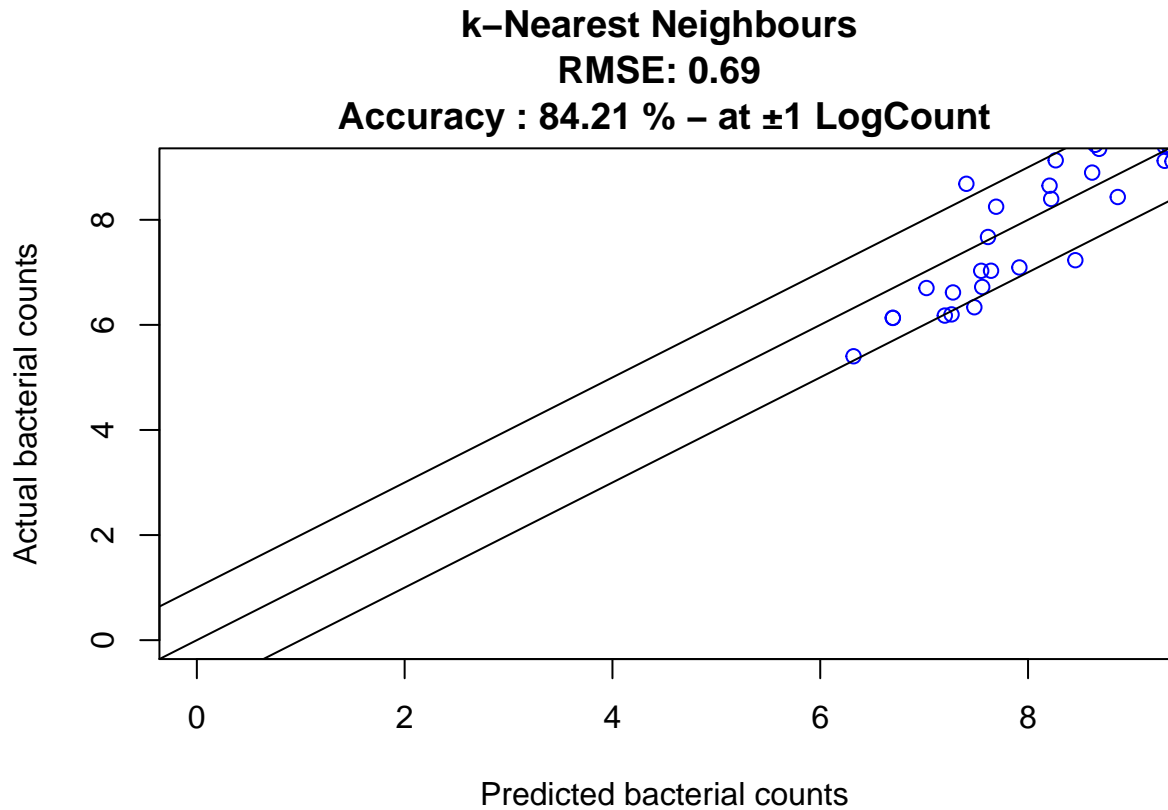


Machine Learning Regression Model Report - FTIR (Chicken Burger)

k-Nearest Neighbours for Total Viable Counts

```
## k-Nearest Neighbors
##
## 90 samples
## 3 predictor
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 81, 80, 81, 81, 79, 82, ...
## Resampling results across tuning parameters:
##
##  k  RMSE      Rsquared  MAE
##  5  0.6191047  0.7551736  0.4804719
##  7  0.6368123  0.7534826  0.5008530
##  9  0.6610862  0.7371926  0.5128284
##
## RMSE was used to select the optimal model using the smallest value.
## The final value used for the model was k = 5.
```

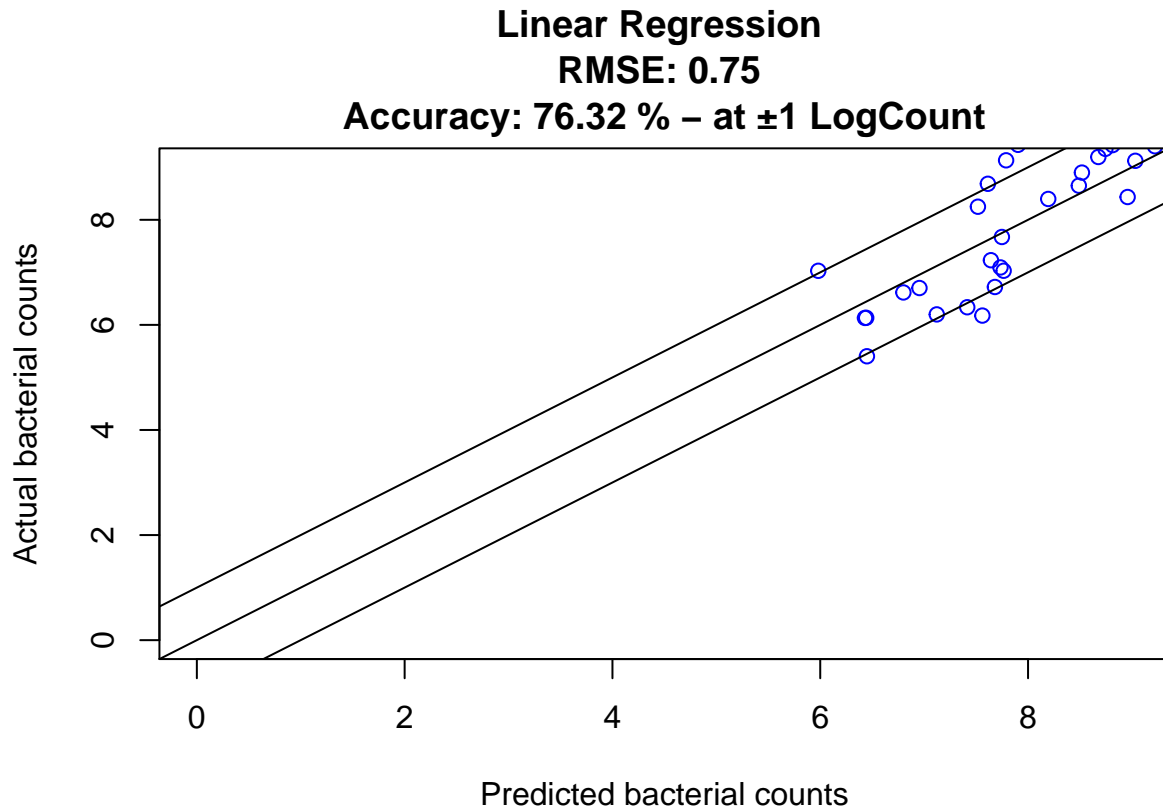
Total Viable Counts distribution - k-Nearest Neighbours



Linear Model for Total Viable Counts

```
## Linear Regression
##
## 90 samples
## 3 predictor
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 80, 81, 82, 81, 81, 81, ...
## Resampling results:
##
##   RMSE      Rsquared  MAE
## 0.7160539 0.688944 0.5979021
##
## Tuning parameter 'intercept' was held constant at a value of TRUE
```

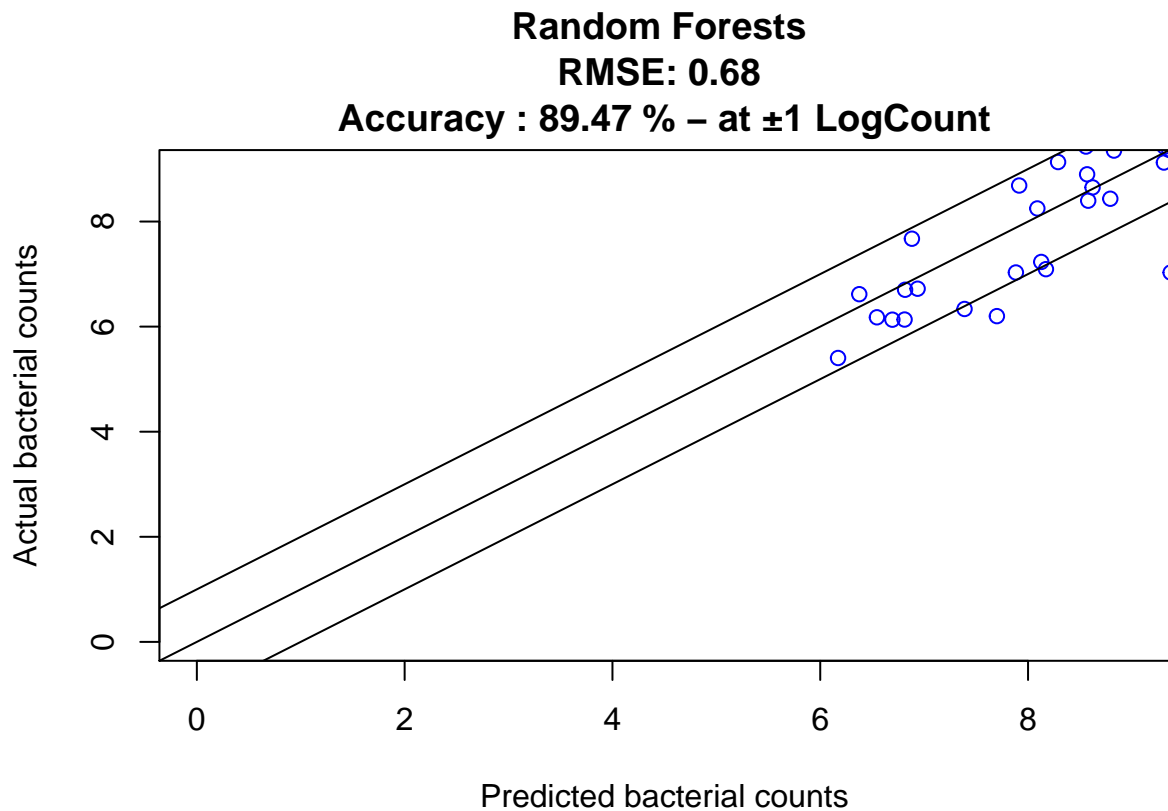
Total Viable Counts distribution - Linear Regression



Random Forest for Total Viable Counts

```
## Random Forest
##
## 90 samples
## 3 predictor
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 81, 82, 82, 81, 81, 80, ...
## Resampling results across tuning parameters:
##
##  mtry  RMSE      Rsquared  MAE
##  2     0.5725139  0.7835897  0.4351155
##  3     0.5604627  0.7839102  0.4301674
##
## RMSE was used to select the optimal model using the smallest value.
## The final value used for the model was mtry = 3.
```

Total Viable Counts distribution - Random Forests



Support Vector Machines with Polynomial Kernel for Total Viable Counts

```
## Support Vector Machines with Polynomial Kernel
##
## 90 samples
## 3 predictor
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 81, 81, 80, 81, 81, 81, ...
## Resampling results across tuning parameters:
##
## degree scale C      RMSE      Rsquared  MAE
## 1       0.001 0.25  1.2311256 0.5560383 0.9430992
## 1       0.001 0.50  1.2171547 0.5587248 0.9312154
## 1       0.001 1.00  1.1955338 0.5595494 0.9103128
## 1       0.010 0.25  1.1426160 0.5734930 0.8591858
## 1       0.010 0.50  1.0696822 0.5920456 0.8098290
## 1       0.010 1.00  0.9653704 0.6044751 0.7320464
## 1       0.100 0.25  0.8365890 0.6117268 0.6481015
## 1       0.100 0.50  0.7876251 0.6198917 0.6169034
```

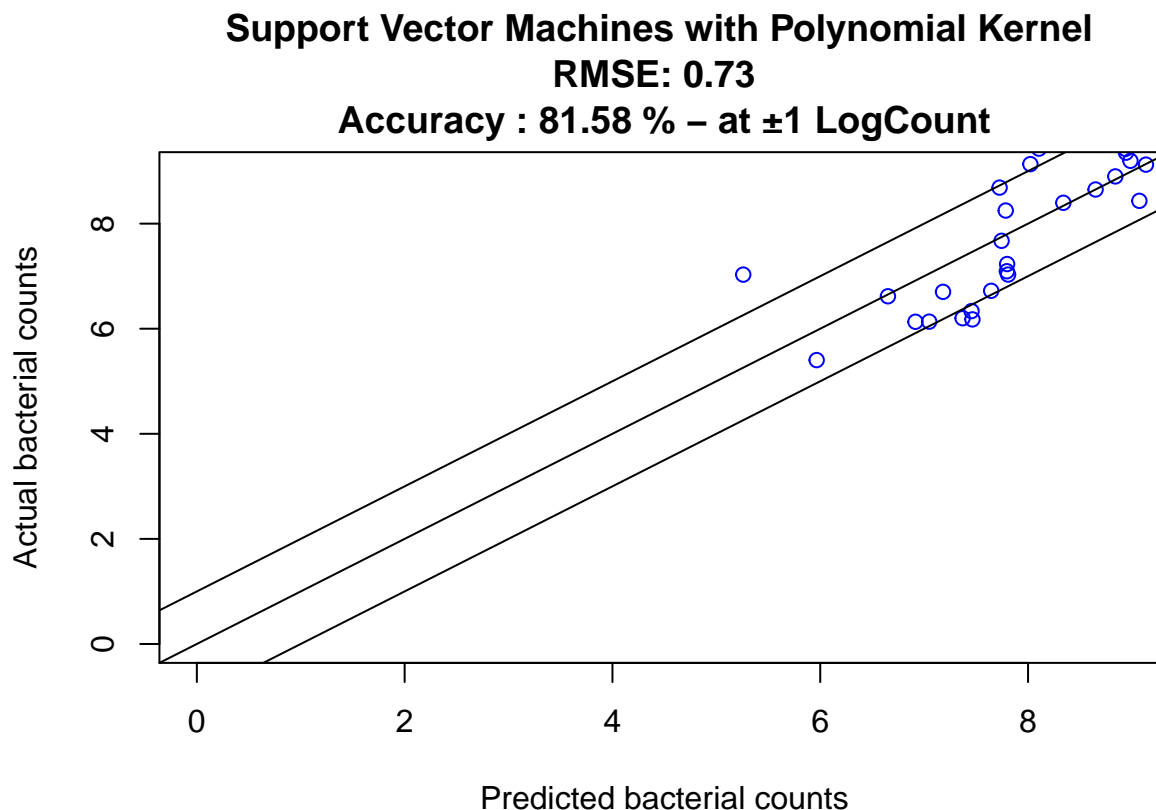
##	1	0.100	1.00	0.7802684	0.6178497	0.6160247
##	2	0.001	0.25	1.2171510	0.5587318	0.9312096
##	2	0.001	0.50	1.1955270	0.5595611	0.9103012
##	2	0.001	1.00	1.1585015	0.5672873	0.8739960
##	2	0.010	0.25	1.0691059	0.5931542	0.8095276
##	2	0.010	0.50	0.9641365	0.6117051	0.7311536
##	2	0.010	1.00	0.8522103	0.6214655	0.6563698
##	2	0.100	0.25	0.7705117	0.6308771	0.6053885
##	2	0.100	0.50	0.7306274	0.6553946	0.5762335
##	2	0.100	1.00	0.6789500	0.7062654	0.5444251
##	3	0.001	0.25	1.2057385	0.5579327	0.9207881
##	3	0.001	0.50	1.1761116	0.5645249	0.8920463
##	3	0.001	1.00	1.1246486	0.5800704	0.8463142
##	3	0.010	0.25	1.0085720	0.6076829	0.7634907
##	3	0.010	0.50	0.8885701	0.6247585	0.6801734
##	3	0.010	1.00	0.8042519	0.6299473	0.6226707
##	3	0.100	0.25	0.6950602	0.6962340	0.5479471
##	3	0.100	0.50	0.6854539	0.7074762	0.5419911
##	3	0.100	1.00	0.8017817	0.6823476	0.5804783

##

RMSE was used to select the optimal model using the smallest value.

The final values used for the model were degree = 2, scale = 0.1 and C = 1.

Total Viable Counts distribution - Support Vector Machines with Polynomial Kernel

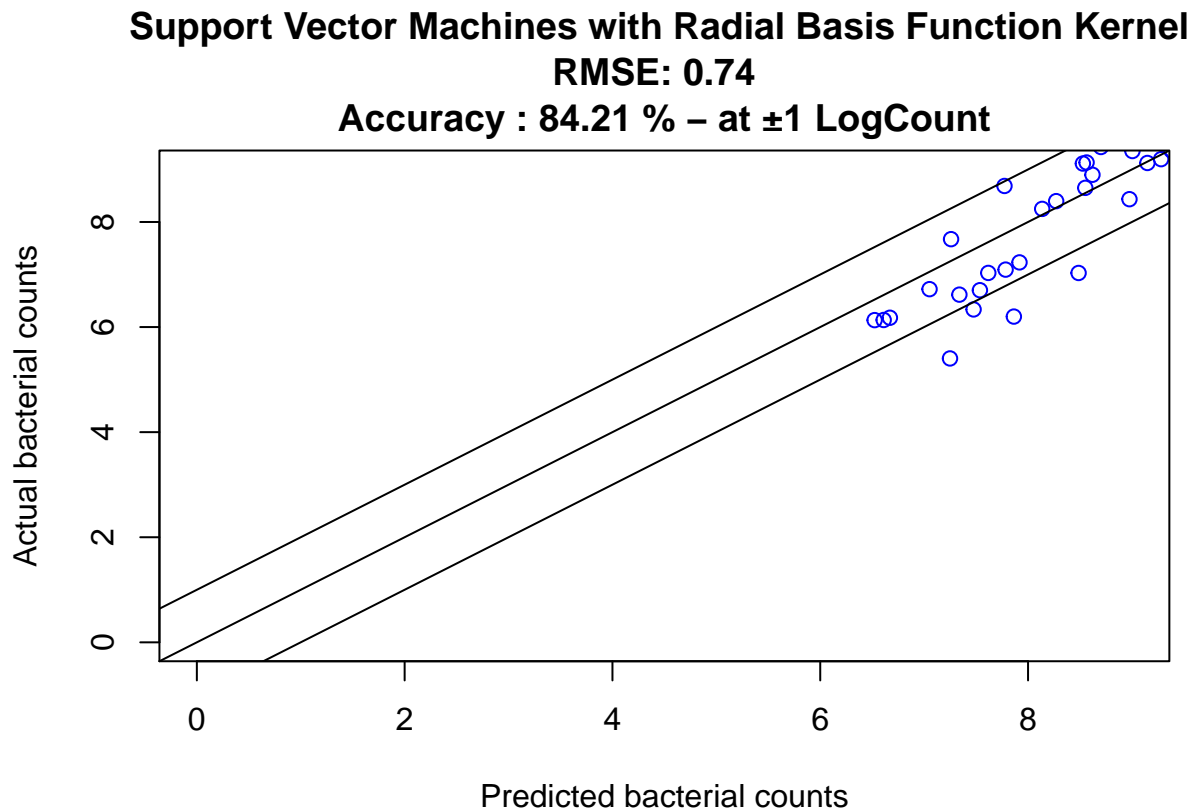


Support Vector Machines with Radial Basis Function Kernel for Total Viable Counts

```
## Support Vector Machines with Radial Basis Function Kernel
##
## 90 samples
## 3 predictor
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 82, 81, 80, 80, 81, 81, ...
## Resampling results across tuning parameters:
##
##  C      RMSE      Rsquared  MAE
##  0.25  0.7668661  0.7167895  0.5889544
##  0.50  0.6762331  0.7369083  0.5041944
##  1.00  0.6288954  0.7553780  0.4600335
##
## Tuning parameter 'sigma' was held constant at a value of 0.99071
## RMSE was used to select the optimal model using the smallest value.
```

```
## The final values used for the model were sigma = 0.99071 and C = 1.
```

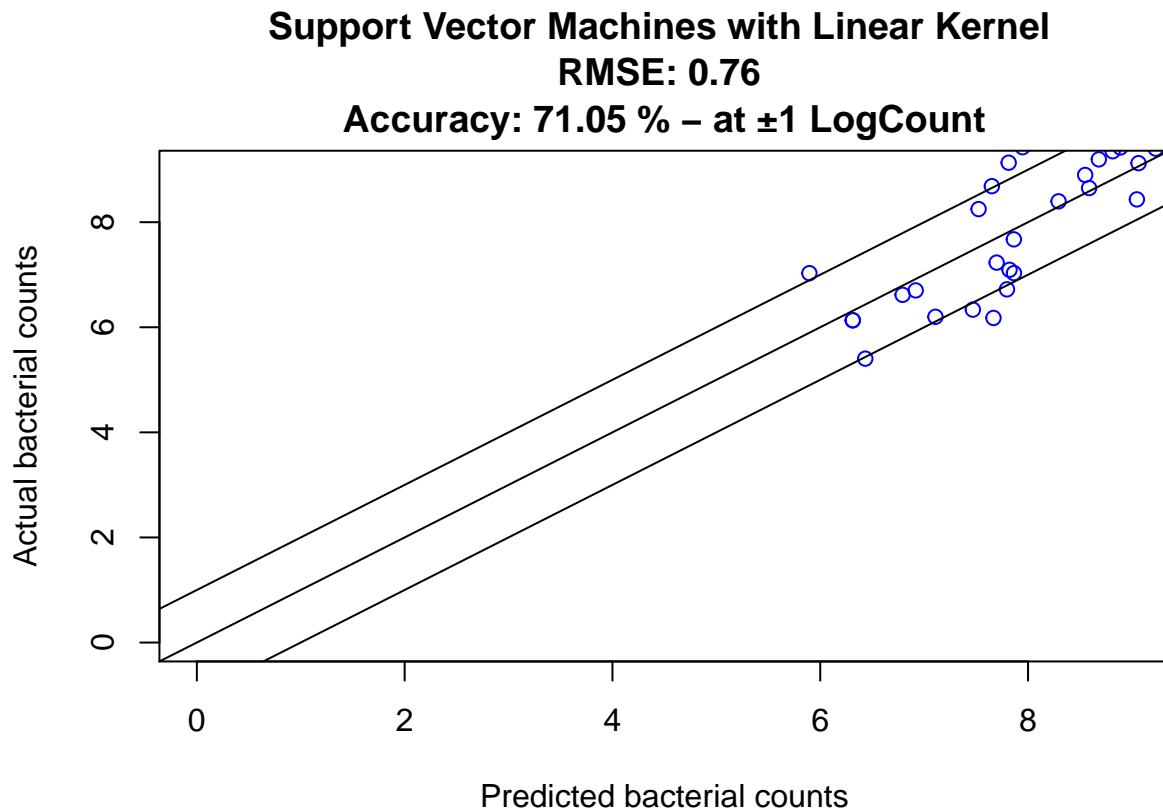
Total Viable Counts distribution - Support Vector Machines with Radial Basis Function Kernel



Support Vector Machines with Linear Kernel for Total Viable Counts

```
## Support Vector Machines with Linear Kernel
##
## 90 samples
## 3 predictor
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 82, 80, 80, 81, 81, 81, ...
## Resampling results:
##
##   RMSE      Rsquared   MAE
## 0.7486569 0.6280973 0.6220538
##
## Tuning parameter 'C' was held constant at a value of 1
```

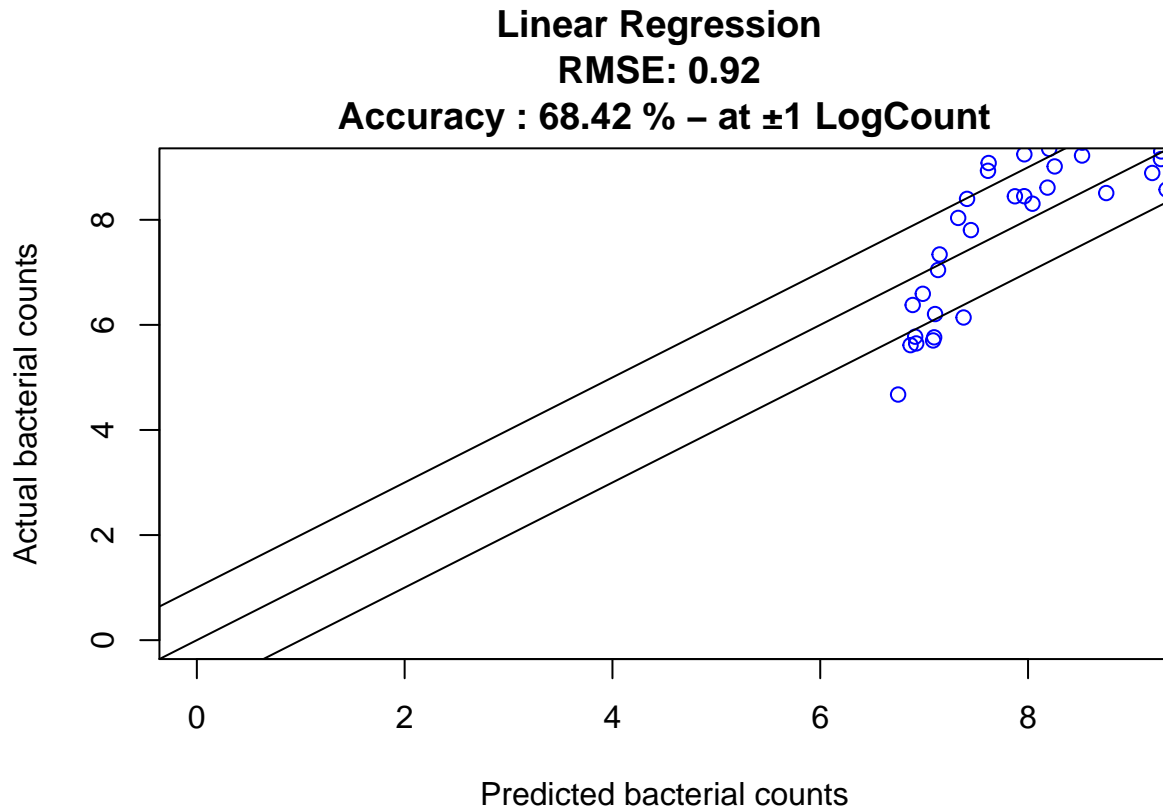
Total Viable Counts distribution - Support Vector Machines with Linear Kernel



Linear Regression for Pseudomonas count

```
## Linear Regression
##
## 90 samples
## 2 predictor
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 80, 81, 82, 81, 81, 81, ...
## Resampling results:
##
##      RMSE      Rsquared   MAE
## 0.835591 0.6215917 0.6720276
##
## Tuning parameter 'intercept' was held constant at a value of TRUE
```

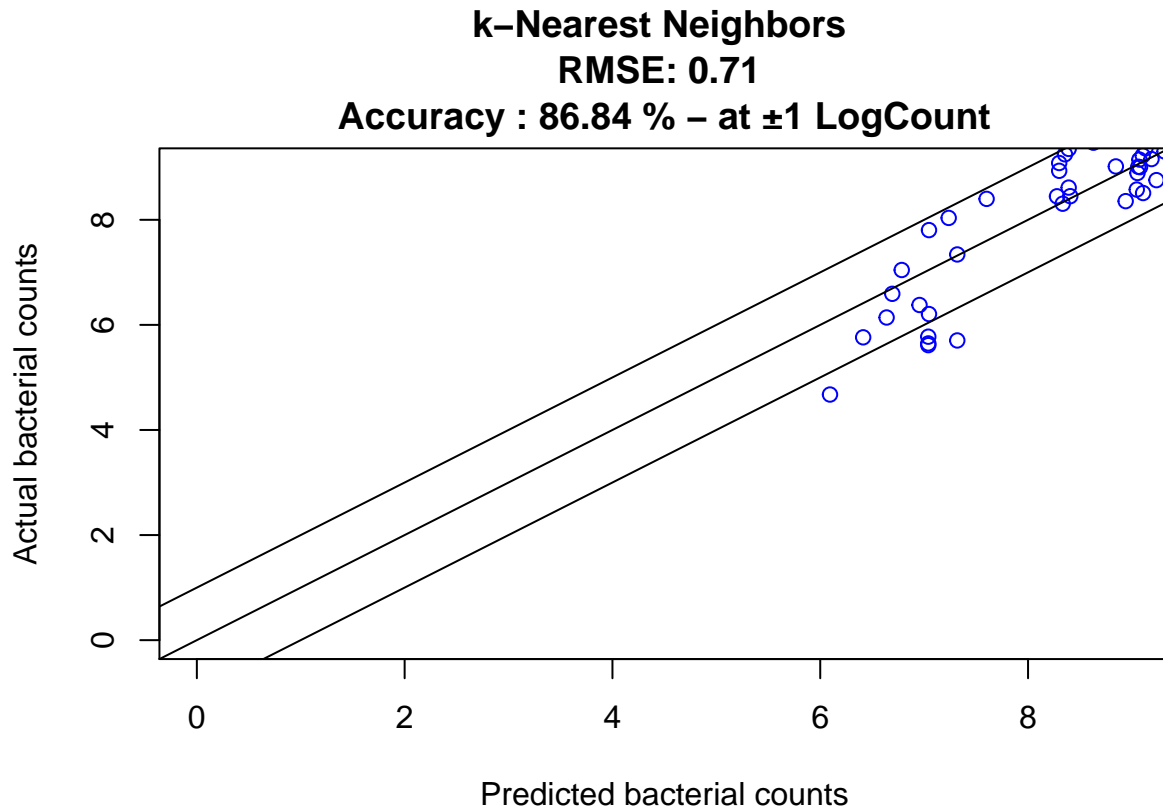

Pseudomonas count distribution - Linear Regression



k-Nearest Neighbors for Pseudomonas count

```
## k-Nearest Neighbors
##
## 90 samples
## 2 predictor
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 81, 80, 82, 81, 82, 82, ...
## Resampling results across tuning parameters:
##
##  k  RMSE      Rsquared  MAE
##  5  0.7571568  0.6636002  0.5788641
##  7  0.7526074  0.6564372  0.5819069
##  9  0.7339070  0.6823211  0.5648194
##
## RMSE was used to select the optimal model using the smallest value.
## The final value used for the model was k = 9.
```

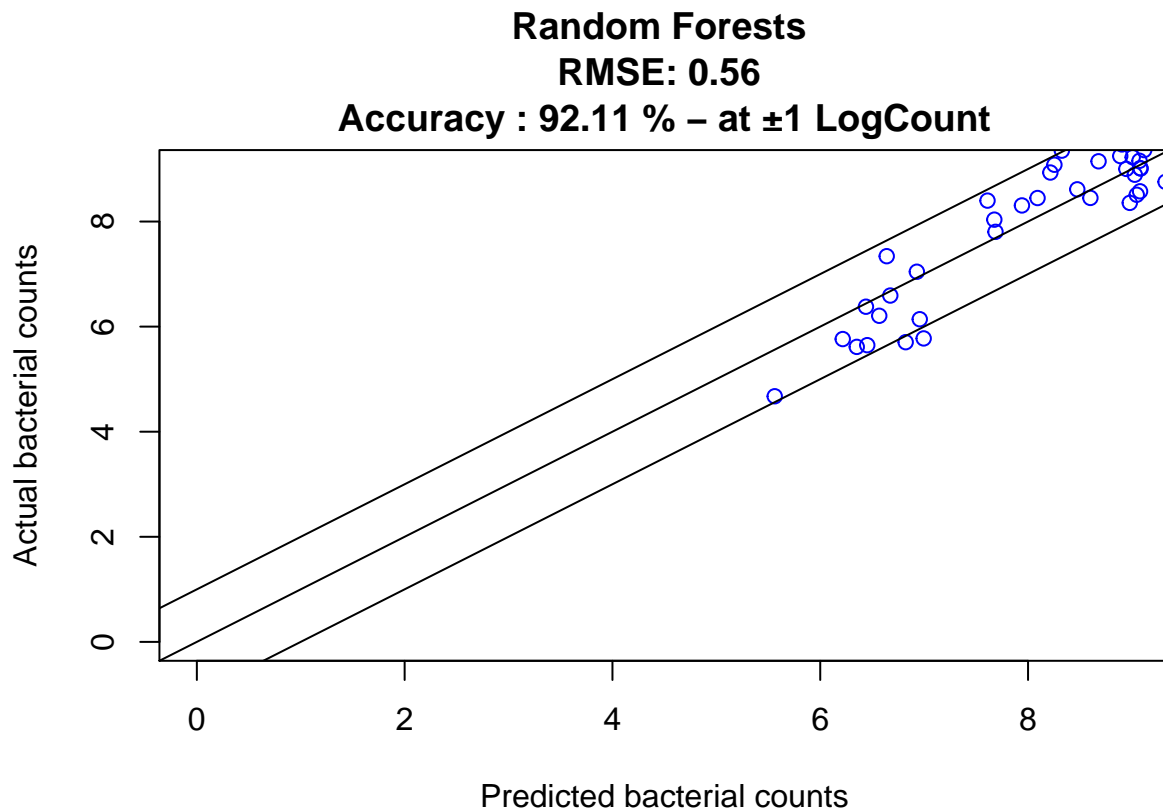
Pseudomonas count distribution - k-Nearest Neighbors



Random Forests for Pseudomonas count

```
## Random Forest
##
## 90 samples
## 2 predictor
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 81, 82, 80, 81, 80, 81, ...
## Resampling results:
##
##   RMSE      Rsquared   MAE
## 0.7419632  0.6740556  0.5714924
##
## Tuning parameter 'mtry' was held constant at a value of 2
```

Pseudomonas count distribution - Random Forests

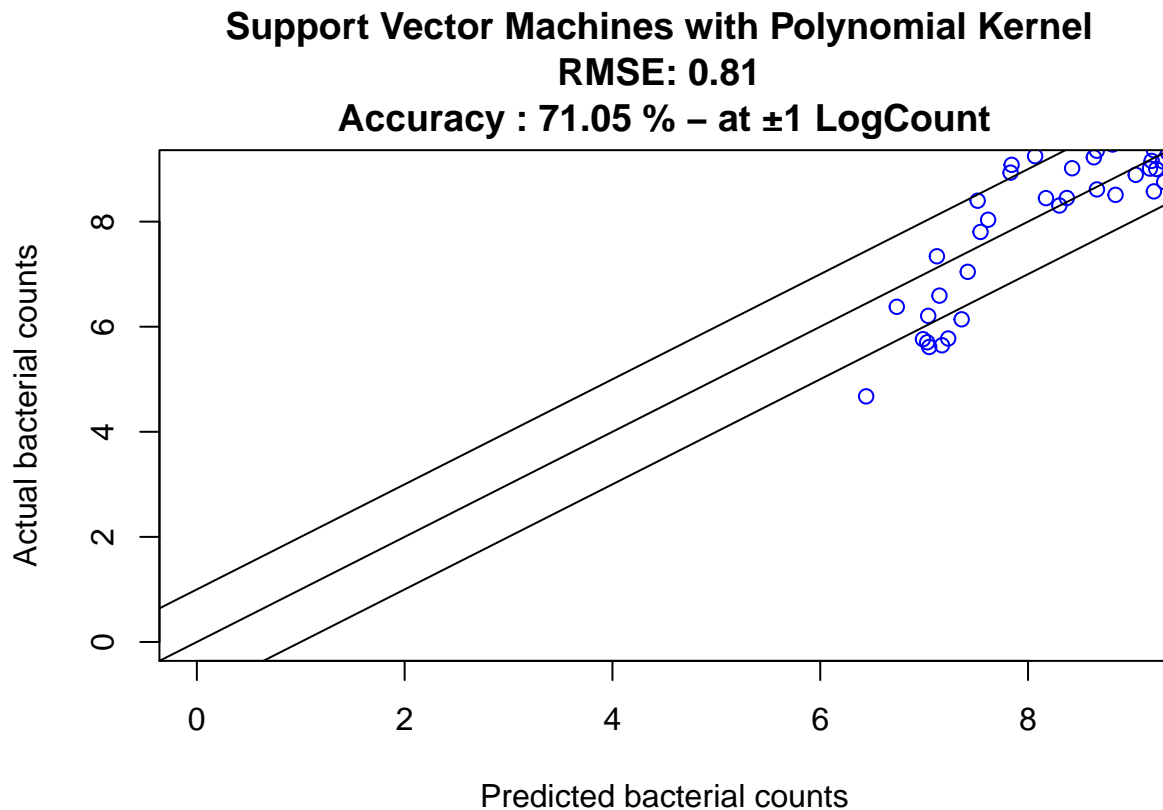


Support Vector Machines with Polynomial Kernel for Pseudomonas count

```
## Support Vector Machines with Polynomial Kernel
##
## 90 samples
## 2 predictor
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 81, 81, 80, 81, 81, 81, ...
## Resampling results across tuning parameters:
##
## degree scale C      RMSE      Rsquared  MAE
## 1      0.001 0.25  1.2983481  0.5049053  1.0243462
## 1      0.001 0.50  1.2868384  0.5034546  1.0143880
## 1      0.001 1.00  1.2669398  0.5053065  0.9947346
## 1      0.010 0.25  1.2133226  0.5155399  0.9459872
## 1      0.010 0.50  1.1500586  0.5098449  0.8905610
## 1      0.010 1.00  1.0488596  0.5306161  0.8186858
## 1      0.100 0.25  0.9471957  0.5272858  0.7403473
## 1      0.100 0.50  0.8919528  0.5432277  0.6931675
```

##	1	0.100	1.00	0.8817733	0.5459385	0.6869787
##	2	0.001	0.25	1.2868386	0.5034366	1.0143848
##	2	0.001	0.50	1.2669406	0.5052870	0.9947285
##	2	0.001	1.00	1.2310739	0.5176511	0.9603960
##	2	0.010	0.25	1.1502582	0.5099523	0.8905916
##	2	0.010	0.50	1.0490142	0.5308054	0.8187324
##	2	0.010	1.00	0.9602793	0.5349908	0.7514314
##	2	0.100	0.25	0.8407208	0.6038151	0.6473915
##	2	0.100	0.50	0.8159893	0.6178273	0.6322046
##	2	0.100	1.00	0.8063575	0.6344522	0.6208134
##	3	0.001	0.25	1.2760890	0.5050415	1.0045063
##	3	0.001	0.50	1.2497636	0.5054974	0.9767334
##	3	0.001	1.00	1.1960583	0.5150169	0.9330297
##	3	0.010	0.25	1.0876595	0.5226547	0.8463643
##	3	0.010	0.50	0.9934795	0.5387080	0.7731184
##	3	0.010	1.00	0.9278288	0.5379077	0.7243191
##	3	0.100	0.25	0.8659318	0.6030276	0.6619882
##	3	0.100	0.50	0.8613557	0.6263359	0.6465256
##	3	0.100	1.00	0.8612081	0.6458813	0.6425685
##						
##	RMSE was used to select the optimal model using the smallest value.					
##	The final values used for the model were degree = 2, scale = 0.1 and C = 1.					

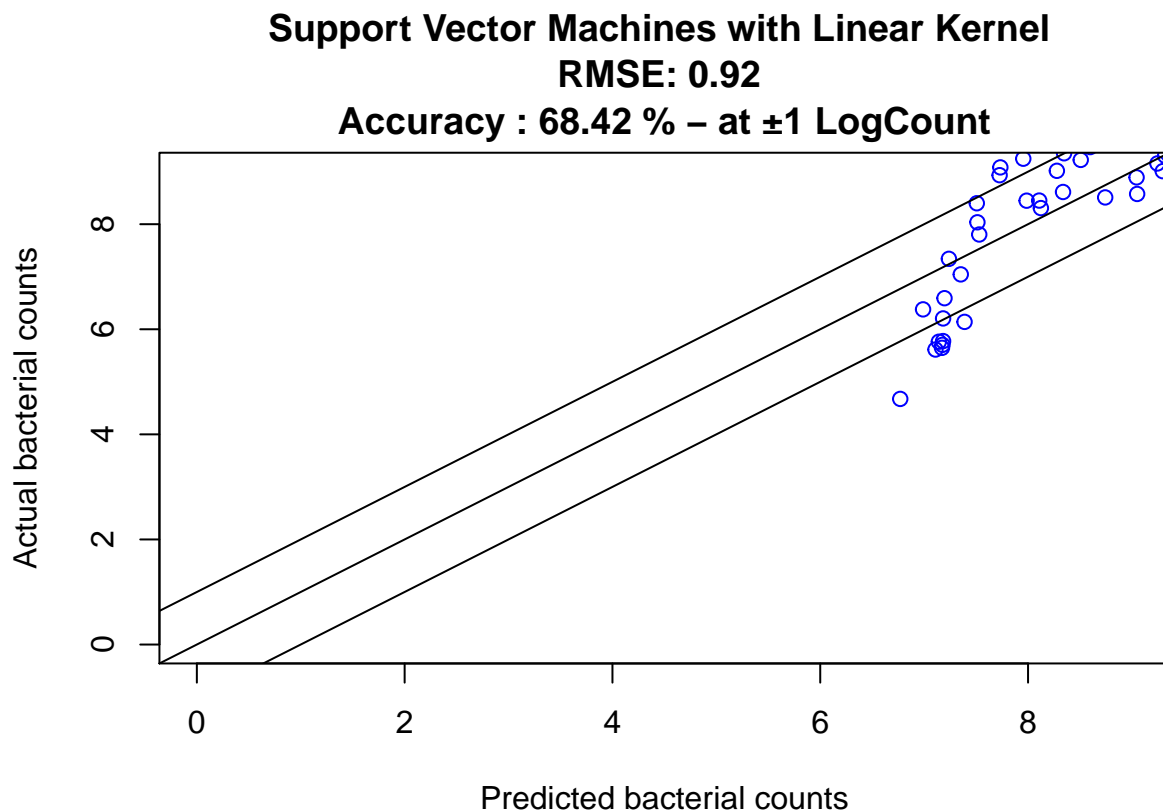
Pseudomonas count distribution - Support Vector Machines with Polynomial Kernel



Support Vector Machines with Linear Kernel for Pseudomonas count

```
## Support Vector Machines with Linear Kernel
##
## 90 samples
## 2 predictor
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 82, 80, 80, 81, 81, 81, ...
## Resampling results:
##
##      RMSE      Rsquared    MAE
## 0.8722094 0.5477718 0.6638681
##
## Tuning parameter 'C' was held constant at a value of 1
```

Pseudomonas count distribution - Support Vector Machines with Linear Kernel

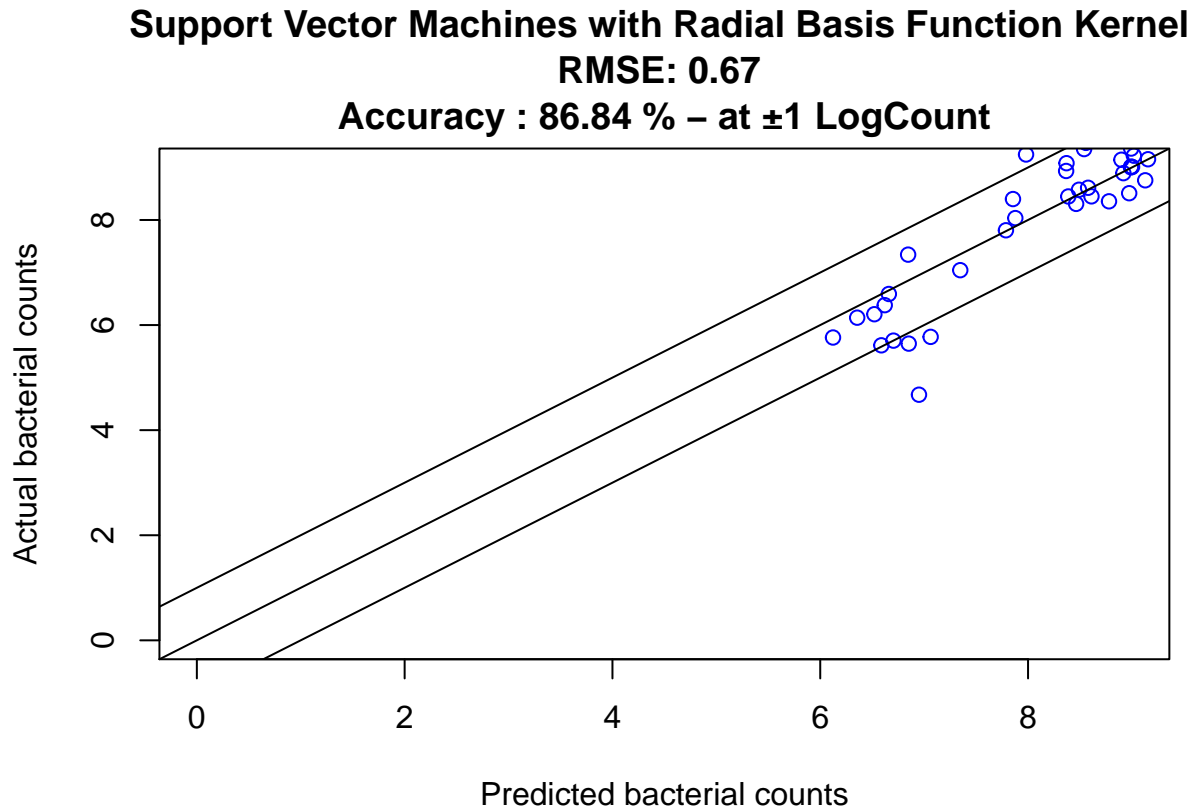


Support Vector Machines with Radial Basis Function Kernel for Pseudomonas count

```
## Support Vector Machines with Radial Basis Function Kernel
##
## 90 samples
## 2 predictor
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 82, 81, 80, 80, 81, 81, ...
## Resampling results across tuning parameters:
##
##  C      RMSE      Rsquared  MAE
##  0.25  0.8106917  0.6958808  0.5923729
##  0.50  0.7632681  0.7055694  0.5573597
##  1.00  0.7614757  0.6901618  0.5564339
##
## Tuning parameter 'sigma' was held constant at a value of 1.860185
## RMSE was used to select the optimal model using the smallest value.
```

```
## The final values used for the model were sigma = 1.860185 and C = 1.
```

Pseudomonas count distribution - Support Vector Machines with Radial Basis Function Kernel

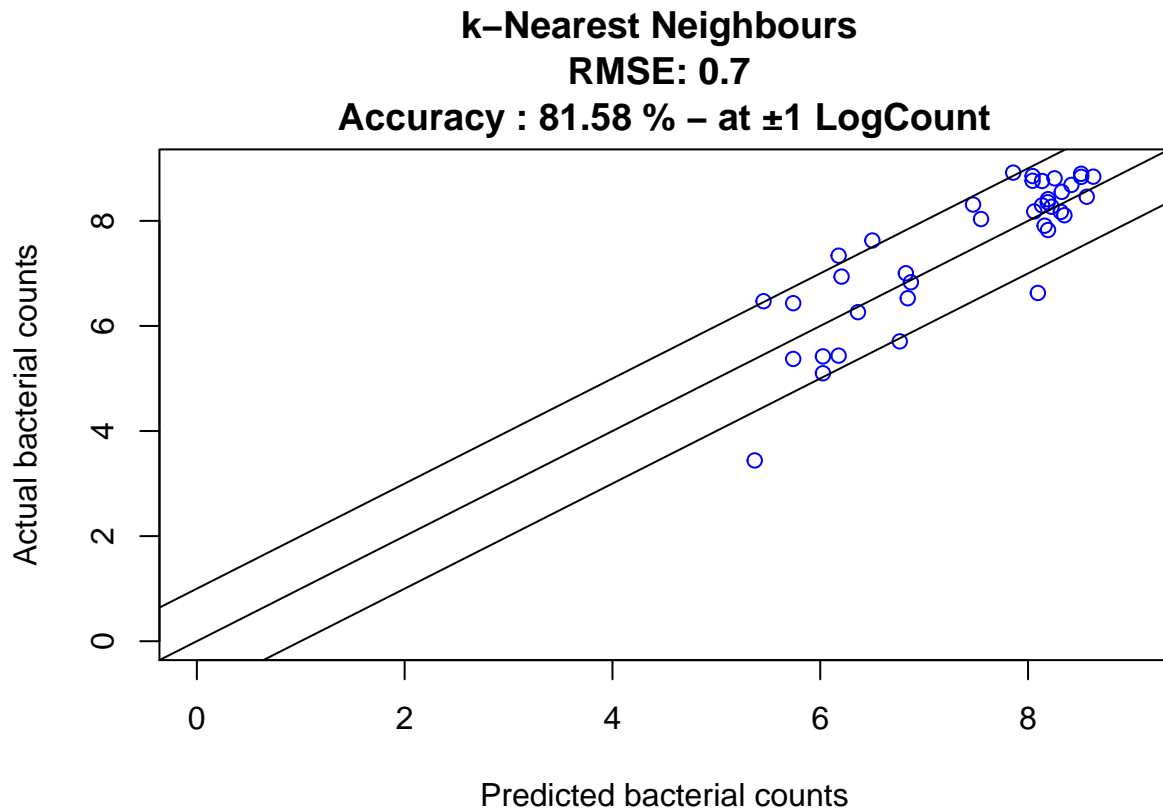


k-Nearest Neighbours for Brochothrix thermosphacta count

```
## k-Nearest Neighbors
##
## 90 samples
## 2 predictor
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 80, 82, 81, 81, 82, 81, ...
## Resampling results across tuning parameters:
##
##  k  RMSE      Rsquared  MAE
##  5  0.6492157  0.7237998  0.4913211
##  7  0.7407354  0.6378233  0.5524963
##  9  0.7364931  0.6543849  0.5543357
##
```

```
## RMSE was used to select the optimal model using the smallest value.
## The final value used for the model was k = 5.
```

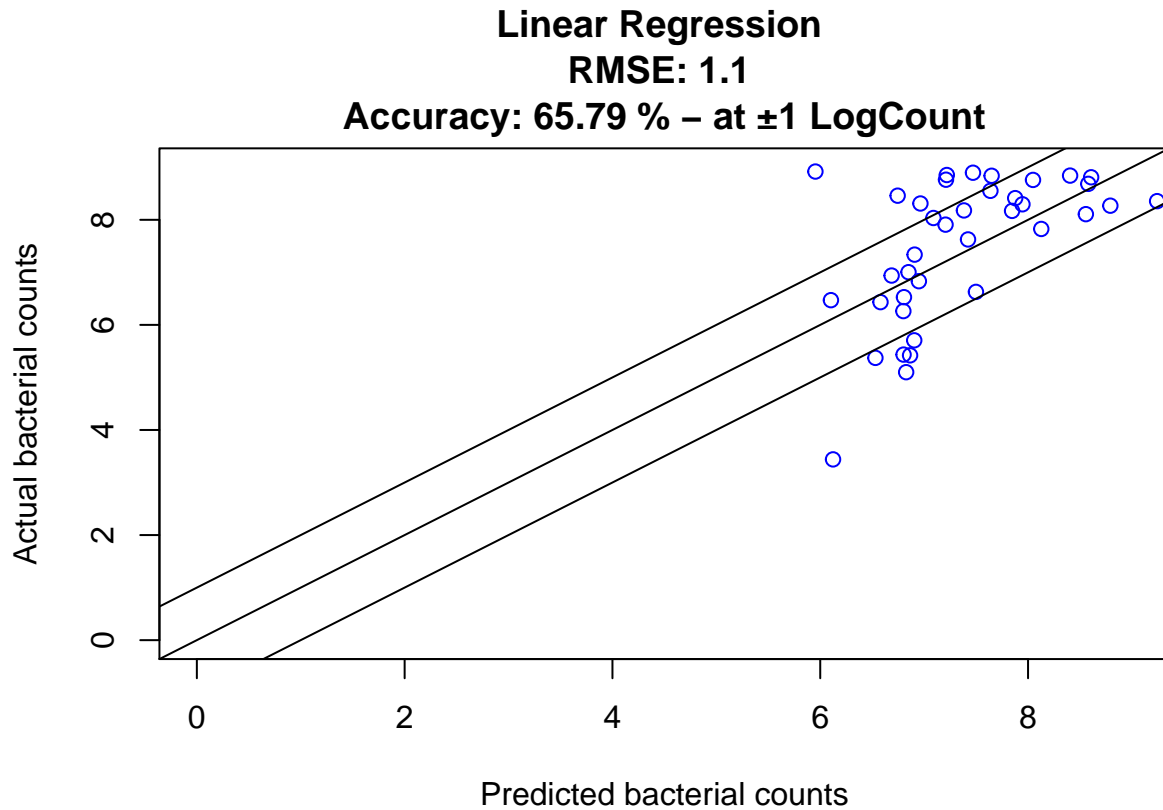
Brochothrix thermosphacta count distribution - k-Nearest Neighbours



Linear Model for Brochothrix thermosphacta count

```
## Linear Regression
##
## 90 samples
## 2 predictor
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 80, 81, 82, 81, 81, 81, ...
## Resampling results:
##
##   RMSE      Rsquared   MAE
## 0.876231  0.5064273  0.7229251
##
## Tuning parameter 'intercept' was held constant at a value of TRUE
```

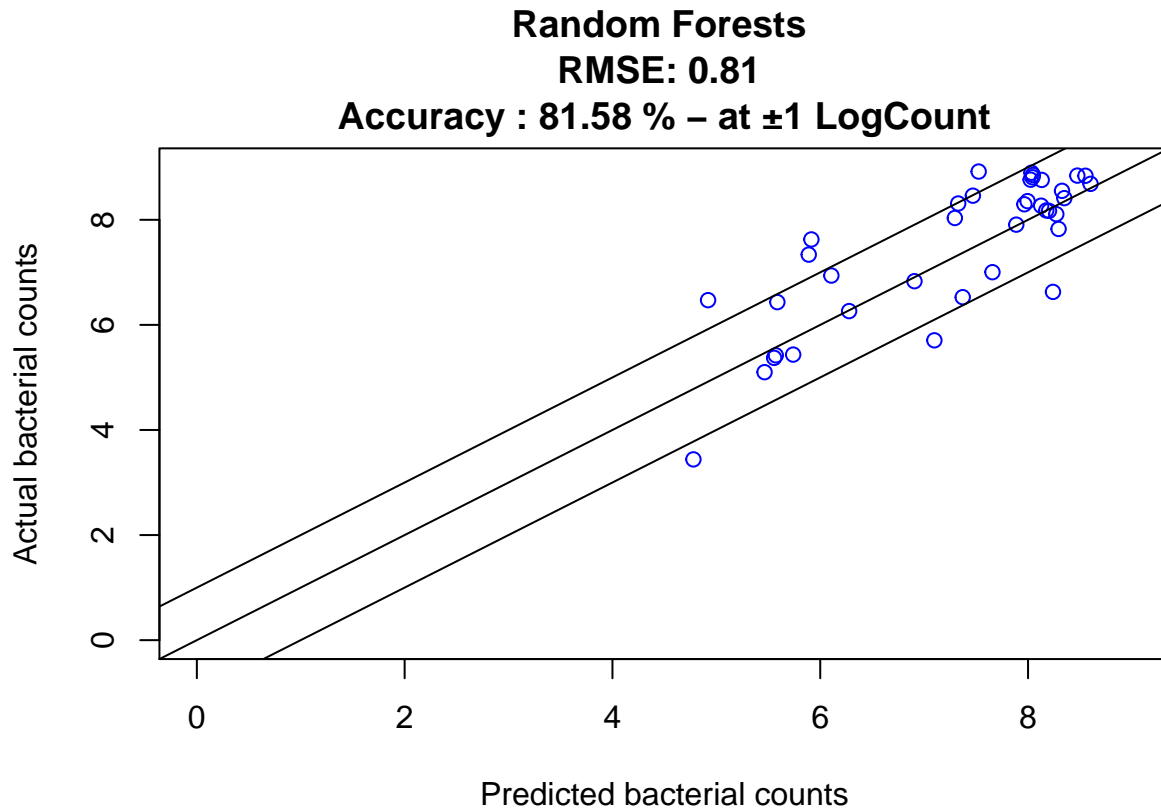

Brochothrix thermosphacta count distribution - Linear Regression



Random Forest for Brochothrix thermosphacta count

```
## Random Forest
##
## 90 samples
## 2 predictor
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 82, 82, 80, 82, 81, 80, ...
## Resampling results:
##
##   RMSE      Rsquared   MAE
## 0.6720012  0.7338889  0.5120875
##
## Tuning parameter 'mtry' was held constant at a value of 2
```

Brochothrix thermosphacta count distribution - Random Forests



Support Vector Machines with Polynomial Kernel for Brochothrix thermosphacta count

```
## Support Vector Machines with Polynomial Kernel
##
## 90 samples
## 2 predictor
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 81, 81, 80, 81, 81, 81, ...
## Resampling results across tuning parameters:
##
## degree scale C RMSE Rsquared MAE
## 1 0.001 0.25 1.2553031 0.4885051 0.8948435
## 1 0.001 0.50 1.2459730 0.4885051 0.8871107
## 1 0.001 1.00 1.2238158 0.4901065 0.8707687
## 1 0.010 0.25 1.1628890 0.4979258 0.8358817
## 1 0.010 0.50 1.1037715 0.4992275 0.7956674
## 1 0.010 1.00 1.0215419 0.5057991 0.7543730
## 1 0.100 0.25 0.9621239 0.5031111 0.7314102
```

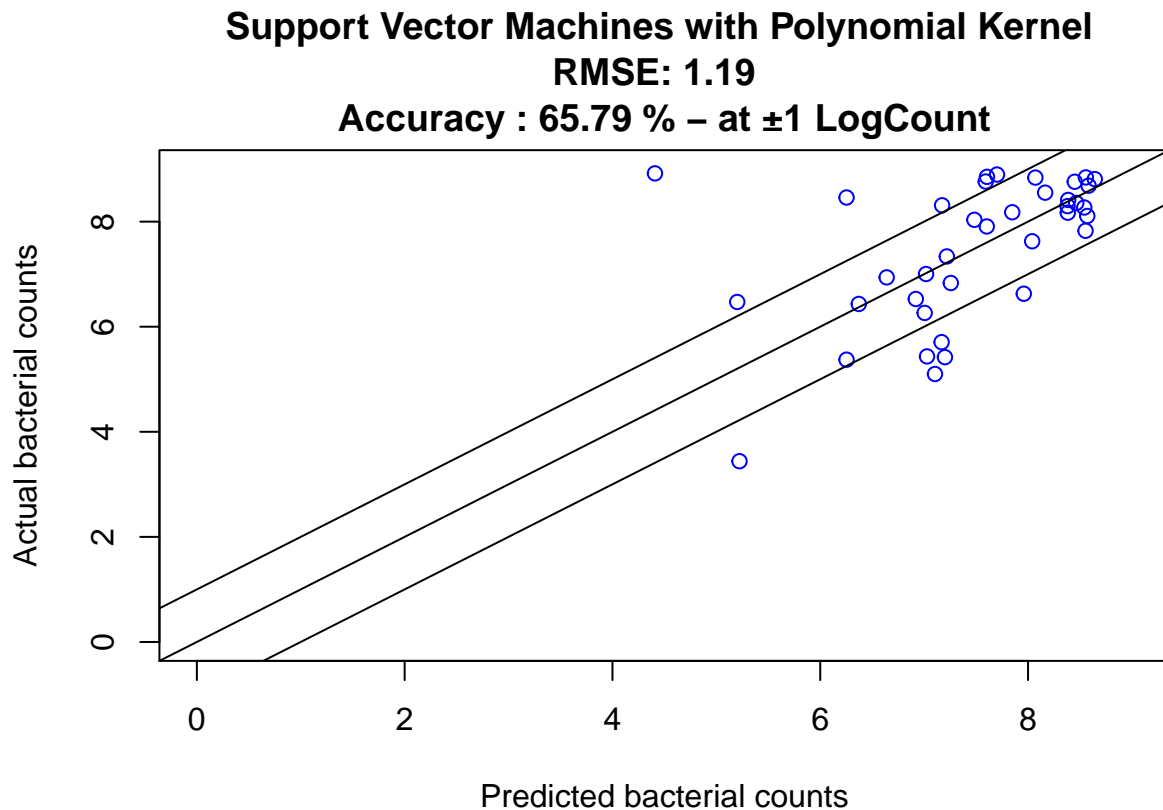
##	1	0.100	0.50	0.9152740	0.5054346	0.7102544
##	1	0.100	1.00	0.9045794	0.5075419	0.7110533
##	2	0.001	0.25	1.2459708	0.4885685	0.8871101
##	2	0.001	0.50	1.2238111	0.4901731	0.8707675
##	2	0.001	1.00	1.1846973	0.4997988	0.8466764
##	2	0.010	0.25	1.1030694	0.5018865	0.7951472
##	2	0.010	0.50	1.0202934	0.5088726	0.7534304
##	2	0.010	1.00	0.9790526	0.5108372	0.7332166
##	2	0.100	0.25	0.8993674	0.5732152	0.6809751
##	2	0.100	0.50	0.8744240	0.6165133	0.6552624
##	2	0.100	1.00	0.8345161	0.6538516	0.6145782
##	3	0.001	0.25	1.2349026	0.4889656	0.8789537
##	3	0.001	0.50	1.2047686	0.4928850	0.8581275
##	3	0.001	1.00	1.1412436	0.4968900	0.8244385
##	3	0.010	0.25	1.0592287	0.5060168	0.7698893
##	3	0.010	0.50	0.9885952	0.5126664	0.7322681
##	3	0.010	1.00	0.9360827	0.5200064	0.7119976
##	3	0.100	0.25	0.8873222	0.6340572	0.6493675
##	3	0.100	0.50	0.8538031	0.6623028	0.6191526
##	3	0.100	1.00	0.8482036	0.6684605	0.6149866

##

RMSE was used to select the optimal model using the smallest value.

The final values used for the model were degree = 2, scale = 0.1 and C = 1.

Brochothrix thermosphacta count distribution - Support Vector Machines with Polynomial Kernel

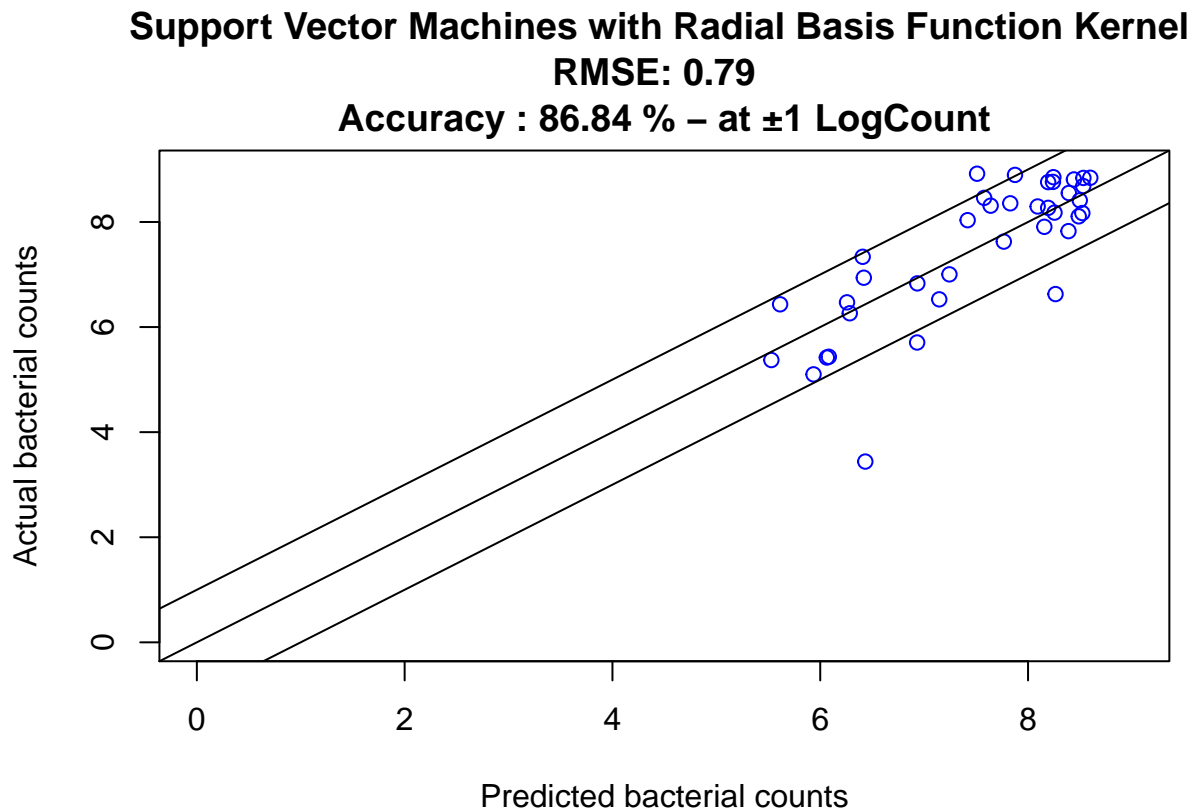


Support Vector Machines with Radial Basis Function Kernel for Brochothrix thermosphacta count

```
## Support Vector Machines with Radial Basis Function Kernel
##
## 90 samples
## 2 predictor
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 82, 81, 80, 80, 81, 81, ...
## Resampling results across tuning parameters:
##
##  C      RMSE      Rsquared  MAE
##  0.25  0.7394682  0.7291462  0.5495196
##  0.50  0.6842274  0.7513929  0.5066947
##  1.00  0.6360243  0.7670038  0.4726799
##
## Tuning parameter 'sigma' was held constant at a value of 1.336064
## RMSE was used to select the optimal model using the smallest value.
```

```
## The final values used for the model were sigma = 1.336064 and C = 1.
```

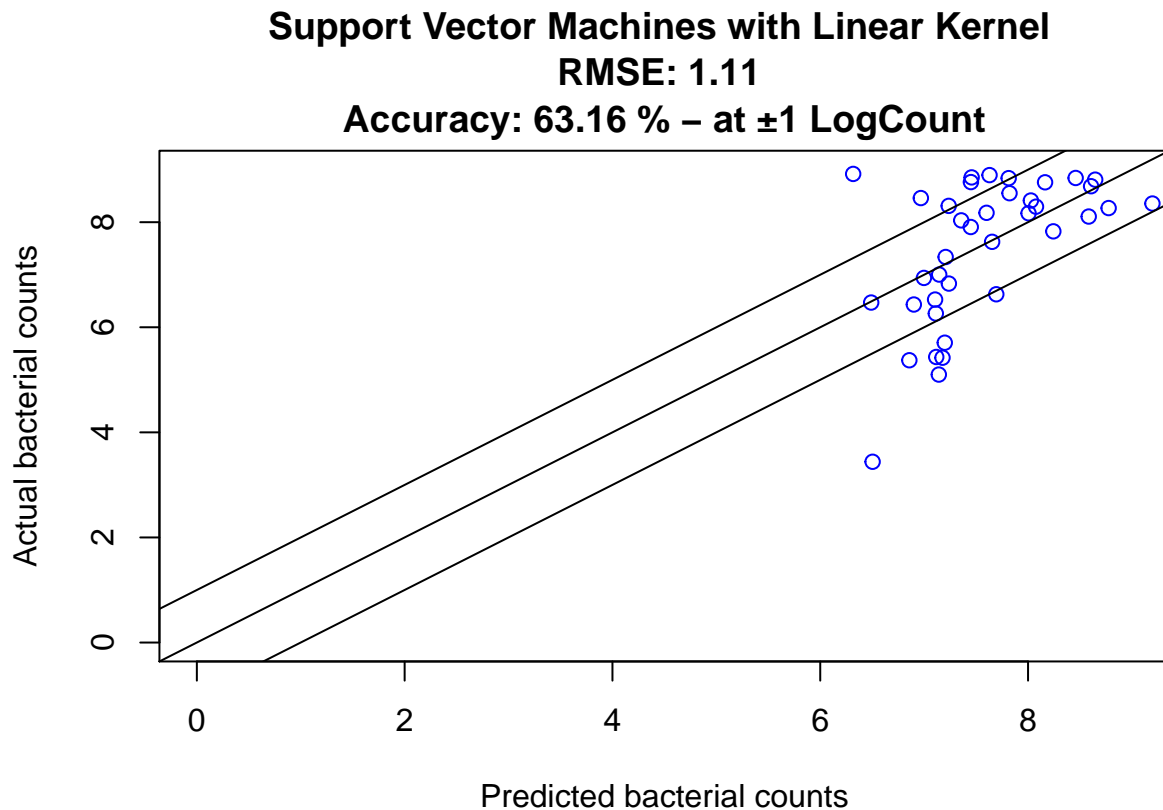
Brochothrix thermosphacta count distribution - Support Vector Machines with Radial Basis Function Kernel



Support Vector Machines with Linear Kernel for Brochothrix thermosphacta count

```
## Support Vector Machines with Linear Kernel
##
## 90 samples
## 2 predictor
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 82, 80, 80, 81, 81, 81, ...
## Resampling results:
##
##   RMSE      Rsquared   MAE
## 0.8827985  0.5157473  0.7245411
##
## Tuning parameter 'C' was held constant at a value of 1
```

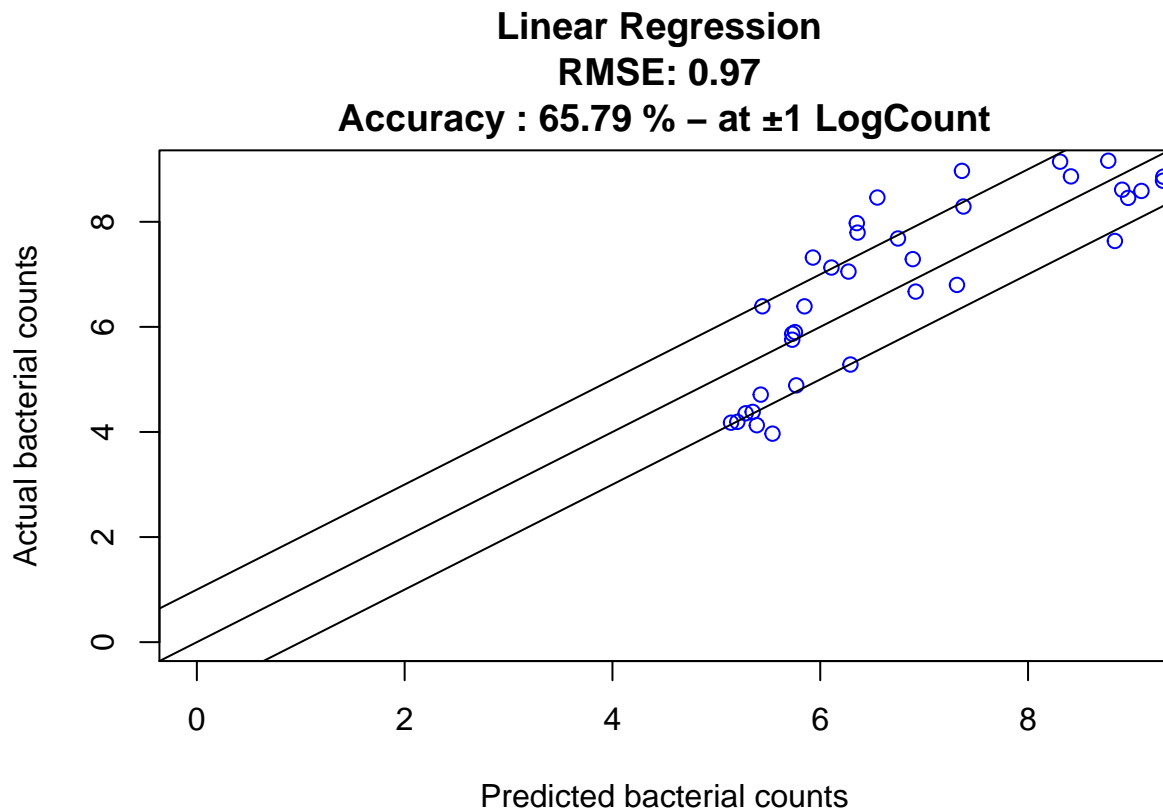
Brochothrix thermosphacta count distribution - Support Vector Machines with Linear Kernel



Linear Regression for Lactic acid bacteria count

```
## Linear Regression
##
## 90 samples
## 2 predictor
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 80, 81, 82, 81, 81, 81, ...
## Resampling results:
##
##      RMSE      Rsquared   MAE
## 0.9060239 0.7492049 0.7856744
##
## Tuning parameter 'intercept' was held constant at a value of TRUE
```

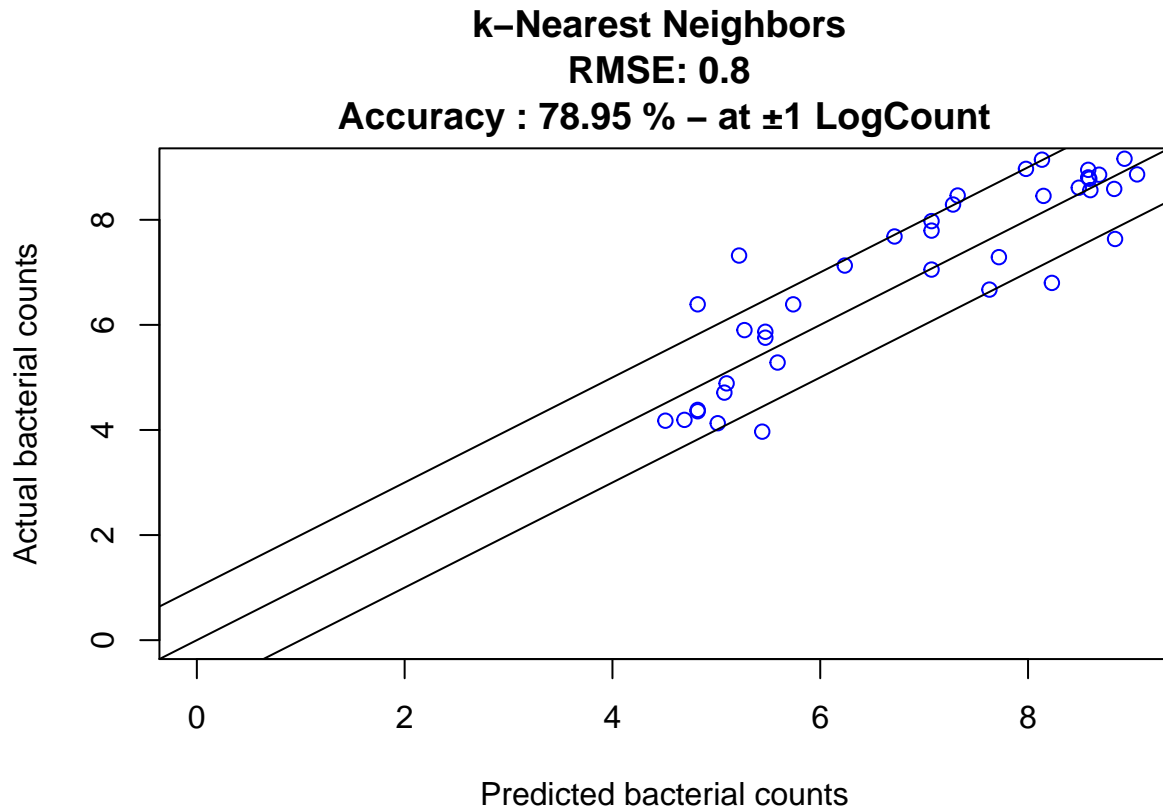
Lactic acid bacteria count distribution - Linear Regression



k-Nearest Neighbors for Lactic acid bacteria count

```
## k-Nearest Neighbors
##
## 90 samples
## 2 predictor
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 82, 81, 80, 81, 80, 82, ...
## Resampling results across tuning parameters:
##
##  k  RMSE      Rsquared  MAE
##  5  0.7764483  0.8094380  0.6132650
##  7  0.7855196  0.8069812  0.6282967
##  9  0.8153230  0.7899636  0.6590856
##
## RMSE was used to select the optimal model using the smallest value.
## The final value used for the model was k = 5.
```

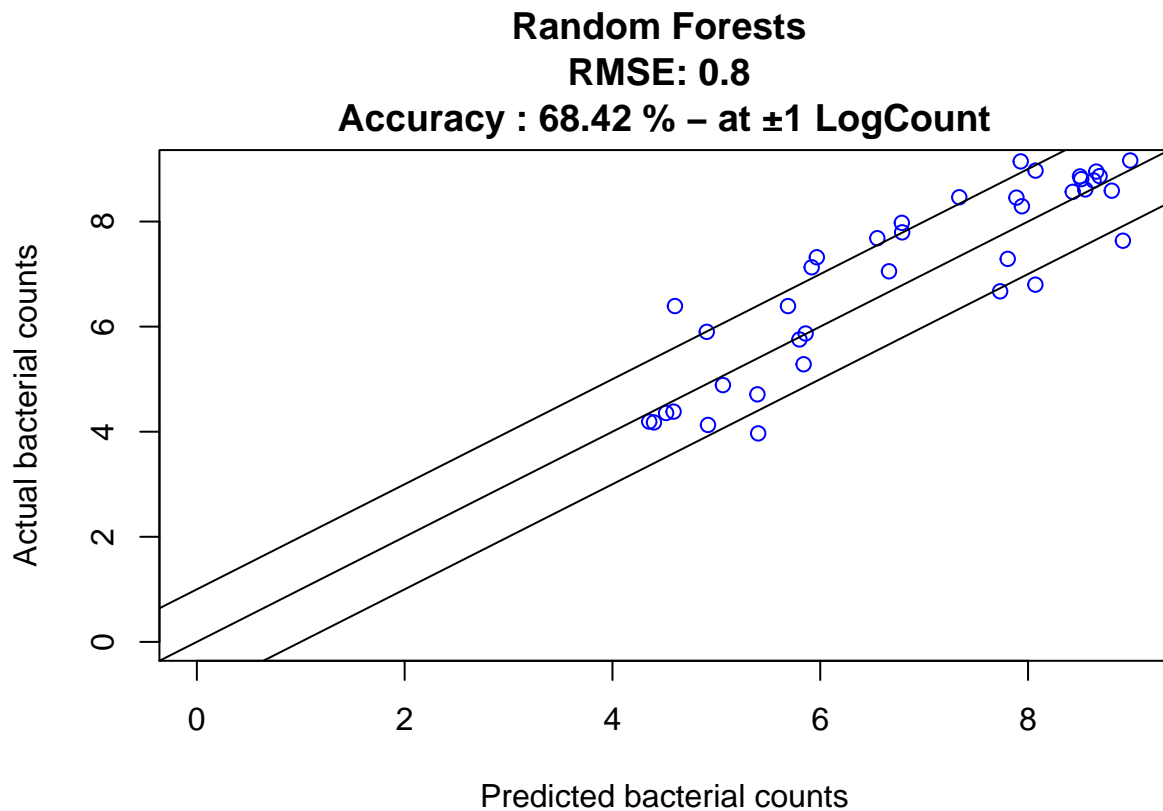
Lactic acid bacteria count distribution - k-Nearest Neighbors



Random Forests for Lactic acid bacteria count

```
## Random Forest
##
## 90 samples
## 2 predictor
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 80, 82, 81, 80, 81, 81, ...
## Resampling results:
##
##   RMSE      Rsquared   MAE
## 0.8311294 0.7609467 0.6678361
##
## Tuning parameter 'mtry' was held constant at a value of 2
```


Lactic acid bacteria count distribution - Random Forests



Support Vector Machines with Polynomial Kernel for Lactic acid bacteria count

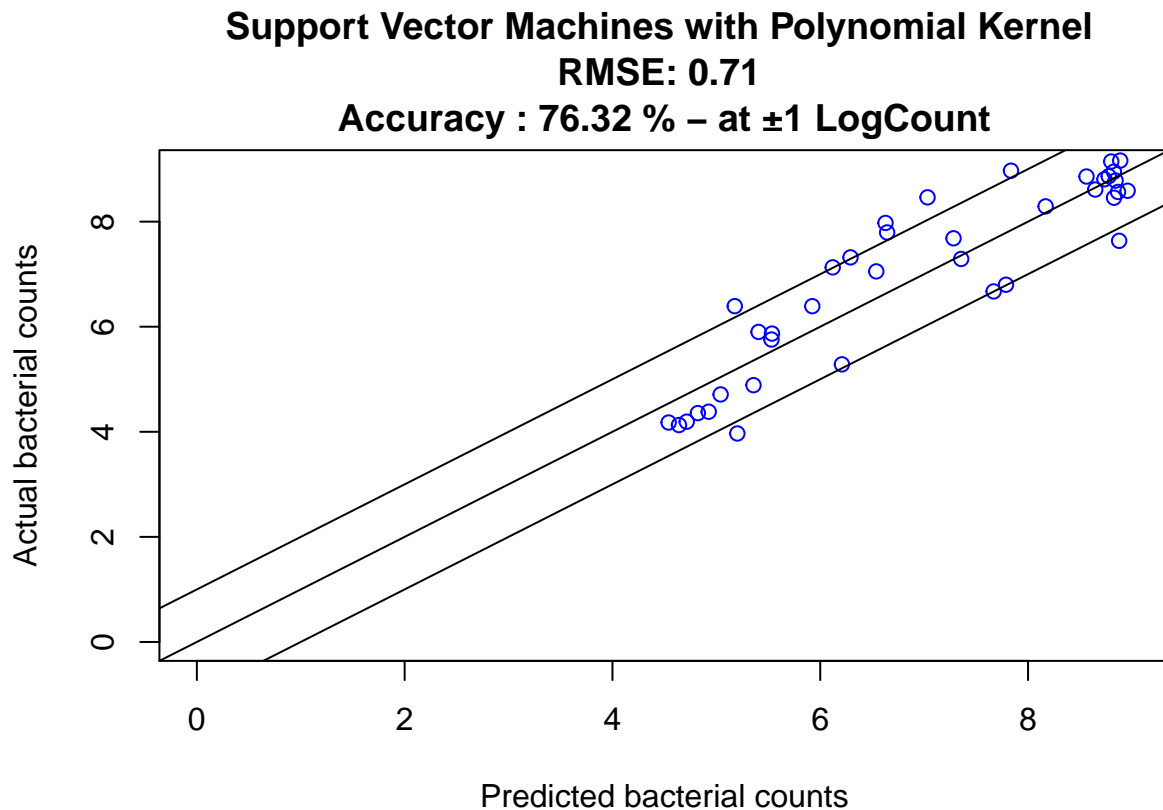
```
## Support Vector Machines with Polynomial Kernel
##
## 90 samples
## 2 predictor
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 81, 81, 80, 81, 81, 81, ...
## Resampling results across tuning parameters:
##
## degree scale C      RMSE      Rsquared  MAE
## 1       0.001 0.25  1.6410029 0.6603675 1.4660358
## 1       0.001 0.50  1.6237707 0.6603675 1.4494524
## 1       0.001 1.00  1.5897140 0.6632060 1.4157924
## 1       0.010 0.25  1.4986038 0.6607264 1.3180474
## 1       0.010 0.50  1.3775591 0.6593698 1.1656762
## 1       0.010 1.00  1.2164865 0.6802256 1.0164361
## 1       0.100 0.25  1.0561894 0.7056929 0.9126649
## 1       0.100 0.50  1.0062978 0.7090261 0.8841818
```

```

## 1      0.100  1.00  0.9712608  0.7211820  0.8445870
## 2      0.001  0.25  1.6237786  0.6601770  1.4494583
## 2      0.001  0.50  1.5897302  0.6630009  1.4158044
## 2      0.001  1.00  1.5267132  0.6606509  1.3502063
## 2      0.010  0.25  1.3783360  0.6573898  1.1662119
## 2      0.010  0.50  1.2196694  0.6779200  1.0184583
## 2      0.010  1.00  1.1077287  0.6964801  0.9457717
## 2      0.100  0.25  0.9191065  0.7475216  0.8070469
## 2      0.100  0.50  0.8631769  0.7703497  0.7473975
## 2      0.100  1.00  0.7926402  0.7964122  0.6774820
## 3      0.001  0.25  1.6064271  0.6626779  1.4324130
## 3      0.001  0.50  1.5575430  0.6605127  1.3830483
## 3      0.001  1.00  1.4712496  0.6612511  1.2848223
## 3      0.010  0.25  1.2895467  0.6741103  1.0788768
## 3      0.010  0.50  1.1670334  0.6797387  0.9845734
## 3      0.010  1.00  1.0404347  0.7078046  0.9065405
## 3      0.100  0.25  0.8245855  0.7939023  0.7292878
## 3      0.100  0.50  0.7695144  0.8169282  0.6724185
## 3      0.100  1.00  0.7573558  0.8248549  0.6425271
##
## RMSE was used to select the optimal model using the smallest value.
## The final values used for the model were degree = 3, scale = 0.1 and C = 1.

```

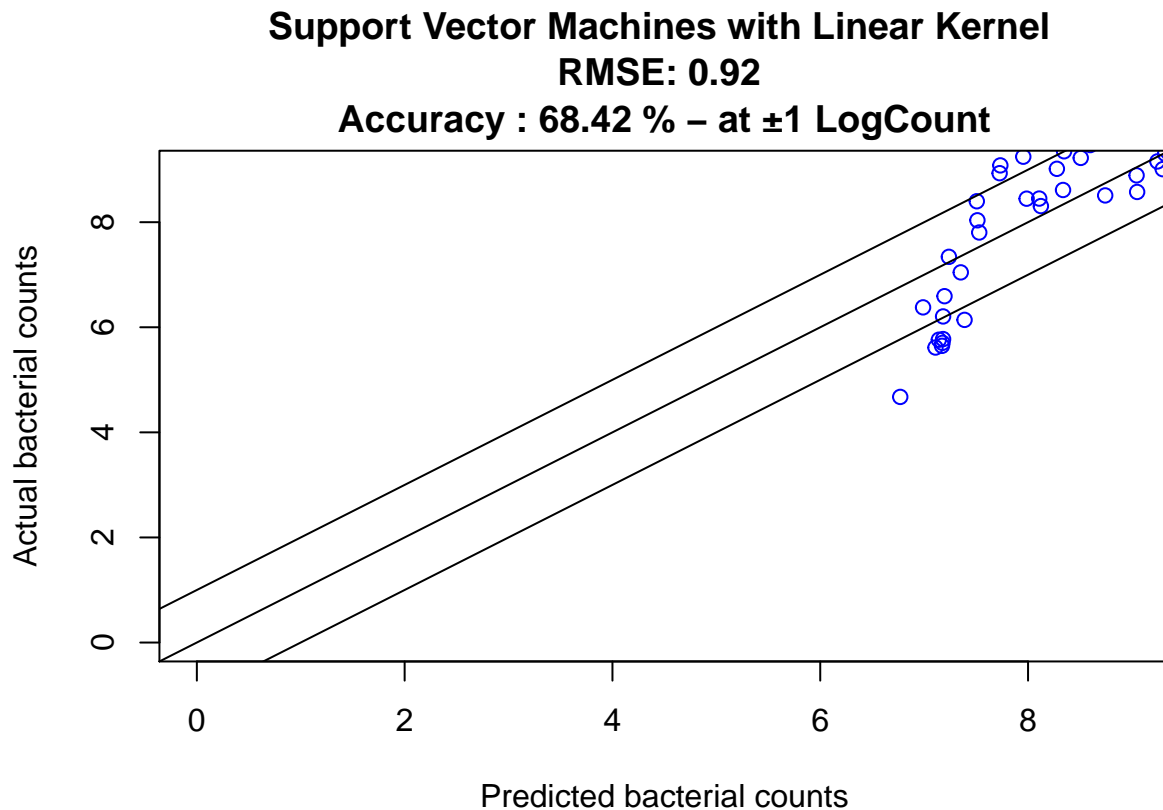
Lactic acid bacteria count distribution - Support Vector Machines with Polynomial Kernel



Support Vector Machines with Linear Kernel for Lactic acid bacteria count

```
## Support Vector Machines with Linear Kernel
##
## 90 samples
## 2 predictor
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 82, 80, 80, 81, 81, 81, ...
## Resampling results:
##
##      RMSE      Rsquared    MAE
## 0.9604258 0.6917079 0.7867821
##
## Tuning parameter 'C' was held constant at a value of 1
```

Lactic acid bacteria count distribution - Support Vector Machines with Linear Kernel



Support Vector Machines with Radial Basis Function Kernel for Lactic acid bacteria count

```
## Support Vector Machines with Radial Basis Function Kernel
##
## 90 samples
## 2 predictor
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 82, 81, 80, 80, 81, 81, ...
## Resampling results across tuning parameters:
##
##  C      RMSE      Rsquared  MAE
##  0.25  0.8887414  0.7525677  0.7161359
##  0.50  0.8327661  0.7759984  0.6518301
##  1.00  0.8234994  0.7773066  0.6338823
##
## Tuning parameter 'sigma' was held constant at a value of 1.219547
## RMSE was used to select the optimal model using the smallest value.
```

The final values used for the model were $\sigma = 1.219547$ and $C = 1$.

Lactic acid bacteria count distribution - Support Vector Machines with Radial Basis Function Kernel

