

Homework – 4

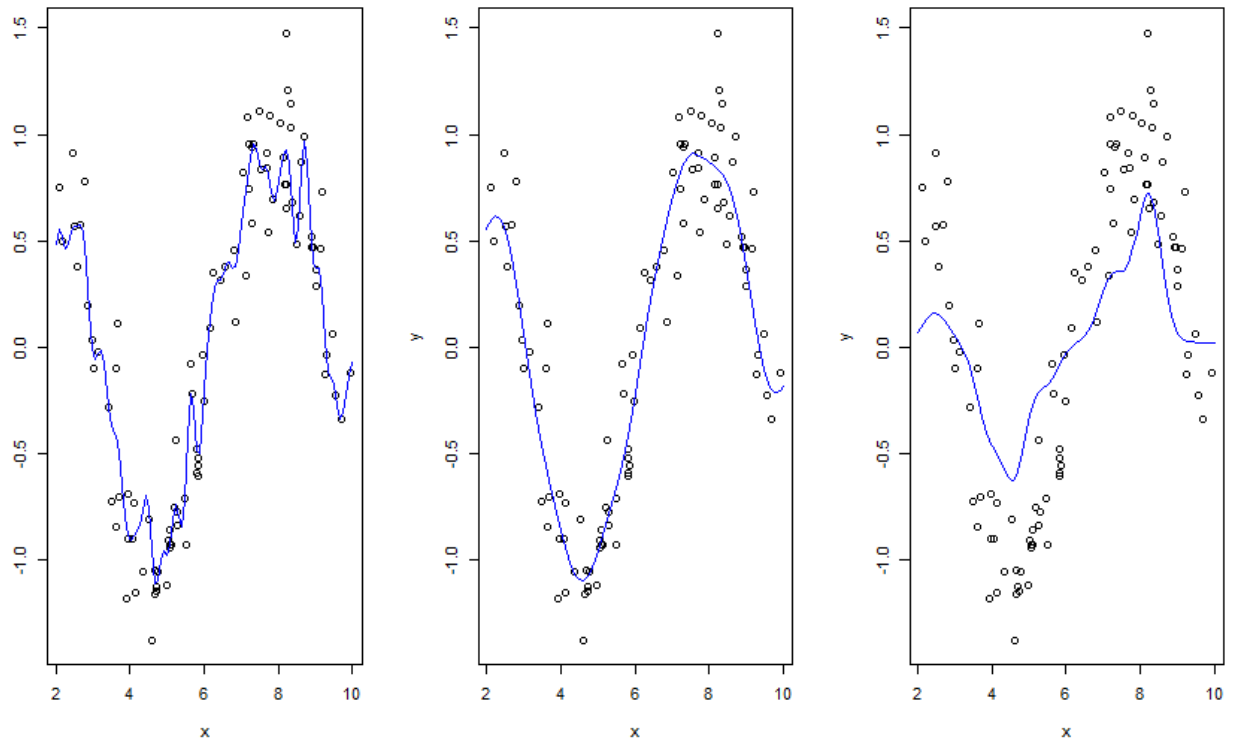
Question 7.1 (a)

Fit different models using a radial basis function and different values of the cost (the c parameter) and epsilon. Plot the fitted curve

Answer:

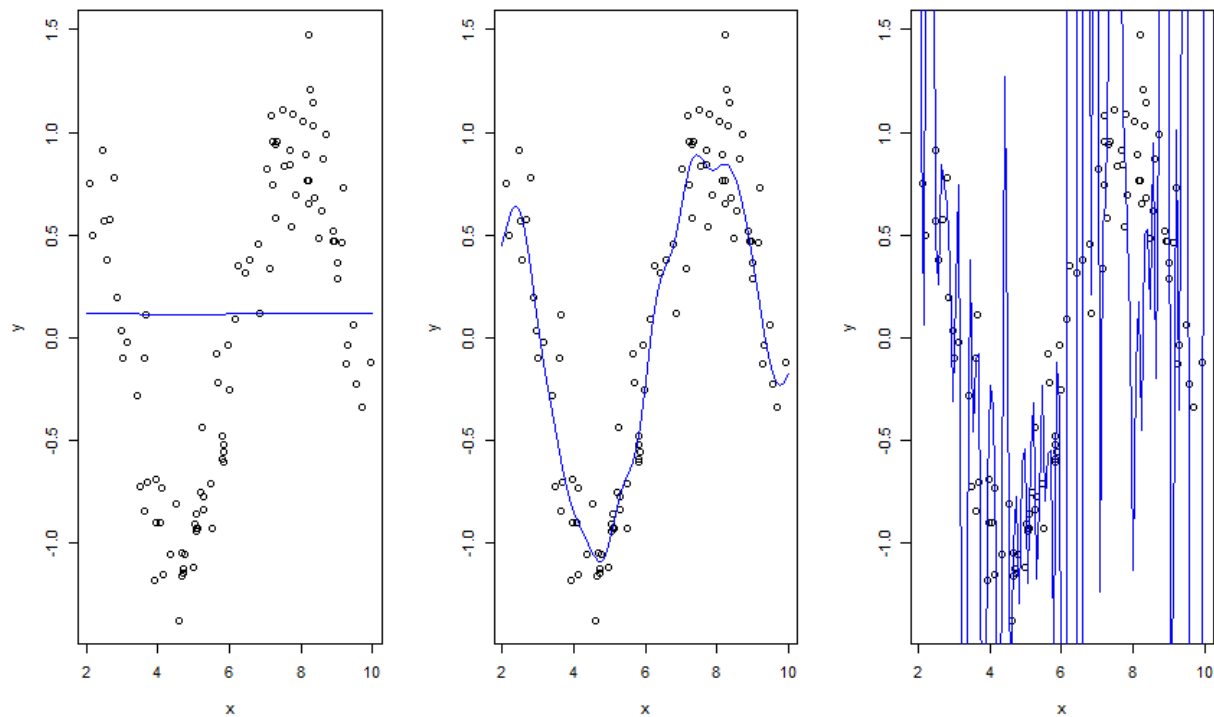
The first 3 plots show change in the epsilon value:

The first plot represents overfitting with smaller epsilon value and last graph represents underfitting with higher epsilon value. We get the below best fit curve in the middle. **The best value of epsilon = 0.1**



The below 3 plots show change in the Cost value:

The first plot represents underfitting with smaller C value and last graph represents overfitting with higher C value. We get the below best fit curve in the middle. **The best value of $C = 1$**

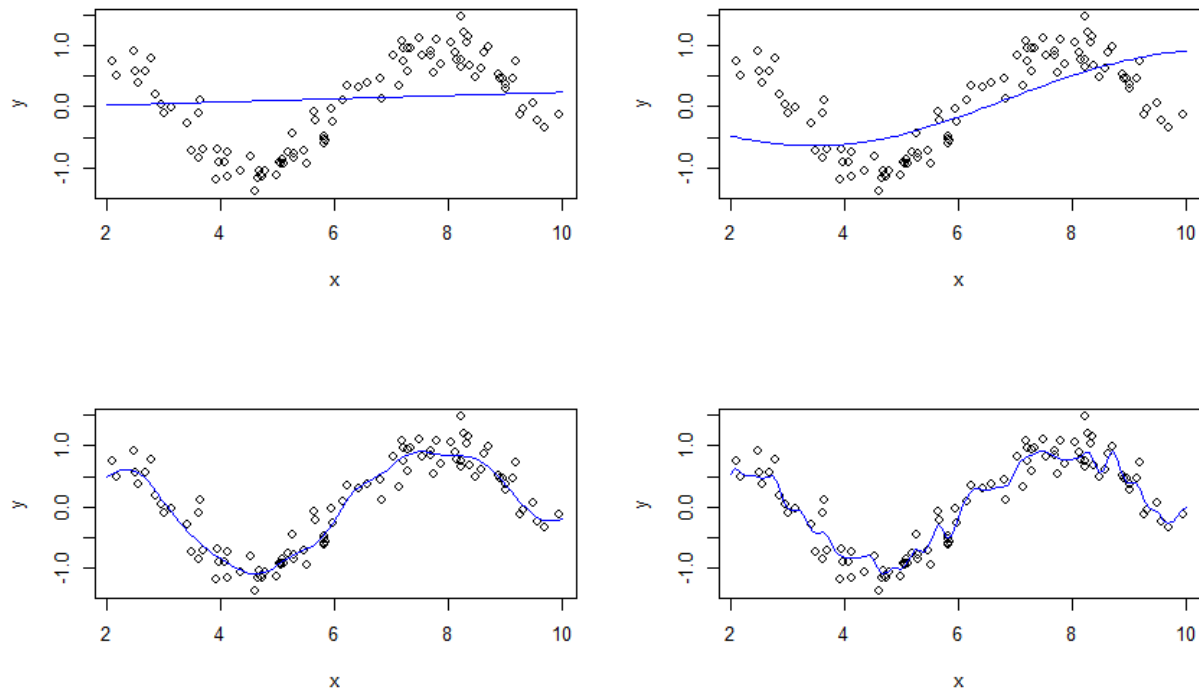


Question 7.1 (b)

Try different values of σ to understand how this parameter changes the model fit. How do the cost, epsilon, and σ values affect the model?

Answer: Using the best values of c and epsilon from 7.1(a), we try to tune sigma values and see that with **sigma = 10** , **C= 1** and **epsilon = 0.1** we get the below best fit curve:

With the **decrease in Cost**, the model will undergo high bias and low variability i.e. **UNDERFITTING** since very small penalty is given. Also, we observe with the decrease in epsilon value, the model begins to overfit. With the increase in sigma seems to overfit the model, however small values underfits the model.



Question 7.2 (a)

Consider KNN and MARS, which model appears to give the best performance?

Answer: Considering both KNN and MARS model, we see that Root Mean Square Error (RMSE) for KNN is 3.1954604 and for MARS model it is 1.2184795, thereby making **MARS model the best performer**.

```
> 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:

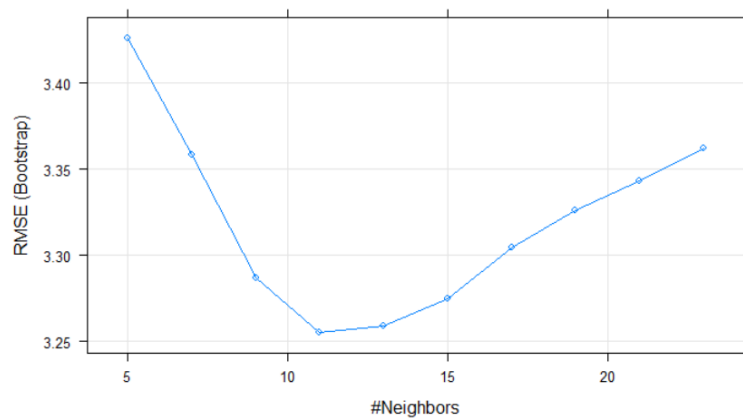
k	RMSE	Rsquared	MAE
5	3.556112	0.5198288	2.839161
7	3.460457	0.5475880	2.777304
9	3.428418	0.5655020	2.752174
11	3.388099	0.5894854	2.717181
13	3.378902	0.6059643	2.713234
15	3.378760	0.6174332	2.721502
17	3.376512	0.6296186	2.729312
19	3.391905	0.6370843	2.754631
21	3.404855	0.6457253	2.776341
23	3.425590	0.6513261	2.788951

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

RMSE and R square for KNN:

```
> postResample(pred = knnPred, obs = testData$y)
      RMSE  Rsquared    MAE
3.1954604 0.6763216 2.5643472
```

Plot of Knn:



******MARS MODEL******

```
> marSTuned
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	4.284557	0.2907768	3.6249495
1	3	3.745343	0.4559584	3.0619808
1	4	3.245863	0.5891338	2.7177850
1	5	2.629813	0.7306695	2.0789777
1	6	2.384633	0.7778715	1.9280078
1	7	1.958668	0.8414514	1.5928906
1	8	1.762501	0.8781308	1.3803270
1	9	1.685097	0.8864650	1.3278093
1	10	1.698655	0.8828539	1.3375487
1	11	1.712238	0.8795209	1.3438979
1	12	1.684415	0.8807914	1.3252383
1	13	1.672263	0.8813845	1.3142691
1	14	1.663376	0.8827605	1.3038362
1	15	1.634537	0.8855884	1.2820001

1	16	1.644353	0.8824488	1.2885712
1	17	1.644353	0.8824488	1.2885712
1	18	1.644353	0.8824488	1.2885712
1	19	1.644353	0.8824488	1.2885712
1	20	1.644353	0.8824488	1.2885712
1	21	1.644353	0.8824488	1.2885712
1	22	1.644353	0.8824488	1.2885712
1	23	1.644353	0.8824488	1.2885712
1	24	1.644353	0.8824488	1.2885712
1	25	1.644353	0.8824488	1.2885712
1	26	1.644353	0.8824488	1.2885712
1	27	1.644353	0.8824488	1.2885712
1	28	1.644353	0.8824488	1.2885712
1	29	1.644353	0.8824488	1.2885712
1	30	1.644353	0.8824488	1.2885712
2	2	4.284557	0.2907768	3.6249495
2	3	3.880966	0.4241772	3.2223793
2	4	3.284656	0.5916369	2.7133834
2	5	2.748910	0.7124206	2.2065683
2	6	2.502461	0.7563797	1.9966779
2	7	2.229125	0.7989121	1.8148853
2	8	2.067839	0.8338152	1.6268420
2	9	1.826997	0.8652168	1.4324910
2	10	1.584590	0.8983887	1.1902973
2	11	1.457277	0.9085165	1.1438142
2	12	1.265827	0.9358851	1.0372929
2	13	1.200899	0.9421594	0.9773092
2	14	1.209770	0.9419917	0.9915414
2	15	1.187278	0.9425942	0.9690146
2	16	1.188954	0.9427666	0.9598889
2	17	1.192742	0.9419037	0.9673360
2	18	1.194431	0.9416624	0.9670779
2	19	1.194431	0.9416624	0.9670779
2	20	1.194431	0.9416624	0.9670779
2	21	1.194431	0.9416624	0.9670779
2	22	1.194431	0.9416624	0.9670779
2	23	1.194431	0.9416624	0.9670779
2	24	1.194431	0.9416624	0.9670779
2	25	1.194431	0.9416624	0.9670779
2	26	1.194431	0.9416624	0.9670779
2	27	1.194431	0.9416624	0.9670779
2	28	1.194431	0.9416624	0.9670779
2	29	1.194431	0.9416624	0.9670779
2	30	1.194431	0.9416624	0.9670779

RMSE was used to select the optimal model using the smallest value.
The final values used for the model were nprune = 15 and degree = 2.

```
> summary(marsTuned)
```

```
Call: earth(x=data.frame[200,10], y=c(16.29,15.08,1...), keepxy=TRUE,
          degree=2, nprune=15)
```

	coefficients
(Intercept)	18.876238
h(0.47762-x1)	-10.654789
h(x1-0.47762)	11.763927
h(0.333521-x2)	-16.042699
h(x2-0.333521)	11.100290
h(0.450485-x3)	10.905837
h(x3-0.450485)	4.130150
h(x3-0.758697)	11.318926
h(0.929743-x4)	-9.969791
h(0.925323-x5)	-5.595141
h(x1-0.47762) * h(x2-0.429713)	-41.248060

```

h(x1-0.47762) * h(0.429713-x2)    -24.788387
h(0.553036-x1) * h(0.333521-x2)    29.499372
h(0.724499-x1) * h(x2-0.333521)    -10.655523
h(x1-0.724499) * h(x2-0.333521)    -27.328765

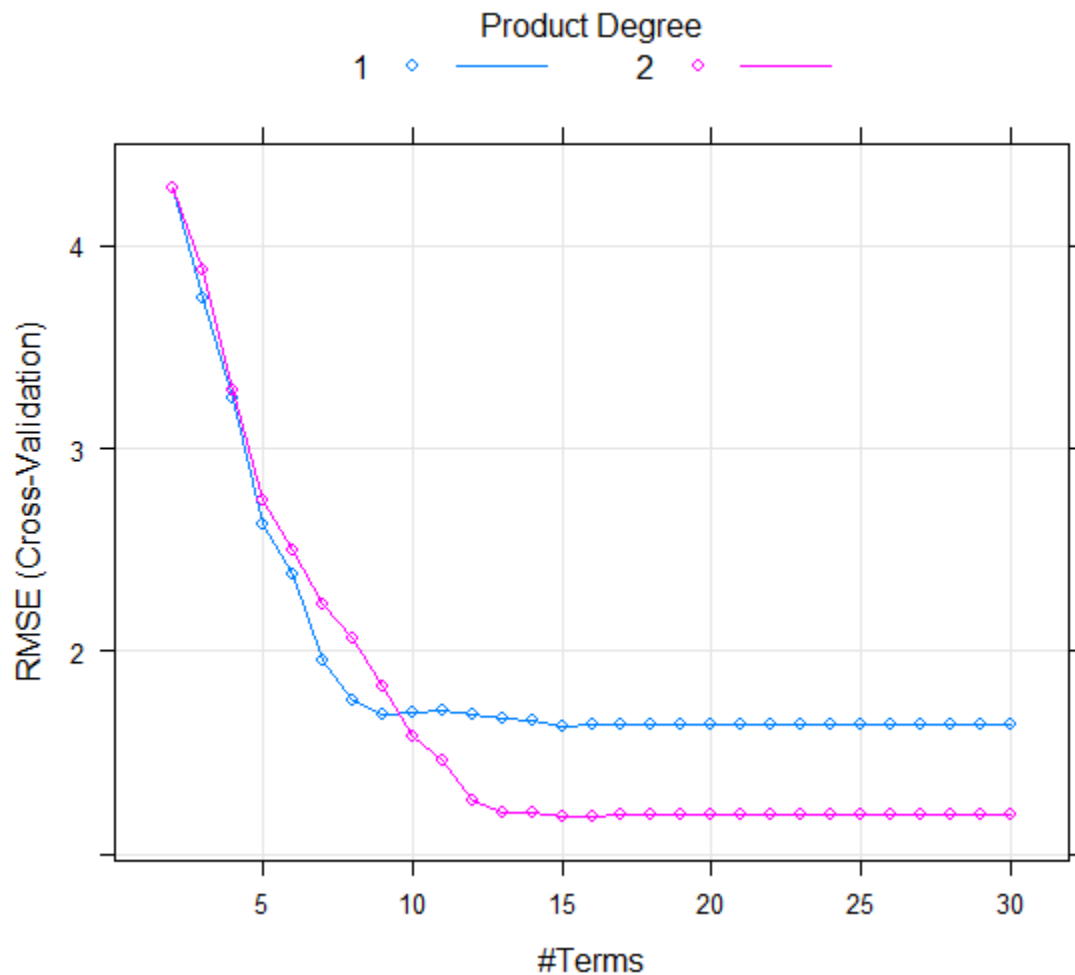
```

```

Selected 15 of 20 terms, and 5 of 10 predictors
Termination condition: Reached nk 21
Importance: x4, x2, x1, x5, x3, x6-unused, x7-unused, x8-unused, ...
Number of terms at each degree of interaction: 1 9 5
GCV 1.510035    RSS 203.0695    GRSq 0.9422094    RSq 0.9607501

```

Plot of MARS:



```

> postResample(pred = marsPred, obs = testData$y)
      RMSE Rsquared      MAE
1.2184795 0.9405195 0.9689160

```

```

> varImp(marSTuned)
earth variable importance

```

```

      Overall
x4      100.00
x2      83.07

```

x1	68.03
x5	55.51
x3	43.99
x6	0.00
x10	0.00
x8	0.00
x9	0.00
x7	0.00

Question 7.2 (b)

Does MARS select the informative predictors (those named X1-X5)?

Answer: Yes, MARS only selects predictors from X1- X5.

Importance: x4, x2, x1, x5, x3, x6-unused, x7-unused, x8-unused, ...

On checking the importance of the variables, we observe:

```
> varImp(marsTuned)
earth variable importance
```

	overall
x4	100.00
x2	83.07
x1	68.03
x5	55.51
x3	43.99
x6	0.00
x10	0.00
x8	0.00
x9	0.00
x7	0.00

Question 7.5 (a)

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

Answer:

On checking the below 4 models we receive the below RMSE values and conclude that **SVM** is the best model, followed by **MARS**, **KNN** and last **Neural Network**:

```
Neural Network: RMSE : [1] 1.481175
MARS: RMSE: [1] 0.976105
SVM: RMSE : [1] 0.8771186
KNN: RMSE : [1] 1.15631
```

*****Neural Network*****

```
> nnetTune
Neural Network
```

```
144 samples
 57 predictor
```

```
Pre-processing: centered (57), scaled (57)
```

```
Resampling: Cross-Validated (10 fold)
```

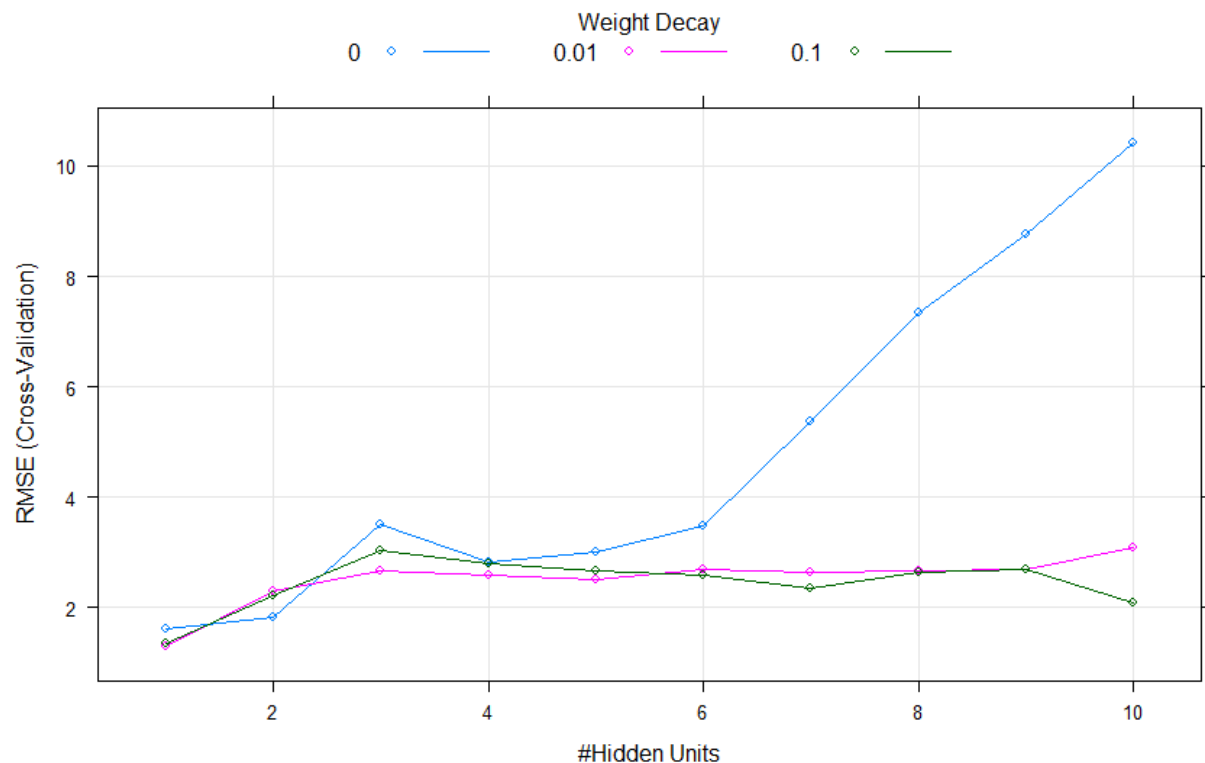
```
Summary of sample sizes: 129, 130, 130, 129, 130, 131, ...
```

```
Resampling results across tuning parameters:
```

decay	size	RMSE	Rsquared	MAE
0.00	1	1.613133	0.29680365	1.274704
0.00	2	1.829547	0.24644535	1.469571
0.00	3	3.514748	0.19934127	2.592703
0.00	4	2.815952	0.27272470	2.243474
0.00	5	3.021870	0.13418450	2.356914
0.00	6	3.478266	0.26920342	2.752366
0.00	7	5.371975	0.03786749	3.908115
0.00	8	7.333995	0.12922071	5.586466
0.00	9	8.754481	0.07477464	6.172310
0.00	10	10.411476	0.13388064	6.777419
0.01	1	1.313547	0.57891130	1.072006
0.01	2	2.305394	0.35672567	1.760655
0.01	3	2.681485	0.30159334	2.060560
0.01	4	2.580796	0.25428844	1.997650
0.01	5	2.513486	0.23123738	1.889188
0.01	6	2.698990	0.24594234	2.031484
0.01	7	2.642295	0.20900749	1.932284
0.01	8	2.672798	0.23740558	2.052299
0.01	9	2.687185	0.30079984	2.094814
0.01	10	3.092851	0.22843847	2.316658
0.10	1	1.360945	0.57819231	1.082098
0.10	2	2.208850	0.40737415	1.727699
0.10	3	3.043843	0.33748370	2.047708
0.10	4	2.796069	0.20667729	2.024215
0.10	5	2.672958	0.27962276	1.888574
0.10	6	2.599611	0.21499006	1.846923
0.10	7	2.344680	0.35088991	1.845712
0.10	8	2.651221	0.26366577	2.011825
0.10	9	2.693228	0.31586094	2.085887
0.10	10	2.093504	0.36036608	1.622409

RMSE was used to select the optimal model using the smallest value.
The final values used for the model were size = 1 and decay = 0.01.

Plot of Neural Networks:



RMSE and R square values:

```
> RMSE
[1] 1.481175
> Rsquared
[1] 0.463877
```

*****MARS Model*****

```
> marstuned2
Multivariate Adaptive Regression spline
```

```
144 samples
57 predictor
```

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

degree	nprune	RMSE	Rsquared	MAE
1	2	1.502409	0.3816048	1.1739426
1	3	1.310604	0.5317297	1.0515917
1	4	1.257524	0.5704640	1.0105068
1	5	1.199891	0.5909569	0.9776183
1	6	1.228152	0.5755721	1.0115693
1	7	1.248118	0.5582910	1.0260538
1	8	1.264259	0.5588769	1.0283702
1	9	1.282930	0.5441876	1.0231224
1	10	1.290678	0.5461481	1.0252852

1	11	1.274922	0.5554307	1.0060641
1	12	1.341004	0.5195106	1.0623705
1	13	1.369019	0.5059586	1.0870393
1	14	1.381312	0.5020588	1.0876543
1	15	1.349563	0.5213324	1.0707806
1	16	1.346936	0.5226876	1.0680519
1	17	1.358106	0.5188035	1.0801521
1	18	1.358106	0.5188035	1.0801521
1	19	1.358106	0.5188035	1.0801521
1	20	1.358106	0.5188035	1.0801521
1	21	1.358106	0.5188035	1.0801521
1	22	1.358106	0.5188035	1.0801521
1	23	1.358106	0.5188035	1.0801521
1	24	1.358106	0.5188035	1.0801521
1	25	1.358106	0.5188035	1.0801521
1	26	1.358106	0.5188035	1.0801521
1	27	1.358106	0.5188035	1.0801521
1	28	1.358106	0.5188035	1.0801521
1	29	1.358106	0.5188035	1.0801521
1	30	1.358106	0.5188035	1.0801521
1	31	1.358106	0.5188035	1.0801521
1	32	1.358106	0.5188035	1.0801521
1	33	1.358106	0.5188035	1.0801521
1	34	1.358106	0.5188035	1.0801521
1	35	1.358106	0.5188035	1.0801521
1	36	1.358106	0.5188035	1.0801521
1	37	1.358106	0.5188035	1.0801521
1	38	1.358106	0.5188035	1.0801521
1	39	1.358106	0.5188035	1.0801521
1	40	1.358106	0.5188035	1.0801521
1	41	1.358106	0.5188035	1.0801521
1	42	1.358106	0.5188035	1.0801521
1	43	1.358106	0.5188035	1.0801521
1	44	1.358106	0.5188035	1.0801521
1	45	1.358106	0.5188035	1.0801521
1	46	1.358106	0.5188035	1.0801521
1	47	1.358106	0.5188035	1.0801521
1	48	1.358106	0.5188035	1.0801521
1	49	1.358106	0.5188035	1.0801521
1	50	1.358106	0.5188035	1.0801521
2	2	1.502409	0.3816048	1.1739426
2	3	1.367764	0.4805279	1.0917356
2	4	1.388190	0.5108278	1.0608128
2	5	1.304490	0.5634132	1.0192828
2	6	1.269676	0.5708952	0.9881550
2	7	1.372822	0.4961310	1.0700828
2	8	1.355434	0.5008839	1.0614555
2	9	1.356070	0.4971033	1.0653667
2	10	1.424864	0.4751246	1.1108653
2	11	1.403176	0.4911517	1.0879520
2	12	1.529606	0.4156696	1.1697298
2	13	1.581811	0.4142080	1.1710376
2	14	1.671390	0.3840484	1.2070565
2	15	1.653477	0.3933017	1.1966139
2	16	1.654954	0.3944623	1.2000589
2	17	1.595685	0.4240096	1.1585922
2	18	1.630129	0.4150621	1.1868511
2	19	1.646315	0.4098851	1.1975194
2	20	1.640001	0.4081172	1.2124948
2	21	1.648272	0.3985678	1.2098688
2	22	1.662832	0.3958711	1.2249462
2	23	1.659475	0.3998134	1.2248941
2	24	1.654106	0.4151083	1.2393631
2	25	1.650484	0.4217019	1.2320061

2	26	1.667116	0.4217100	1.2428794
2	27	1.667116	0.4217100	1.2428794
2	28	1.667116	0.4217100	1.2428794
2	29	1.667116	0.4217100	1.2428794
2	30	1.667116	0.4217100	1.2428794
2	31	1.667116	0.4217100	1.2428794
2	32	1.667116	0.4217100	1.2428794
2	33	1.667116	0.4217100	1.2428794
2	34	1.667116	0.4217100	1.2428794
2	35	1.667116	0.4217100	1.2428794
2	36	1.667116	0.4217100	1.2428794
2	37	1.667116	0.4217100	1.2428794
2	38	1.667116	0.4217100	1.2428794
2	39	1.667116	0.4217100	1.2428794
2	40	1.667116	0.4217100	1.2428794
2	41	1.667116	0.4217100	1.2428794
2	42	1.667116	0.4217100	1.2428794
2	43	1.667116	0.4217100	1.2428794
2	44	1.667116	0.4217100	1.2428794
2	45	1.667116	0.4217100	1.2428794
2	46	1.667116	0.4217100	1.2428794
2	47	1.667116	0.4217100	1.2428794
2	48	1.667116	0.4217100	1.2428794
2	49	1.667116	0.4217100	1.2428794
2	50	1.667116	0.4217100	1.2428794

RMSE was used to select the optimal model using the smallest value.
The final values used for the model were nprune = 5 and degree = 1.

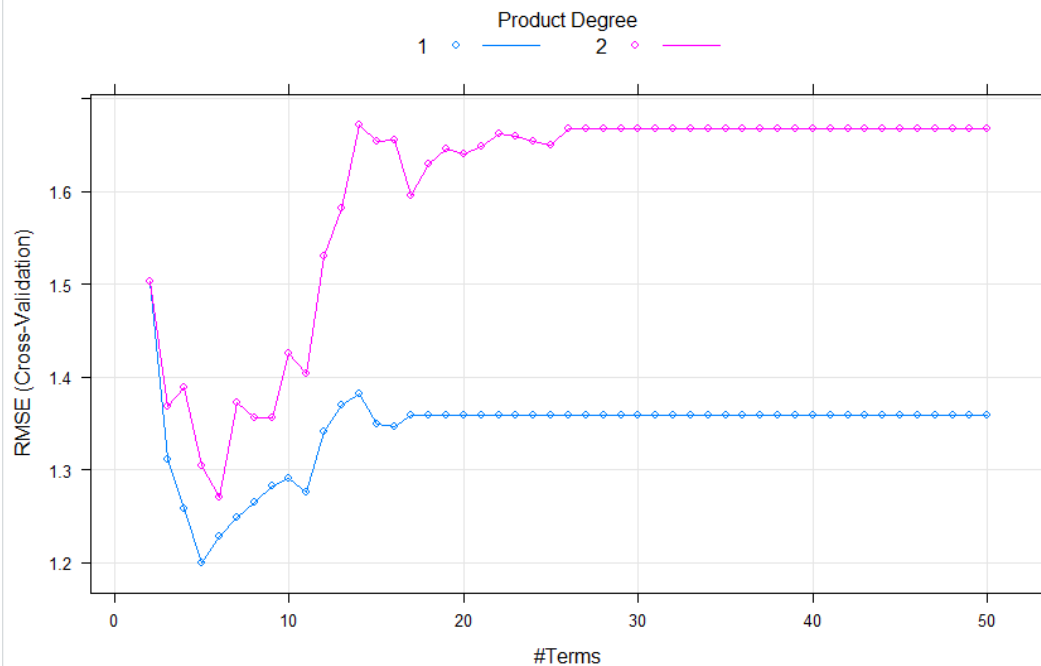
> `summary(marsTuned2)`

Call: `earth(x=data.frame[144,57], y=c(38,42.03,41.4...), keepxy=TRUE, degree=1, nprune=5)`

	coefficients
(Intercept)	38.260768
h(-1.01531-ManufacturingProcess09)	-1.102648
h(ManufacturingProcess09- -1.01531)	0.541082
h(-0.992785-ManufacturingProcess13)	1.660157
h(ManufacturingProcess32- -1.01272)	1.158230

Selected 5 of 21 terms, and 3 of 57 predictors
Termination condition: RSq changed by less than 0.001 at 21 terms
Importance: ManufacturingProcess32, ManufacturingProcess09, ManufacturingProcess13, BiologicalMaterial01-unused, ...
Number of terms at each degree of interaction: 1 4 (additive model)
GCV 1.39529 RSS 176.5914 GRSq 0.6048384 RSq 0.6478156

Plot of MARS:



RMSE and R square values:

```
> RMSE
[1] 0.976105
> Rsquared
[1,] 0.6829522
```

*****SVM Model*****

```
> svmRTuned
Support Vector Machines with Radial Basis Function Kernel
```

```
144 samples
57 predictor
```

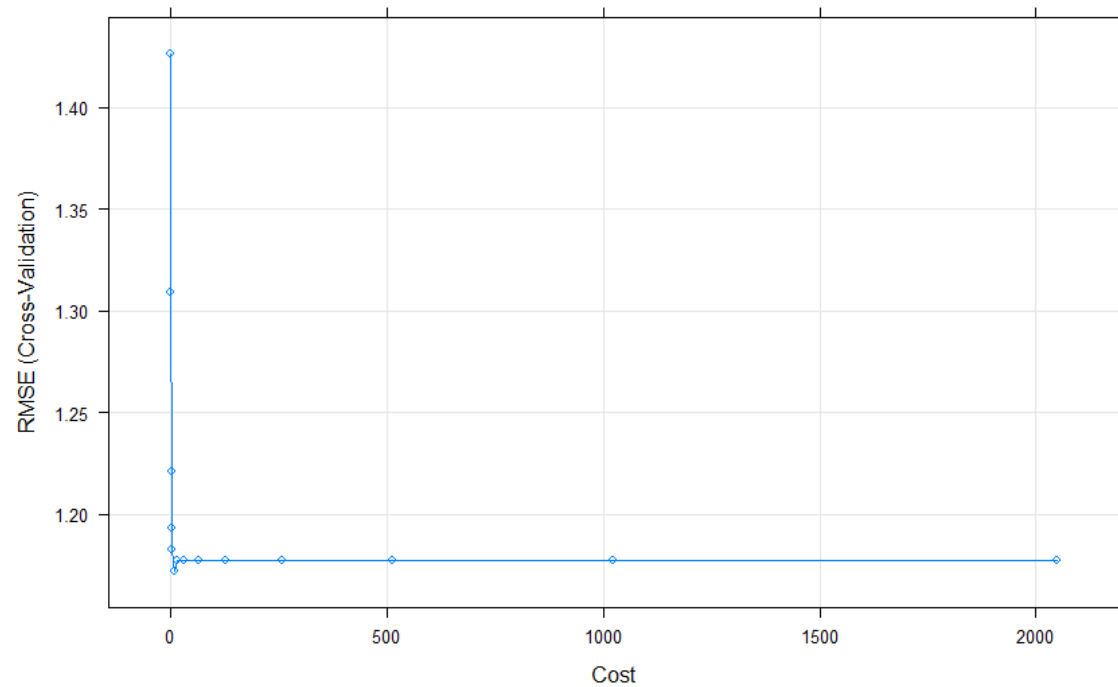
```
Pre-processing: centered (57), scaled (57)
Resampling: Cross-Validated (10 fold)
Summary of sample sizes: 130, 129, 129, 130, 130, 130, ...
Resampling results across tuning parameters:
```

C	RMSE	Rsquared	MAE
0.25	1.426182	0.4970065	1.1598629
0.50	1.309048	0.5496127	1.0666378
1.00	1.221146	0.5934250	0.9951853
2.00	1.193059	0.6075233	0.9669143
4.00	1.182927	0.6120168	0.9609258
8.00	1.172228	0.6192141	0.9549031
16.00	1.177742	0.6161415	0.9607608
32.00	1.177742	0.6161415	0.9607608
64.00	1.177742	0.6161415	0.9607608
128.00	1.177742	0.6161415	0.9607608
256.00	1.177742	0.6161415	0.9607608

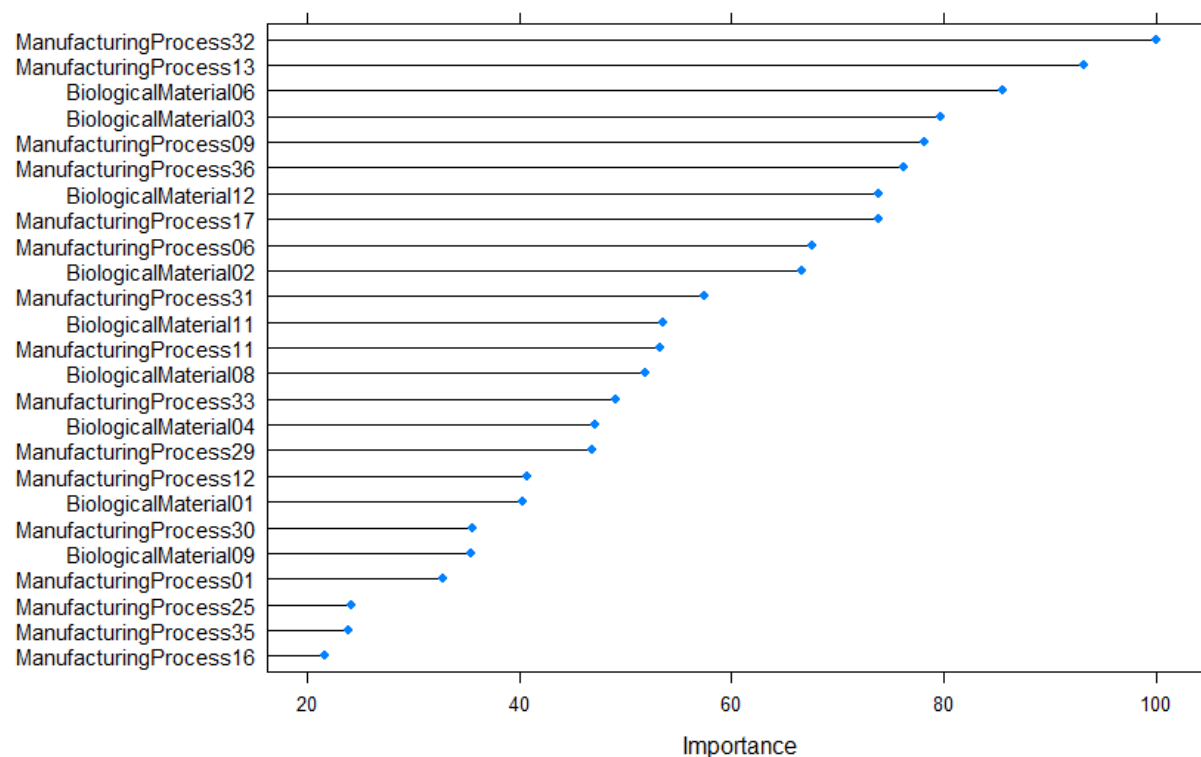
512.00	1.177742	0.6161415	0.9607608
1024.00	1.177742	0.6161415	0.9607608
2048.00	1.177742	0.6161415	0.9607608

Tuning parameter 'sigma' was held constant at a value of 0.01457755
RMSE was used to select the optimal model using the smallest value.
The final values used for the model were sigma = 0.01457755 and C = 8.

Plot of SVM:



Plot of important predictors:



RMSE and R square values:

```
> RMSE
[1] 0.8771186
> Rsquared
[1] 0.7410714
```

*****KNN Model*****

```
> knnTune
k-Nearest Neighbors
```

```
144 samples
56 predictor
```

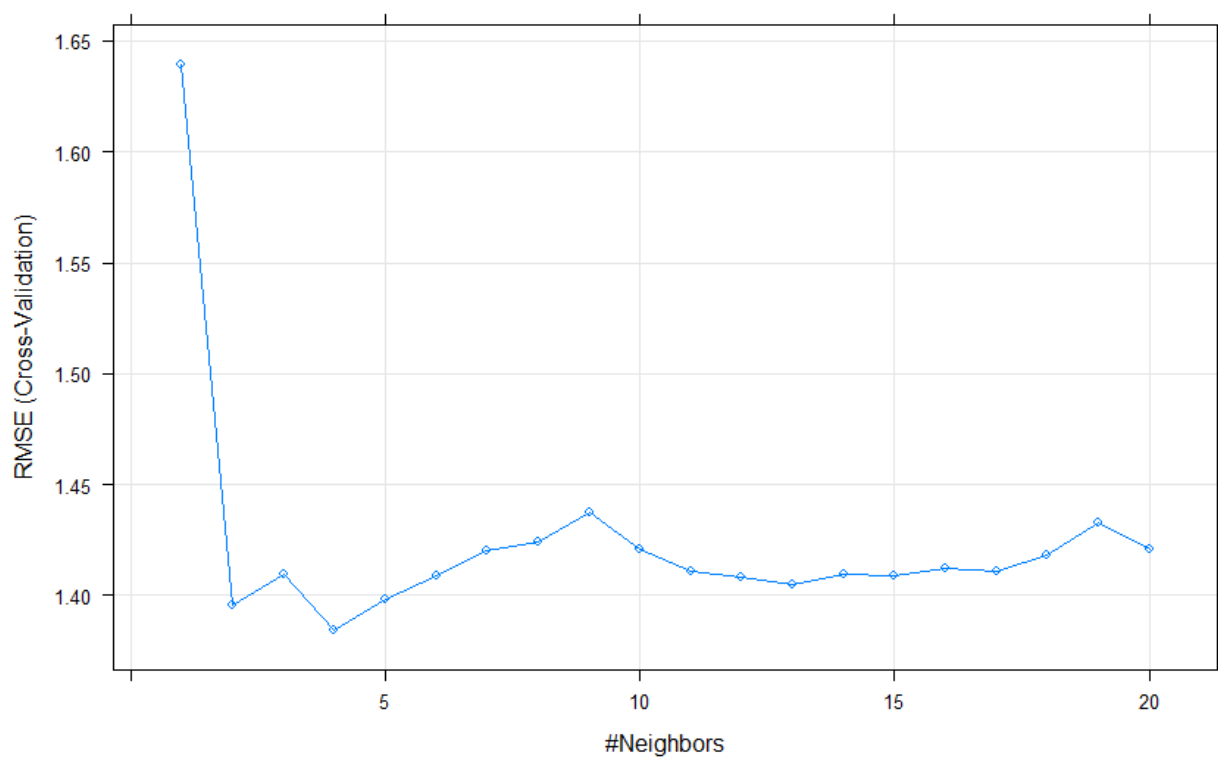
```
Pre-processing: centered (56), scaled (56)
Resampling: Cross-Validated (10 fold)
Summary of sample sizes: 129, 130, 130, 129, 130, 131, ...
Resampling results across tuning parameters:
```

k	RMSE	Rsquared	MAE
1	1.639293	0.3430869	1.262014
2	1.395296	0.4752058	1.114661
3	1.409294	0.4485807	1.097158
4	1.384346	0.4858396	1.086574
5	1.398517	0.4581576	1.106972
6	1.409157	0.4454810	1.121231
7	1.420295	0.4388996	1.151864
8	1.423832	0.4398441	1.163044

9	1.437183	0.4287864	1.172073
10	1.421155	0.4378686	1.155454
11	1.411128	0.4473777	1.152830
12	1.408270	0.4500300	1.151142
13	1.404617	0.4550758	1.146724
14	1.409763	0.4514934	1.147584
15	1.409020	0.4589753	1.139574
16	1.411879	0.4619994	1.139984
17	1.410879	0.4721659	1.137554
18	1.418117	0.4677082	1.145305
19	1.432810	0.4603145	1.154873
20	1.421041	0.4750207	1.150003

RMSE was used to select the optimal model using the smallest value.
The final value used for the model was $k = 4$.

Plot of KNN:



RMSE and R square values:

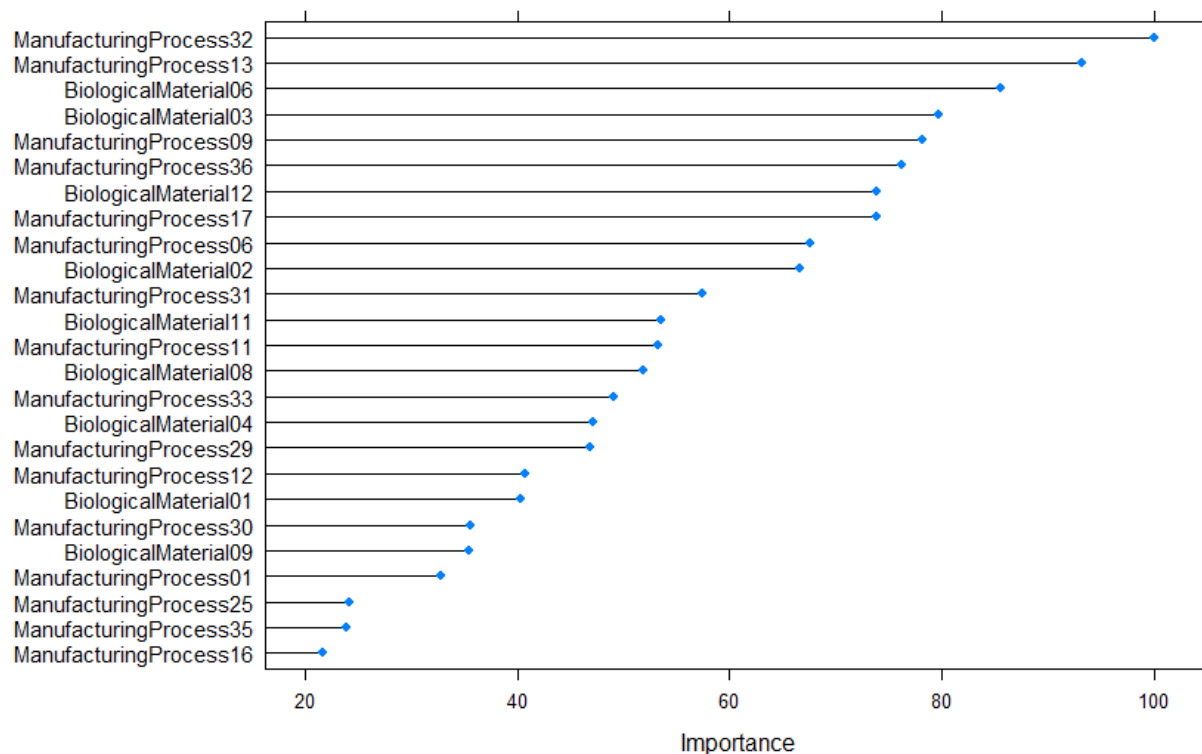
```
> RMSE
[1] 1.15631
> Rsquared
[1] 0.5810843
```

Question 7.5 (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?

Answer:

SVM being the most optimal nonlinear regression model has the below important predictors:



ManufacturingProcess variables dominate the list for SVM.

From previous homework

Model	RMSE
Lm	10.93
Lasso	1.82
Ridge	1.83
Enet	2.11

We see that Lasso is the best linear model on the Chemical Manufacturing Process data. Comparing the predictors of lasso and SVM we get:

- LASSO

ManufacturingProcess variables dominate the list for Lasso as well.

```
> varImp(lasso_model, lambda = cv$lambda.min)
```

	Overall
BiologicalMaterial01	0.000000000
BiologicalMaterial02	0.000000000
BiologicalMaterial03	0.112708621
BiologicalMaterial04	0.000000000
BiologicalMaterial05	0.000000000
BiologicalMaterial06	0.000000000
BiologicalMaterial07	0.009509862
BiologicalMaterial08	0.000000000
BiologicalMaterial09	0.000000000
BiologicalMaterial10	0.000000000
BiologicalMaterial11	0.000000000
BiologicalMaterial12	0.000000000
ManufacturingProcess01	0.000000000
ManufacturingProcess02	0.000000000
ManufacturingProcess03	0.000000000
ManufacturingProcess04	0.162928695
ManufacturingProcess05	0.000000000
ManufacturingProcess06	0.085777342
ManufacturingProcess07	0.062973310
ManufacturingProcess08	0.000000000
ManufacturingProcess09	0.284614864
ManufacturingProcess10	0.000000000
ManufacturingProcess11	0.000000000
ManufacturingProcess12	0.000000000
ManufacturingProcess13	0.096286395
ManufacturingProcess14	0.000000000
ManufacturingProcess15	0.000000000
ManufacturingProcess16	0.000000000
ManufacturingProcess17	0.357619767
ManufacturingProcess18	0.000000000
ManufacturingProcess19	0.000000000
ManufacturingProcess20	0.000000000
ManufacturingProcess21	0.000000000
ManufacturingProcess22	0.000000000
ManufacturingProcess23	0.008925333
ManufacturingProcess24	0.093393325
ManufacturingProcess25	0.000000000
ManufacturingProcess26	0.000000000
ManufacturingProcess27	0.000000000
ManufacturingProcess28	0.000000000
ManufacturingProcess29	0.591763124
ManufacturingProcess30	0.137948363
ManufacturingProcess31	0.000000000
ManufacturingProcess32	0.747713305
ManufacturingProcess33	0.000000000
ManufacturingProcess34	0.076817805
ManufacturingProcess35	0.000000000
ManufacturingProcess36	0.179127984
ManufacturingProcess37	0.221060479
ManufacturingProcess38	0.000000000
ManufacturingProcess39	0.048027780
ManufacturingProcess40	0.000000000
ManufacturingProcess41	0.000000000
ManufacturingProcess42	0.000000000
ManufacturingProcess43	0.051966758
ManufacturingProcess44	0.000000000
ManufacturingProcess45	0.061329224

- SVM

```
> varImp(svmRTuned)$importance
```

```
Overall
BiologicalMaterial01 40.2779608
BiologicalMaterial02 66.5824394
BiologicalMaterial03 79.6906796
BiologicalMaterial04 47.1507324
BiologicalMaterial05 10.8623772
BiologicalMaterial06 85.5635314
BiologicalMaterial07 3.3351954
BiologicalMaterial08 51.8451978
BiologicalMaterial09 35.4803625
BiologicalMaterial10 21.5067030
BiologicalMaterial11 53.5969206
BiologicalMaterial12 73.8215317
ManufacturingProcess01 32.7592301
ManufacturingProcess02 10.8197488
ManufacturingProcess03 3.4911254
ManufacturingProcess04 21.0223053
ManufacturingProcess05 4.2172945
ManufacturingProcess06 67.5571363
ManufacturingProcess07 0.2771389
ManufacturingProcess08 0.1033685
ManufacturingProcess09 78.2091653
ManufacturingProcess10 14.5255441
ManufacturingProcess11 53.2271800
ManufacturingProcess12 40.7319774
ManufacturingProcess13 93.1932828
ManufacturingProcess14 8.4507257
ManufacturingProcess15 19.0578586
ManufacturingProcess16 21.6730438
ManufacturingProcess17 73.7853670
ManufacturingProcess18 17.2068235
ManufacturingProcess19 5.2462448
ManufacturingProcess20 20.4856909
ManufacturingProcess21 12.2021501
ManufacturingProcess22 0.6078945
ManufacturingProcess23 2.4651551
ManufacturingProcess24 15.8760370
ManufacturingProcess25 24.2331286
ManufacturingProcess26 13.7209560
ManufacturingProcess27 16.1986253
ManufacturingProcess28 17.3060225
ManufacturingProcess29 46.7965363
ManufacturingProcess30 35.5739492
ManufacturingProcess31 57.4009288
ManufacturingProcess32 100.0000000
ManufacturingProcess33 49.0972274
ManufacturingProcess34 7.6558269
ManufacturingProcess35 23.9400984
ManufacturingProcess36 76.2131059
ManufacturingProcess37 13.1438491
ManufacturingProcess38 1.4337566
ManufacturingProcess39 0.4978371
ManufacturingProcess40 1.5448843
ManufacturingProcess41 0.7734379
ManufacturingProcess42 0.0000000
ManufacturingProcess43 5.9478364
ManufacturingProcess44 1.7741678
ManufacturingProcess45 0.1311078
```

Looking at top 20 important predictors of SVM

```
> varImp(svmRTuned)
loess r-squared variable importance

  only 20 most important variables shown (out of 57)

              overall
ManufacturingProcess32 100.00
ManufacturingProcess13  93.19
BiologicalMaterial06    85.56
BiologicalMaterial03    79.69
ManufacturingProcess09  78.21
ManufacturingProcess36  76.21
BiologicalMaterial12    73.82
ManufacturingProcess17  73.79
ManufacturingProcess06  67.56
BiologicalMaterial02    66.58
ManufacturingProcess31  57.40
BiologicalMaterial11    53.60
ManufacturingProcess11  53.23
BiologicalMaterial08    51.85
ManufacturingProcess33  49.10
BiologicalMaterial04    47.15
ManufacturingProcess29  46.80
ManufacturingProcess12  40.73
BiologicalMaterial01    40.28
ManufacturingProcess30  35.57
```

*****Homework Code*****

```
## We will use packages: caret, earth, kernlab, and nnet
install.packages(c("caret", "earth", "kernlab", "nnet"))
```

```
set.seed(1)
x <- runif(100, min = 2, max = 10)
y <- sin(x) + rnorm(length(x)) * .25
sinData <- data.frame(x = x, y = y)
plot(x, y)
```

```
## Create a grid of x values to use for prediction
```

```
dataGrid <- data.frame(x = seq(2, 10, length = 100))
```

```

library(kernlab)
par(mfrow = c(1,3))

rbfSVM <- ksvm(x = x, y = y, data = sinData, kernel = "rbfdot", kpar = "automatic",
               C = 1, epsilon = 0.001)
modelPrediction <- predict(rbfSVM, newdata = dataGrid)
plot(x,y)
points(x = dataGrid$x, y = modelPrediction[,1], type = "l", col = "blue")

rbfSVM <- ksvm(x = x, y = y, data = sinData, kernel = "rbfdot", kpar = "automatic",
               C = 1, epsilon = 0.1)
modelPrediction <- predict(rbfSVM, newdata = dataGrid)
plot(x,y)
points(x = dataGrid$x, y = modelPrediction[,1], type = "l", col = "blue")

rbfSVM2 <- ksvm(x = x, y = y, data = sinData, kernel = "rbfdot", kpar = "automatic",
                C = 1, epsilon = 1)
modelPrediction2 <- predict(rbfSVM2, newdata = dataGrid)
plot(x,y)
points(x = dataGrid$x, y = modelPrediction2[,1], type = "l", col = "blue")

-----
par(mfrow = c(1,3))
rbfSVM3 <- ksvm(x = x, y = y, data = sinData, kernel = "rbfdot", kpar = "automatic",
                C = 0.0001, epsilon = 0.1)
modelPrediction3 <- predict(rbfSVM3, newdata = dataGrid)
plot(x,y)
points(x = dataGrid$x, y = modelPrediction3[,1], type = "l", col = "blue")

rbfSVM4 <- ksvm(x = x, y = y, data = sinData, kernel = "rbfdot", kpar = "automatic",
                C = 1, epsilon = 0.1)
modelPrediction4 <- predict(rbfSVM4, newdata = dataGrid)
plot(x,y)
points(x = dataGrid$x, y = modelPrediction4[,1], type = "l", col = "blue")

```

```
rbfSVM5 <- ksvm(x = x, y = y, data = sinData, kernel ="rbfdot", kpar = "automatic",  
               C = 10000000, epsilon = 0.1)  
modelPrediction5 <- predict(rbfSVM5, newdata = dataGrid)  
plot(x,y)  
points(x = dataGrid$x, y = modelPrediction5[,1], type = "l", col = "blue")
```

#7.1(b)

```
par(mfrow = c(2,2))  
rbfSVM6 <- ksvm(x = x, y = y, data = sinData, kernel ="rbfdot", kpar = list(sigma =  
0.001), C = 1, epsilon = 0.1)  
modelPrediction6 <- predict(rbfSVM6, newdata = dataGrid)  
plot(x, y)  
points(x = dataGrid$x, y = modelPrediction6[,1],type = "l", col = "blue")
```

```
rbfSVM7 <- ksvm(x = x, y = y, data = sinData, kernel ="rbfdot", kpar = list(sigma = 0.1),  
C = 1, epsilon = 0.1)  
modelPrediction7 <- predict(rbfSVM7, newdata = dataGrid)  
plot(x, y)  
points(x = dataGrid$x, y = modelPrediction7[,1],type = "l", col = "blue")
```

```
rbfSVM8 <- ksvm(x = x, y = y, data = sinData, kernel ="rbfdot", kpar = list(sigma = 10),  
C = 1, epsilon = 0.1)  
modelPrediction8 <- predict(rbfSVM8, newdata = dataGrid)  
plot(x, y)  
points(x = dataGrid$x, y = modelPrediction8[,1],type = "l", col = "blue")
```

```
rbfSVM9 <- ksvm(x = x, y = y, data = sinData, kernel ="rbfdot", kpar = list(sigma =  
100), C = 1, epsilon = 0.1)  
modelPrediction9 <- predict(rbfSVM9, newdata = dataGrid)  
plot(x, y)  
points(x = dataGrid$x, y = modelPrediction9[,1],type = "l", col = "blue")
```

#7.2 (a)

```
library(mlbench)
```

```
library(caret)
```

```
set.seed(1)
```

```
trainingData <- mlbench.friedman1(200, sd = 1)
```

```
trainingData$x <- data.frame(trainingData$x)
```

```
featurePlot(trainingData$x, trainingData$y)
```

```
testData <- mlbench.friedman1(5000, sd = 1)
```

```
testData$x <- data.frame(testData$x)
```

##knn model

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

```
knnModel
```

```
knnPred <- predict(knnModel, newdata = testData$x)
```

```
plot(knnModel)
```

```
postResample(pred = knnPred, obs = testData$y)
```

##MARS model

```
library(earth)
```

```
library(AppliedPredictiveModeling)
```

```
marsGrid <- expand.grid(.degree = 1:2, .nprune = 2:30)
```

```
set.seed(1)
```

```
marsTuned <- train(trainingData$x, trainingData$y,method = "earth", tuneGrid =  
marsGrid, trControl = trainControl(method = "cv"))
```

```
marsTuned
```

```
summary(marsTuned)
```

```
marsPred <- predict(marsTuned, newdata = testData$x)
```

```
plotmo(marsTuned)
```

```
plot(marsTuned)
```

```
varImp(marsTuned)
```

```
postResample(pred = marsPred, obs = testData$y)
```

##7.5

```
library(RANN)
```

```
data("ChemicalManufacturingProcess")
```

```
predictors<-subset(ChemicalManufacturingProcess, select = -Yield)
```

```
yield<-subset(ChemicalManufacturingProcess, select="Yield")
```

```
P1<- preProcess(predictors,method=c("knnImpute"))
```

```
Predictors1 <- predict(P1,predictors)
```

```
P2<- preProcess(Predictors1, method = c("center","scale"))
```

```
Predictors2 <- predict(P2,Predictors1)
```

```
Split<-createDataPartition(yield$Yield, p=0.8, list = FALSE)
```

```
TrainP<- Predictors2[Split,]
```

```
TrainY<-yield[Split,]
```

```
TestP<- Predictors2[-Split,]
```

```
TestY<-yield[-Split,]
```

##Neural Network with resampling

```
nnetGrid <- expand.grid(.decay = c(0, 0.01, .1),  
                        .size = c(1:10))
```

```
set.seed(1)
```

```
ctrl <- trainControl(method = "cv", number = 10)
```

```
nnetTune <- train(TrainP, TrainY,  
                  method = "nnet",  
                  tuneGrid = nnetGrid,  
                  trControl = ctrl,  
                  preProc = c("center", "scale"),
```

```
linout = TRUE,  
trace = FALSE,  
MaxNWts = 10 * (ncol(TrainP) + 1) + 10 + 1,  
maxit = 500)
```

```
nnetTune  
plot(nnetTune)
```

```
Pred=predict(nnetTune, TestP)  
SSEnnet=mean((TestY-Pred)^2)  
RMSE=sqrt(SSEnnet)  
Rsquared=(cor(TestY, Pred))^2  
RMSE  
Rsquared
```

```
##MARS with resampling
```

```
library(earth)  
library(AppliedPredictiveModeling)
```

```
marsGrid2 <- expand.grid(.degree = 1:2, .nprune = 2:50)  
set.seed(1)
```

```
marsTuned2 <- train(TrainP, TrainY,  
  method = "earth",  
  tuneGrid = marsGrid2,  
  trControl = trainControl(method = "cv"))
```

```
marsTuned2  
summary(marsTuned2)  
predict(marsTuned2, newdata = TestP)  
plot(marsTuned2)
```

```
varImp(marsTuned2)
```



```

Pred=predict(marsTuned2, TestP)
SSEmars=mean((TestY-Pred)^2)
RMSE=sqrt(SSEmars)
Rsquared=(cor(TestY, Pred))^2
RMSE
Rsquared

```

##SVM

```

install.packages("kernlab")
library(kernlab)
library(AppliedPredictiveModeling)

```

```

svmRTuned <- train(TrainP, TrainY,
                  method = "svmRadial",
                  preProc = c("center", "scale"),
                  tuneLength = 14,
                  trControl = trainControl(method = "cv"))

```

```

svmRTuned
plot(svmRTuned)

```

The subobject named finalModel contains the model created by the ksvm
function:

```

svmRTuned$finalModel

```

```

important=varImp(svmRTuned)
plot(important, top = 25, scales = list(y = list(cex = .95)))

```

```

Pred=predict(svmRTuned, TestP)
SSEsvm=mean((TestY-Pred)^2)
RMSE=sqrt(SSEsvm)
Rsquared=(cor(TestY, Pred))^2

```

RMSE
Rsquared

##knn

```
library(AppliedPredictiveModeling)
library(caret)
knnDescr <- TrainP[, -nearZeroVar(TrainP)]
set.seed(1)
knnTune <- train(knnDescr,
                 TrainY,
                 method = "knn",
                 # Center and scaling will occur for new predictions too
                 preProc = c("center", "scale"),
                 tuneGrid = data.frame(.k = 1:20),
                 trControl = trainControl(method = "cv"))
knnTune
plot(knnTune)
```

```
Pred=predict(knnTune, TestP)
SSEknn=mean((TestY-Pred)^2)
RMSE=sqrt(SSEknn)
Rsquared=(cor(TestY, Pred))^2
RMSE
Rsquared
```

#-----

```
#lasso
set.seed(1)
cv <- cv.glmnet(as.matrix(TrainP), TrainY, alpha = 1,
               nfolds=3, standardize = TRUE)
plot(cv)
cv$lambda.min
```

```
varImp(lasso_model, lambda = cv$lambda.min)
```