to create data:

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:

library(caret)  
library(mlbench)  
  
set.seed(200)  
trainingData <- mlbench.friedman1(200, sd = 1)  
## We convert the 'x' data from a matrix to a data frame  
## One reason is that this will give the columns names.  
trainingData$x <- data.frame(trainingData$x)  
## Look at the data using  
caret::featurePlot(trainingData$x, trainingData$y)



## or other methods.  
  
## This creates a list with a vector 'y' and a matrix  
## of predictors 'x'. Also simulate a large test set to  
## estimate the true error rate with good precision:  
testData <- mlbench.friedman1(5000, sd = 1)  
testData$x <- data.frame(testData$x)

Tune several models on these data. For example:

library(caret)  
knnModel <- train(x = trainingData$x,  
 y = trainingData$y,  
 method = "knn",  
 preProc = c("center", "scale"),  
 tuneLength = 10)  
  
knnModel

#> 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 3.466085 0.5121775 2.816838  
#> 7 3.349428 0.5452823 2.727410  
#> 9 3.264276 0.5785990 2.660026  
#> 11 3.214216 0.6024244 2.603767  
#> 13 3.196510 0.6176570 2.591935  
#> 15 3.184173 0.6305506 2.577482  
#> 17 3.183130 0.6425367 2.567787  
#> 19 3.198752 0.6483184 2.592683  
#> 21 3.188993 0.6611428 2.588787  
#> 23 3.200458 0.6638353 2.604529  
#>   
#> RMSE was used to select the optimal model using the smallest value.  
#> The final value used for the model was k = 17.

knnPred <- predict(knnModel, newdata = testData$x)  
## The function 'postResample' can be used to get the test set  
## perforamnce values  
postResample(pred = knnPred, obs = testData$y)

#> RMSE Rsquared MAE   
#> 3.2040595 0.6819919 2.5683461

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

#### Using a Neural Network model

First, we remove predictors to ensure that the maximum absolute pairwise correlation between the predictors is less than 0.75.

tooHigh <- findCorrelation(cor(trainingData$x), cutoff = .75)  
  
tooHigh

#> integer(0)

Since the correlation vector is empty, there are no predictors to remove. We can now fit a neural network model using the existing training set.

# Resource: Chapter 7.5 of textbook "Applied Predictive Modeling" by KJ  
  
## Create a specific candidate set of models to evaluate:  
nnetGrid <- expand.grid(.decay = c(0, 0.01, .1),  
 .size = c(1:10),  
 .bag = FALSE)  
  
# We can use caret to perform a grid search using 10-fold cross-validation.  
# The train function generates a resampling estimate of performance. Because  
# the training set size is not small, 10-fold cross-validation should produce  
# reasonable estimates of model performance. The function trainControl specifies  
# the type of resampling:  
ctrl <- trainControl(method = "cv", number = 10)  
  
nnetTune <- train(trainingData$x, trainingData$y,  
 method = "avNNet",  
 tuneGrid = nnetGrid,  
 trControl = ctrl,  
 ## Automatically standardize data prior to modeling  
 ## and prediction  
 preProc = c("center", "scale"),  
 linout = TRUE,  
 trace = FALSE,  
 MaxNWts = 10 \* (ncol(trainingData$x) + 1) + 10 + 1,  
 maxit = 500)  
  
nnetTune

#> Model Averaged Neural Network   
#>   
#> 200 samples  
#> 10 predictor  
#>   
#> Pre-processing: centered (10), scaled (10)   
#> Resampling: Cross-Validated (10 fold)   
#> Summary of sample sizes: 180, 180, 180, 180, 180, 180, ...   
#> Resampling results across tuning parameters:  
#>   
#> decay size RMSE Rsquared MAE   
#> 0.00 1 2.434845 0.7683498 1.921367  
#> 0.00 2 2.497822 0.7558233 1.993325  
#> 0.00 3 2.037885 0.8419795 1.609413  
#> 0.00 4 1.900063 0.8584928 1.529545  
#> 0.00 5 2.176661 0.8092998 1.628603  
#> 0.00 6 2.743381 0.7255103 1.988222  
#> 0.00 7 3.496229 0.6401273 2.493454  
#> 0.00 8 4.034891 0.5941657 2.749735  
#> 0.00 9 4.221796 0.5137164 2.800450  
#> 0.00 10 4.682342 0.5848908 2.818883  
#> 0.01 1 2.437231 0.7689665 1.934978  
#> 0.01 2 2.510986 0.7596191 1.988260  
#> 0.01 3 1.999944 0.8419567 1.555751  
#> 0.01 4 2.003357 0.8445288 1.549723  
#> 0.01 5 2.104801 0.8296459 1.664982  
#> 0.01 6 2.314704 0.7997307 1.857949  
#> 0.01 7 2.341101 0.8072335 1.872758  
#> 0.01 8 2.205611 0.8163107 1.748153  
#> 0.01 9 2.262921 0.8146166 1.776693  
#> 0.01 10 2.453311 0.7709666 1.981977  
#> 0.10 1 2.450897 0.7652309 1.942945  
#> 0.10 2 2.489399 0.7606443 1.997060  
#> 0.10 3 2.200693 0.8155496 1.786599  
#> 0.10 4 2.059322 0.8432340 1.651716  
#> 0.10 5 2.189025 0.8133603 1.729453  
#> 0.10 6 2.215091 0.8128993 1.757966  
#> 0.10 7 2.209521 0.8196474 1.786772  
#> 0.10 8 2.317124 0.8010433 1.826655  
#> 0.10 9 2.286711 0.7928430 1.849002  
#> 0.10 10 2.238560 0.8113030 1.787851  
#>   
#> 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.

Predict using the test data set and get the model’s performance values

nnetPred <- predict(nnetTune, newdata = testData$x)  
## The function 'postResample' can be used to get the test set  
## performance values  
postResample(pred = nnetPred, obs = testData$y)

#> RMSE Rsquared MAE   
#> 2.496722 0.784618 1.685182

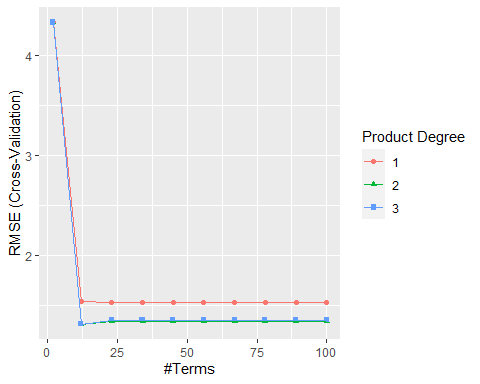
#### Using a Multivariate Adaptive Regression Splines (MARS) model

# Resource: Chapter 7.5 of textbook "Applied Predictive Modeling" by KJ  
# Resource: http://uc-r.github.io/mars  
  
library(earth)  
library(dplyr)  
  
## Create a specific candidate set of models to evaluate:  
marsGrid <- expand.grid(degree = 1:3,  
 nprune = seq(2, 100, length.out = 10) %>% floor()  
 )  
  
# We can use caret to perform a grid search using 10-fold cross-validation.  
# The train function generates a resampling estimate of performance. Because  
# the training set size is not small, 10-fold cross-validation should produce  
# reasonable estimates of model performance. The function trainControl specifies  
# the type of resampling:  
ctrl <- trainControl(method = "cv", number = 10)  
  
  
# cross validated model  
tuned\_mars <- train(  
 x = trainingData$x,  
 y = trainingData$y,  
 method = "earth",  
 metric = "RMSE",  
 trControl = ctrl,  
 tuneGrid = marsGrid  
)  
  
tuned\_mars

#> Multivariate Adaptive Regression Spline   
#>   
#> 200 samples  
#> 10 predictor  
#>   
#> No pre-processing  
#> Resampling: Cross-Validated (10 fold)   
#> Summary of sample sizes: 180, 180, 180, 180, 180, 180, ...   
#> Resampling results across tuning parameters:  
#>   
#> degree nprune RMSE Rsquared MAE   
#> 1 2 4.334325 0.2599883 3.607719  
#> 1 12 1.545349 0.8992979 1.243771  
#> 1 23 1.529405 0.9018457 1.223874  
#> 1 34 1.529405 0.9018457 1.223874  
#> 1 45 1.529405 0.9018457 1.223874  
#> 1 56 1.529405 0.9018457 1.223874  
#> 1 67 1.529405 0.9018457 1.223874  
#> 1 78 1.529405 0.9018457 1.223874  
#> 1 89 1.529405 0.9018457 1.223874  
#> 1 100 1.529405 0.9018457 1.223874  
#> 2 2 4.334325 0.2599883 3.607719  
#> 2 12 1.312883 0.9284253 1.063321  
#> 2 23 1.340821 0.9285264 1.050274  
#> 2 34 1.340821 0.9285264 1.050274  
#> 2 45 1.340821 0.9285264 1.050274  
#> 2 56 1.340821 0.9285264 1.050274  
#> 2 67 1.340821 0.9285264 1.050274  
#> 2 78 1.340821 0.9285264 1.050274  
#> 2 89 1.340821 0.9285264 1.050274  
#> 2 100 1.340821 0.9285264 1.050274  
#> 3 2 4.334325 0.2599883 3.607719  
#> 3 12 1.312883 0.9284253 1.063321  
#> 3 23 1.356568 0.9267847 1.068755  
#> 3 34 1.356568 0.9267847 1.068755  
#> 3 45 1.356568 0.9267847 1.068755  
#> 3 56 1.356568 0.9267847 1.068755  
#> 3 67 1.356568 0.9267847 1.068755  
#> 3 78 1.356568 0.9267847 1.068755  
#> 3 89 1.356568 0.9267847 1.068755  
#> 3 100 1.356568 0.9267847 1.068755  
#>   
#> 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.

Plot the MARS model results

ggplot(tuned\_mars)



Show the best tuned MARS model

# best chosen MARS model  
tuned\_mars$bestTune

#> nprune degree  
#> 12 12 2

Predict using the test data set and get the model’s performance values

marsPred <- predict(tuned\_mars, newdata = testData$x)  
## The function 'postResample' can be used to get the test set  
## performance values  
postResample(pred = marsPred, obs = testData$y)

#> RMSE Rsquared MAE   
#> 1.2803060 0.9335241 1.0168673

#### Using a Support Vector Machines (SVM) model

# Resource: Chapter 7.5 of textbook "Applied Predictive Modeling" by KJ  
  
library(kernlab)  
  
  
# We can use caret to perform a grid search using 10-fold cross-validation.  
# The train function generates a resampling estimate of performance. Because  
# the training set size is not small, 10-fold cross-validation should produce  
# reasonable estimates of model performance. The function trainControl specifies  
# the type of resampling:  
ctrl <- trainControl(method = "cv", number = 10)  
  
  
svmRTuned <- train(trainingData$x, trainingData$y,  
 method = "svmRadial",  
 preProc = c("center", "scale"),  
 tuneLength = 14,  
 trControl = ctrl)  
  
svmRTuned

#> Support Vector Machines with Radial Basis Function Kernel   
#>   
#> 200 samples  
#> 10 predictor  
#>   
#> Pre-processing: centered (10), scaled (10)   
#> Resampling: Cross-Validated (10 fold)   
#> Summary of sample sizes: 180, 180, 180, 180, 180, 180, ...   
#> Resampling results across tuning parameters:  
#>   
#> C RMSE Rsquared MAE   
#> 0.25 2.469506 0.7985704 1.979900  
#> 0.50 2.217035 0.8125018 1.766726  
#> 1.00 2.051120 0.8325247 1.618837  
#> 2.00 1.965427 0.8450934 1.539666  
#> 4.00 1.897161 0.8563701 1.500170  
#> 8.00 1.862883 0.8615845 1.475808  
#> 16.00 1.861693 0.8623909 1.474581  
#> 32.00 1.861693 0.8623909 1.474581  
#> 64.00 1.861693 0.8623909 1.474581  
#> 128.00 1.861693 0.8623909 1.474581  
#> 256.00 1.861693 0.8623909 1.474581  
#> 512.00 1.861693 0.8623909 1.474581  
#> 1024.00 1.861693 0.8623909 1.474581  
#> 2048.00 1.861693 0.8623909 1.474581  
#>   
#> Tuning parameter 'sigma' was held constant at a value of 0.06192511  
#> RMSE was used to select the optimal model using the smallest value.  
#> The final values used for the model were sigma = 0.06192511 and C = 16.

Predict using the test data set and get the model’s performance values

svmPred <- predict(svmRTuned, newdata = testData$x)  
## The function 'postResample' can be used to get the test set  
## performance values  
postResample(pred = svmPred, obs = testData$y)

#> RMSE Rsquared MAE   
#> 2.0712382 0.8260501 1.5732943

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

Comparing all used models we can see that the **MARS** model yields the best performance in terms of the lowest **RMSE = 1.2803060**.

| Model | RMSE | Rsquared | MAE |
| --- | --- | --- | --- |
| KNN | 3.2040595 | 0.6819919 | 2.5683461 |
| Neural Network (avNNet) | 2.1930855 | 0.8113903 | 1.6402075 |
| MARS | **1.2803060** | 0.9335241 | 1.0168673 |
| SVM | 2.0793977 | 0.8249453 | 1.5796370 |

## KJ 7.5 (Nonlinear Regression Models)

**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.**

Load libraries used for Exercise 6.3

library(RANN)  
library(dplyr)  
library(naniar)  
library(caret)

#### Load the data

library(AppliedPredictiveModeling)  
data(ChemicalManufacturingProcess)  
df\_raw <- ChemicalManufacturingProcess

#### Perform imputation of missing values

# check variables for missing values  
# gg\_miss\_var(df\_raw)

preProcess\_impute <- preProcess(df\_raw, method ="knnImpute")  
df <- predict(preProcess\_impute, newdata = df\_raw)

# check variables for missing values  
# gg\_miss\_var(df)

#### Remove near zero variance predictors

Predictors that have one unique value (i.e. are zero variance predictors) or predictors that are have both of the following characteristics: they have very few unique values relative to the number of samples and the ratio of the frequency of the most common value to the frequency of the second most common value is large.

df <- df %>% select(!caret::nearZeroVar(.))

#### Splitting data in to training and test set

# Create the training and test datasets  
set.seed(100)  
# Step 1: Get row numbers for the training data  
trainRowNumbers <- createDataPartition(df$Yield, p=0.8, list=FALSE)  
# Step 2: Create the training dataset  
trainData <- df[trainRowNumbers,]  
# Step 3: Create the test dataset  
testData <- df[-trainRowNumbers,]

#### Data preprocess applying centering and scaling

preProcValues <- preProcess(trainData, method = c("center", "scale"))  
trainTransformed <- predict(preProcValues, trainData)  
testTransformed <- predict(preProcValues, testData)  
  
xTrain <- trainTransformed %>% select(-Yield)  
yTrain <- trainTransformed %>% select(Yield)  
  
xTest <- testTransformed %>% select(-Yield)  
yTest <- testTransformed %>% select(Yield)

#### Fit a KNN model

knnChemModel <- train(x = xTrain,  
 y = yTrain$Yield,  
 method = "knn",  
 preProc = c("center", "scale"),  
 tuneLength = 10)  
  
knnChemModel

#> k-Nearest Neighbors   
#>   
#> 144 samples  
#> 56 predictor  
#>   
#> Pre-processing: centered (56), scaled (56)   
#> Resampling: Bootstrapped (25 reps)   
#> Summary of sample sizes: 144, 144, 144, 144, 144, 144, ...   
#> Resampling results across tuning parameters:  
#>   
#> k RMSE Rsquared MAE   
#> 5 0.7729445 0.4007219 0.6155921  
#> 7 0.7815333 0.3869367 0.6257886  
#> 9 0.7793118 0.3914364 0.6269750  
#> 11 0.7788873 0.3934229 0.6297394  
#> 13 0.7820317 0.3930332 0.6349738  
#> 15 0.7867647 0.3851576 0.6386412  
#> 17 0.7873253 0.3889346 0.6392012  
#> 19 0.7909364 0.3831876 0.6429651  
#> 21 0.7911040 0.3889180 0.6416521  
#> 23 0.7925310 0.3925148 0.6427579  
#>   
#> RMSE was used to select the optimal model using the smallest value.  
#> The final value used for the model was k = 5.

knnChemPred <- predict(knnChemModel, newdata = xTest)  
## The function 'postResample' can be used to get the test set  
## perforamnce values  
postResample(pred = knnChemPred, obs = yTest$Yield)

#> RMSE Rsquared MAE   
#> 0.6501442 0.4623051 0.5205731

#### Fit a Neural Network model

First, we remove predictors to ensure that the maximum absolute pairwise correlation between the predictors is less than 0.75.

tooHigh <- findCorrelation(cor(xTrain), cutoff = .75)  
  
tooHigh

#> [1] 2 4 6 7 1 11 43 30 29 41 40 20 26 24 21 53 37 36 56 42 51

Since the correlation vector is not empty, there are predictors to be removed. After removal, generate a new training and test sets of predictors.

trainXnnet <- xTrain[, -tooHigh]  
testXnnet <- xTest[, -tooHigh]

We can now fit a neural network model using the existing training set.

# Resource: Chapter 7.5 of textbook "Applied Predictive Modeling" by KJ  
  
## Create a specific candidate set of models to evaluate:  
nnetGrid <- expand.grid(.decay = c(0, 0.01, .1),  
 .size = c(1:10),  
 .bag = FALSE)  
  
# We can use caret to perform a grid search using 10-fold cross-validation.  
# The train function generates a resampling estimate of performance. Because  
# the training set size is not small, 10-fold cross-validation should produce  
# reasonable estimates of model performance. The function trainControl specifies  
# the type of resampling:  
ctrl <- trainControl(method = "cv", number = 10)  
  
nnetChemTune <- train(xTrain, yTrain$Yield,  
 method = "avNNet",  
 tuneGrid = nnetGrid,  
 trControl = ctrl,  
 ## Automatically standardize data prior to modeling  
 ## and prediction  
 preProc = c("center", "scale"),  
 linout = TRUE,  
 trace = FALSE,  
 MaxNWts = 10 \* (ncol(trainXnnet) + 1) + 10 + 1,  
 maxit = 500)  
  
nnetChemTune

#> Model Averaged Neural Network   
#>   
#> 144 samples  
#> 56 predictor  
#>   
#> Pre-processing: centered (56), scaled (56)   
#> Resampling: Cross-Validated (10 fold)   
#> Summary of sample sizes: 130, 129, 129, 129, 131, 129, ...   
#> Resampling results across tuning parameters:  
#>   
#> decay size RMSE Rsquared MAE   
#> 0.00 1 0.7482484 0.5157903 0.5740126  
#> 0.00 2 0.7670906 0.5273524 0.6228174  
#> 0.00 3 0.7637153 0.4955543 0.6265964  
#> 0.00 4 0.7452890 0.5685729 0.5967578  
#> 0.00 5 0.8359766 0.4617132 0.6987576  
#> 0.00 6 0.7416037 0.5544016 0.6147103  
#> 0.00 7 NaN NaN NaN  
#> 0.00 8 NaN NaN NaN  
#> 0.00 9 NaN NaN NaN  
#> 0.00 10 NaN NaN NaN  
#> 0.01 1 0.7955973 0.5175823 0.6293428  
#> 0.01 2 0.7960410 0.5555520 0.6448632  
#> 0.01 3 0.7166066 0.6183926 0.5596929  
#> 0.01 4 0.6805917 0.6109865 0.5386482  
#> 0.01 5 0.6185713 0.6635756 0.4948506  
#> 0.01 6 0.6797687 0.6151501 0.5380404  
#> 0.01 7 NaN NaN NaN  
#> 0.01 8 NaN NaN NaN  
#> 0.01 9 NaN NaN NaN  
#> 0.01 10 NaN NaN NaN  
#> 0.10 1 0.7325230 0.5480941 0.5885330  
#> 0.10 2 0.6751114 0.6177832 0.5525322  
#> 0.10 3 0.6788970 0.6116242 0.5669672  
#> 0.10 4 0.6410899 0.6367564 0.5099966  
#> 0.10 5 0.6817571 0.6272634 0.5366705  
#> 0.10 6 0.5983899 0.6787830 0.4756949  
#> 0.10 7 NaN NaN NaN  
#> 0.10 8 NaN NaN NaN  
#> 0.10 9 NaN NaN NaN  
#> 0.10 10 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 = 6, decay = 0.1 and bag = FALSE.

Predict using the test data set and get the model’s performance values

nnetChemPred <- predict(nnetChemTune, newdata = xTest)  
## The function 'postResample' can be used to get the test set  
## performance values  
postResample(pred = nnetChemPred, obs = yTest$Yield)

#> RMSE Rsquared MAE   
#> 0.5594510 0.6676931 0.4589402

#### Fit a MARS model

# Resource: Chapter 7.5 of textbook "Applied Predictive Modeling" by KJ  
# Resource: http://uc-r.github.io/mars  
  
library(earth)  
library(dplyr)  
  
## Create a specific candidate set of models to evaluate:  
marsGrid <- expand.grid(degree = 1:3,  
 nprune = seq(2, 100, length.out = 10) %>% floor()  
 )  
  
# We can use caret to perform a grid search using 10-fold cross-validation.  
# The train function generates a resampling estimate of performance. Because  
# the training set size is not small, 10-fold cross-validation should produce  
# reasonable estimates of model performance. The function trainControl specifies  
# the type of resampling:  
ctrl <- trainControl(method = "cv", number = 10)  
  
  
# cross validated model  
tuned\_ChemMARS <- train(  
 x = xTrain,  
 y = yTrain$Yield,  
 method = "earth",  
 metric = "RMSE",  
 trControl = ctrl,  
 tuneGrid = marsGrid  
)  
  
tuned\_ChemMARS

#> Multivariate Adaptive Regression Spline   
#>   
#> 144 samples  
#> 56 predictor  
#>   
#> No pre-processing  
#> Resampling: Cross-Validated (10 fold)   
#> Summary of sample sizes: 131, 129, 131, 130, 130, 128, ...   
#> Resampling results across tuning parameters:  
#>   
#> degree nprune RMSE Rsquared MAE   
#> 1 2 0.7311847 0.4797663 0.5765448  
#> 1 12 0.6268401 0.6363518 0.4961724  
#> 1 23 0.6777858 0.5923480 0.5317603  
#> 1 34 0.6777858 0.5923480 0.5317603  
#> 1 45 0.6777858 0.5923480 0.5317603  
#> 1 56 0.6777858 0.5923480 0.5317603  
#> 1 67 0.6777858 0.5923480 0.5317603  
#> 1 78 0.6777858 0.5923480 0.5317603  
#> 1 89 0.6777858 0.5923480 0.5317603  
#> 1 100 0.6777858 0.5923480 0.5317603  
#> 2 2 0.7311847 0.4797663 0.5765448  
#> 2 12 0.7864332 0.5169358 0.6064500  
#> 2 23 0.8559298 0.4818783 0.6329810  
#> 2 34 0.9532541 0.4772605 0.6638981  
#> 2 45 0.9532541 0.4772605 0.6638981  
#> 2 56 0.9532541 0.4772605 0.6638981  
#> 2 67 0.9532541 0.4772605 0.6638981  
#> 2 78 0.9532541 0.4772605 0.6638981  
#> 2 89 0.9532541 0.4772605 0.6638981  
#> 2 100 0.9532541 0.4772605 0.6638981  
#> 3 2 0.7244312 0.4928378 0.5711214  
#> 3 12 0.7410723 0.5707312 0.5533310  
#> 3 23 0.9362855 0.5341917 0.6469362  
#> 3 34 0.9672974 0.5340704 0.6539555  
#> 3 45 0.9672974 0.5340704 0.6539555  
#> 3 56 0.9672974 0.5340704 0.6539555  
#> 3 67 0.9672974 0.5340704 0.6539555  
#> 3 78 0.9672974 0.5340704 0.6539555  
#> 3 89 0.9672974 0.5340704 0.6539555  
#> 3 100 0.9672974 0.5340704 0.6539555  
#>   
#> RMSE was used to select the optimal model using the smallest value.  
#> The final values used for the model were nprune = 12 and degree = 1.

Predict using the test data set and get the model’s performance values

marsChemPred <- predict(tuned\_ChemMARS, newdata = xTest)  
## The function 'postResample' can be used to get the test set  
## performance values  
postResample(pred = marsChemPred, obs = yTest$Yield)

#> RMSE Rsquared MAE   
#> 0.5754156 0.6002260 0.4630585

#### Fit an SVM model

# Resource: Chapter 7.5 of textbook "Applied Predictive Modeling" by KJ  
  
library(kernlab)  
  
  
# We can use caret to perform a grid search using 10-fold cross-validation.  
# The train function generates a resampling estimate of performance. Because  
# the training set size is not small, 10-fold cross-validation should produce  
# reasonable estimates of model performance. The function trainControl specifies  
# the type of resampling:  
ctrl <- trainControl(method = "cv", number = 10)  
  
  
svmChemRTuned <- train(xTrain, yTrain$Yield,  
 method = "svmRadial",  
 preProc = c("center", "scale"),  
 tuneLength = 14,  
 trControl = ctrl)  
  
svmChemRTuned

#> Support Vector Machines with Radial Basis Function Kernel   
#>   
#> 144 samples  
#> 56 predictor  
#>   
#> Pre-processing: centered (56), scaled (56)   
#> Resampling: Cross-Validated (10 fold)   
#> Summary of sample sizes: 130, 129, 129, 132, 129, 129, ...   
#> Resampling results across tuning parameters:  
#>   
#> C RMSE Rsquared MAE   
#> 0.25 0.7748155 0.4982164 0.6333898  
#> 0.50 0.7066847 0.5452049 0.5836571  
#> 1.00 0.6654443 0.5830103 0.5500636  
#> 2.00 0.6434370 0.6058495 0.5263888  
#> 4.00 0.6304889 0.6168851 0.5087674  
#> 8.00 0.6226799 0.6238696 0.5038193  
#> 16.00 0.6226799 0.6238696 0.5038193  
#> 32.00 0.6226799 0.6238696 0.5038193  
#> 64.00 0.6226799 0.6238696 0.5038193  
#> 128.00 0.6226799 0.6238696 0.5038193  
#> 256.00 0.6226799 0.6238696 0.5038193  
#> 512.00 0.6226799 0.6238696 0.5038193  
#> 1024.00 0.6226799 0.6238696 0.5038193  
#> 2048.00 0.6226799 0.6238696 0.5038193  
#>   
#> Tuning parameter 'sigma' was held constant at a value of 0.01532961  
#> RMSE was used to select the optimal model using the smallest value.  
#> The final values used for the model were sigma = 0.01532961 and C = 8.

Predict using the test data set and get the model’s performance values

svmChemPred <- predict(svmChemRTuned, newdata = xTest)  
## The function 'postResample' can be used to get the test set  
## performance values  
postResample(pred = svmChemPred, obs = yTest$Yield)

#> RMSE Rsquared MAE   
#> 0.5648427 0.5929463 0.4521138

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

Comparing all used models we can see that the **Neural Network (avNNet)** model yields the best performance in terms of the lowest RMSE = 0.5594510.

| Model | RMSE | Rsquared | MAE |
| --- | --- | --- | --- |
| KNN | 0.6501442 | 0.4623051 | 0.5205731 |
| Neural Network (avNNet) | **0.5594510** | 0.6676931 | 0.4589402 |
| MARS | 0.5754156 | 0.6002260 | 0.4630585 |
| SVM | 0.5682649 | 0.5880968 | 0.4506714 |

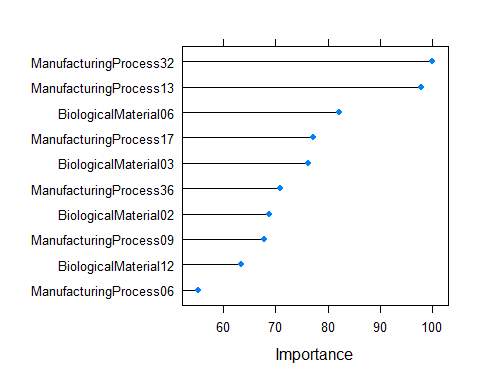
### b. Which predictors are most important in the optimal nonlinear regression model? Do either the biological or process variables dominate the list? How do the top ten important predictors compare to the top ten predictors from the optimal linear model?

* The **Neural Network (avNNet)** model yields the best performance in terms of the lowest RMSE = 0.5594510. For such model, below are the predictors in order of importance. A plot of them is also provided.
* The comparison of the top ten most important predictor between the NNET model and the Linear Model shows that the most important predictor is the "ManufacturingProcess32". The rest of the predictors are ranked differently between the 2 models. The NNET model captured only one biological predictor "BiologicalMaterial11" in the top 10 list. While the Linear Model ranked 4 biological predictors in the top 10.

| Importance | Linear Model Top Predictors | Overall | NNET Model Predictors | Overall |
| --- | --- | --- | --- | --- |

`1|ManufacturingProcess32 |4.0148629 | ManufacturingProcess32 |100.00000`  
 2|ManufacturingProcess33 |2.5534232 | ManufacturingProcess13 |97.83640  
 3|ManufacturingProcess28 |2.2725763 | BiologicalMaterial06 |82.21744  
 4|ManufacturingProcess37 |2.1891986 | ManufacturingProcess17 |77.26777  
 5|ManufacturingProcess13 |2.0341703 | BiologicalMaterial03 |76.21094  
 6|ManufacturingProcess07 |1.7731421 | ManufacturingProcess36 |70.96498  
 7|BiologicalMaterial05 |1.6380685 | BiologicalMaterial02 |68.78876  
 8|ManufacturingProcess04 |1.6338725 | ManufacturingProcess09 |67.86384  
 9|ManufacturingProcess16 |1.5879600 | BiologicalMaterial12 |63.36203  
 10|BiologicalMaterial11 |1.5688048 | ManufacturingProcess06 |55.15443

plot(caret::varImp(nnetChemTune), top = 10)

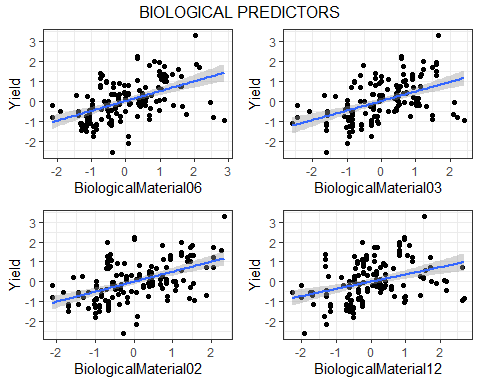


caret::varImp(nnetChemTune)

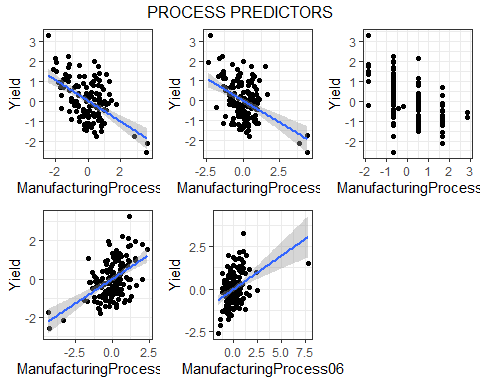
#> loess r-squared variable importance  
#>   
#> only 20 most important variables shown (out of 56)  
#>   
#> Overall  
#> ManufacturingProcess32 100.00  
#> ManufacturingProcess13 97.84  
#> BiologicalMaterial06 82.22  
#> ManufacturingProcess17 77.27  
#> BiologicalMaterial03 76.21  
#> ManufacturingProcess36 70.96  
#> BiologicalMaterial02 68.79  
#> ManufacturingProcess09 67.86  
#> BiologicalMaterial12 63.36  
#> ManufacturingProcess06 55.15  
#> BiologicalMaterial04 54.31  
#> ManufacturingProcess33 49.35  
#> ManufacturingProcess31 47.56  
#> ManufacturingProcess11 45.87  
#> BiologicalMaterial11 42.44  
#> BiologicalMaterial08 41.89  
#> ManufacturingProcess29 41.45  
#> BiologicalMaterial01 41.19  
#> BiologicalMaterial09 39.70  
#> ManufacturingProcess02 37.13

### 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?

library(gridExtra)  
  
top9nnetPred <- trainTransformed %>%  
 select(Yield,   
 ManufacturingProcess13,  
 BiologicalMaterial06,  
 ManufacturingProcess17,  
 BiologicalMaterial03,  
 ManufacturingProcess36,  
 BiologicalMaterial02,  
 ManufacturingProcess09,  
 BiologicalMaterial12,  
 ManufacturingProcess06)  
  
plt01 <- top9nnetPred %>%  
 ggplot(aes(x = ManufacturingProcess13, y = Yield)) +  
 geom\_point() + geom\_smooth(method = "lm") + theme\_bw()  
  
plt02 <- top9nnetPred %>%  
 ggplot(aes(x = BiologicalMaterial06, y = Yield)) +  
 geom\_point()+ geom\_smooth(method = "lm") + theme\_bw()  
  
plt03 <- top9nnetPred %>%  
 ggplot(aes(x = ManufacturingProcess17, y = Yield)) +  
 geom\_point() + geom\_smooth(method = "lm") + theme\_bw()  
  
plt04 <- top9nnetPred %>%  
 ggplot(aes(x = BiologicalMaterial03, y = Yield)) +  
 geom\_point() + geom\_smooth(method = "lm") + theme\_bw()  
  
plt05 <- top9nnetPred %>%  
 ggplot(aes(x = ManufacturingProcess36, y = Yield)) +  
 geom\_point() + theme\_bw()  
  
plt06 <- top9nnetPred %>%  
 ggplot(aes(x = BiologicalMaterial02, y = Yield)) +  
 geom\_point() + geom\_smooth(method = "lm") + theme\_bw()  
  
plt07 <- top9nnetPred %>%  
 ggplot(aes(x = ManufacturingProcess09, y = Yield)) +  
 geom\_point() + geom\_smooth(method = "lm") + theme\_bw()  
  
plt08 <- top9nnetPred %>%  
 ggplot(aes(x = BiologicalMaterial12, y = Yield)) +  
 geom\_point() + geom\_smooth(method = "lm") + theme\_bw()  
  
plt09 <- top9nnetPred %>%  
 ggplot(aes(x = ManufacturingProcess06, y = Yield)) +  
 geom\_point() + geom\_smooth(method = "lm") + theme\_bw()  
  
# Biological Predictors  
grid.arrange(plt02, plt04, plt06, plt08, nrow = 2, top = "BIOLOGICAL PREDICTORS")



# Process Predictors  
grid.arrange(plt01, plt03, plt05, plt07, plt09,  
 nrow = 2, top = "PROCESS PREDICTORS")



We use scatter plots between the top predictors and the response for the TOP 9 predictors that are unique to the optimal nonlinear regression model.

The conclusion is:

* All four Biological predictors (BiologicalMaterial02, BiologicalMaterial36, BiologicalMaterial06, BiologicalMaterial12) appear to have low positive correlation to the response variable.
* The ManufacturingProcess13 and ManufacturingProcess17 appear to have low negative correlation to the response within a limited interval in each case. Also, there are a few outliers outside of the intervals.
* Predictor ManufacturingProcess17 appears to have no correlation to the response. The points seem to form parallel vertical lines every 2.5 units. I am not sure why this predictor would come up in the top 10 predictors for the optimal non-linear regression model.
* Process predictors ManufacturingProcess09 and ManufacturingProcess06 seem to have a low positive correlation within a limited interval in each case.

## KJ 8.1 (Regression Trees and Rule-Based Models)

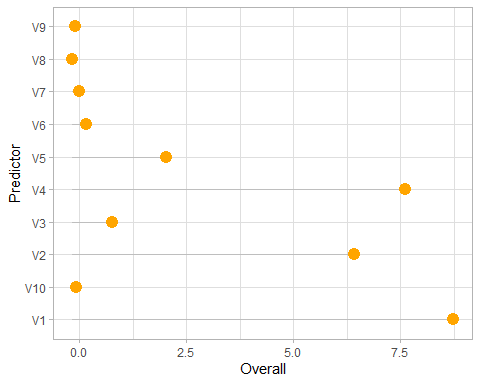
**Recreate the simulated data from Exercise 7.2:**

library(mlbench)  
set.seed(200)  
simulated <- mlbench.friedman1(200, sd = 1)  
simulated <- cbind(simulated$x, simulated$y)  
simulated <- as.data.frame(simulated)  
colnames(simulated)[ncol(simulated)] <- "y"  
head(simulated)

#> V1 V2 V3 V4 V5 V6 V7  
#> 1 0.5337724 0.6478064 0.85078526 0.18159957 0.92903976 0.36179060 0.8266609  
#> 2 0.5837650 0.4381528 0.67272659 0.66924914 0.16379784 0.45305931 0.6489601  
#> 3 0.5895783 0.5879065 0.40967108 0.33812728 0.89409334 0.02681911 0.1785614  
#> 4 0.6910399 0.2259548 0.03335447 0.06691274 0.63744519 0.52500637 0.5133614  
#> 5 0.6673315 0.8188985 0.71676079 0.80324287 0.08306864 0.22344157 0.6644906  
#> 6 0.8392937 0.3862983 0.64618857 0.86105431 0.63038947 0.43703891 0.3360117  
#> V8 V9 V10 y  
#> 1 0.4214081 0.59111440 0.5886216 18.46398  
#> 2 0.8446239 0.92819306 0.7584008 16.09836  
#> 3 0.3495908 0.01759542 0.4441185 17.76165  
#> 4 0.7970260 0.68986918 0.4450716 13.78730  
#> 5 0.9038919 0.39696995 0.5500808 18.42984  
#> 6 0.6489177 0.53116033 0.9066182 20.85817

### a. Fit a random forest model to all of the predictors, then estimate the variable importance scores:

library(randomForest)  
#library(caret)  
library(tibble)  
model1 <- randomForest(y ~., data = simulated, importance = TRUE, ntree = 1000)  
rfImp1 <- varImp(model1, scale = FALSE)  
  
rfImp1 <- tibble::rownames\_to\_column(rfImp1, "Predictors")  
  
rfImp1 %>%  
 mutate(name = fct\_reorder(Predictors, Overall)) %>%  
 ggplot(aes(x = name, y = Overall)) +  
 geom\_segment(aes(x=Predictors, xend=Predictors, y=min(Overall), yend= Overall), color = "grey") +  
 geom\_point(color = "orange", size = 4) +  
 xlab("Predictor") +  
 theme\_light() +  
 coord\_flip()



Did the random forest model significantly use the uninformative predictors (V6-V10)?

### b. Now add an additional predictor that is highly correlated with one of the informative predictors. For example:

> simulated$duplicate1 <- simulated$V1 + rnorm(200) \* .1  
> cor(simulated$duplicate1, simulated$V1)

Fit another random forest model to these data. Did the importance score for change?

What happens when you add another predictor that is also highly correlated with ?

### c. Use the cforest function in the party package to fit a random forest model using conditional inference trees. The party package function varimp can calculate predictor importance. The conditional argument of that function toggles between the traditional importance measure and the modified version described in Strobl et al. (2007). Do these importances show the same pattern as the traditional random forest model?

### d. Repeat this process with different tree models, such as boosted trees and Cubist. Does the same pattern occur?

## KJ 8.2 (Regression Trees and Rule-Based Models)

**Use a simulation to show tree bias with different granularities.**

## KJ 8.3 (Regression Trees and Rule-Based Models)

## KJ 8.7 (Regression Trees and Rule-Based Models)

**In stochastic gradient boosting the bagging fraction and learning rate will govern the construction of the trees as they are guided by the gradient. Althouth the optimal values of these paramaters should be obtained through the tuning process, it is helpful to understand how the magnitudes of these parameters affect magnitudes of variable importance. Figure 8.24 provides the variable importance plots for boosting using two extreme values for the bagging fraction (0.1 and 0.9) and the learning rate (0.1 and 0.9) for the solubility data. The left-hand plot has both parameters set to 0.1, and the right-hand plot has both set to 0.9:**

### a. Why does the model on the right focus its importance on just the first few of predictors, whereas the model on the left spreads importance across more predictors?

### b. Which model do you think would be more predictive of other samples?

### c. How would increasing interaction depth affect the slope of predictor importance for either model in Fig. 8.24?

# Week 6

## HW BATCH #2 - Market Basket Analysis / Recommender Systems (a simple problem)

**I am assigning one simple problem on market basket analysis / recommender systems.**

**Imagine 10000 receipts sitting on your table. Each receipt represents a transcation with items that were purchased. The receipt is a representation of stuff that went into a customer’s basket - and therefore ‘Market Basket Analysis’.**

**That is exactly what the Groceries Data Set contains: a collection of receipts with each line representing 1 receipt and the items purchased. Each line is called a**

**and each column in a row represents an**

**Here is the dataset =**[GroceryDataSet.csv](https://bbhosted.cuny.edu/bbcswebdav/pid-8461316-dt-announcement-rid-389564218_1/xid-389564218_1)**(comma separated file)**

**You assignment is to use R to mine the data for association rules. You should report support confidence and lift and your top 10 rules by lift. Turn in as you would the other problems from HA and KJ. You should packaged this with your HW#2 set.**

**NOTE: Bonus - Use a Python Library in addition to R and get a Bonus.**

## References