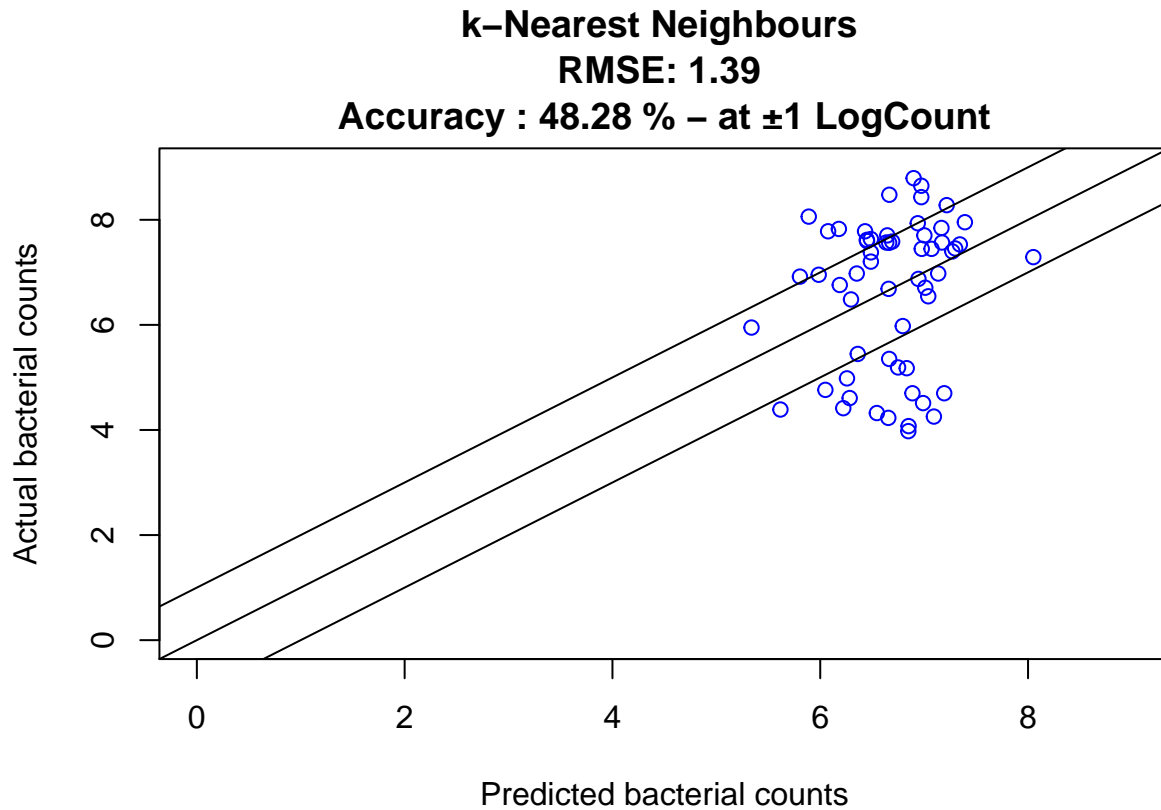


# Machine Learning Regression Model Report - FTIR (Chicken Thigh Fillet)

## k-Nearest Neighbours for Total Viable Counts

```
## k-Nearest Neighbors
##
## 140 samples
## 87 predictor
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 127, 127, 126, 126, 126, 126, ...
## Resampling results across tuning parameters:
##
##  k  RMSE      Rsquared    MAE
##  5  1.286339  0.05576910  1.064429
##  7  1.259468  0.07755742  1.037543
##  9  1.275517  0.07948775  1.059139
##
## RMSE was used to select the optimal model using the smallest value.
## The final value used for the model was k = 7.
```

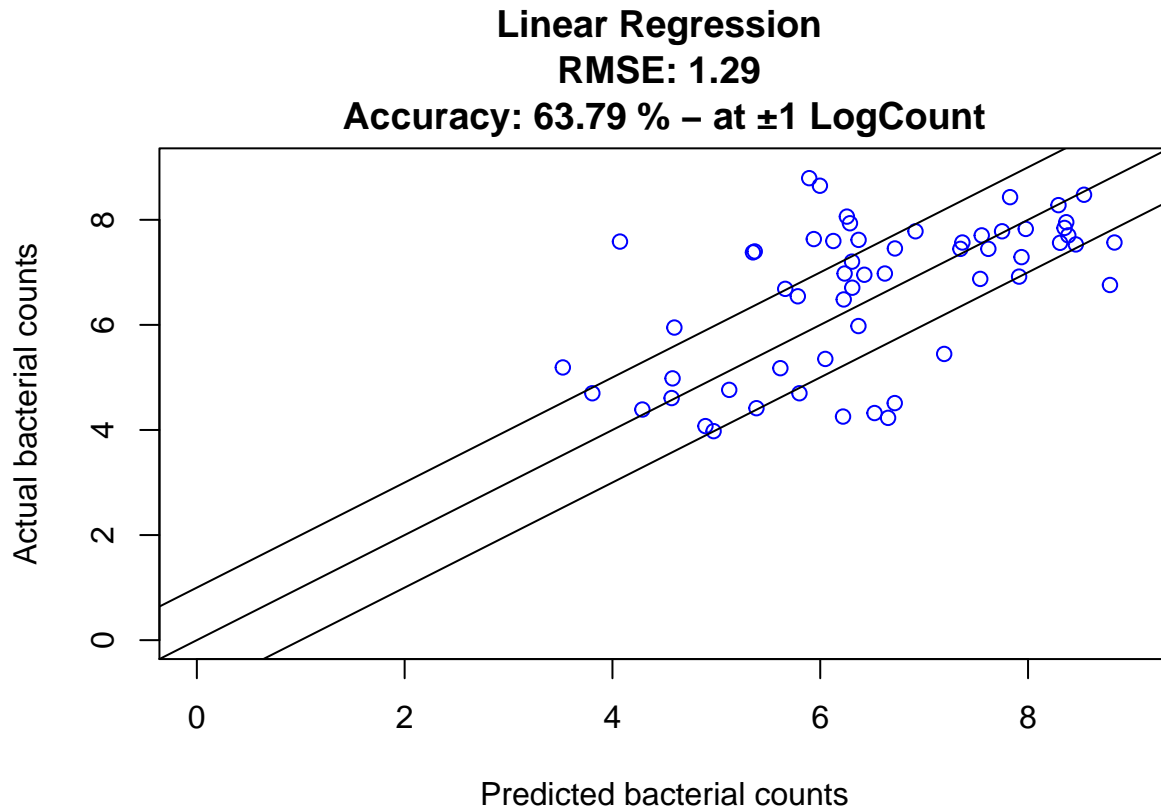
## Total Viable Counts distribution - k-Nearest Neighbours



## Linear Model for Total Viable Counts

```
## Linear Regression
##
## 140 samples
## 87 predictor
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 125, 125, 126, 128, 126, 127, ...
## Resampling results:
##
##   RMSE      Rsquared   MAE
## 1.647184  0.2650452  1.204469
##
## Tuning parameter 'intercept' was held constant at a value of TRUE
```

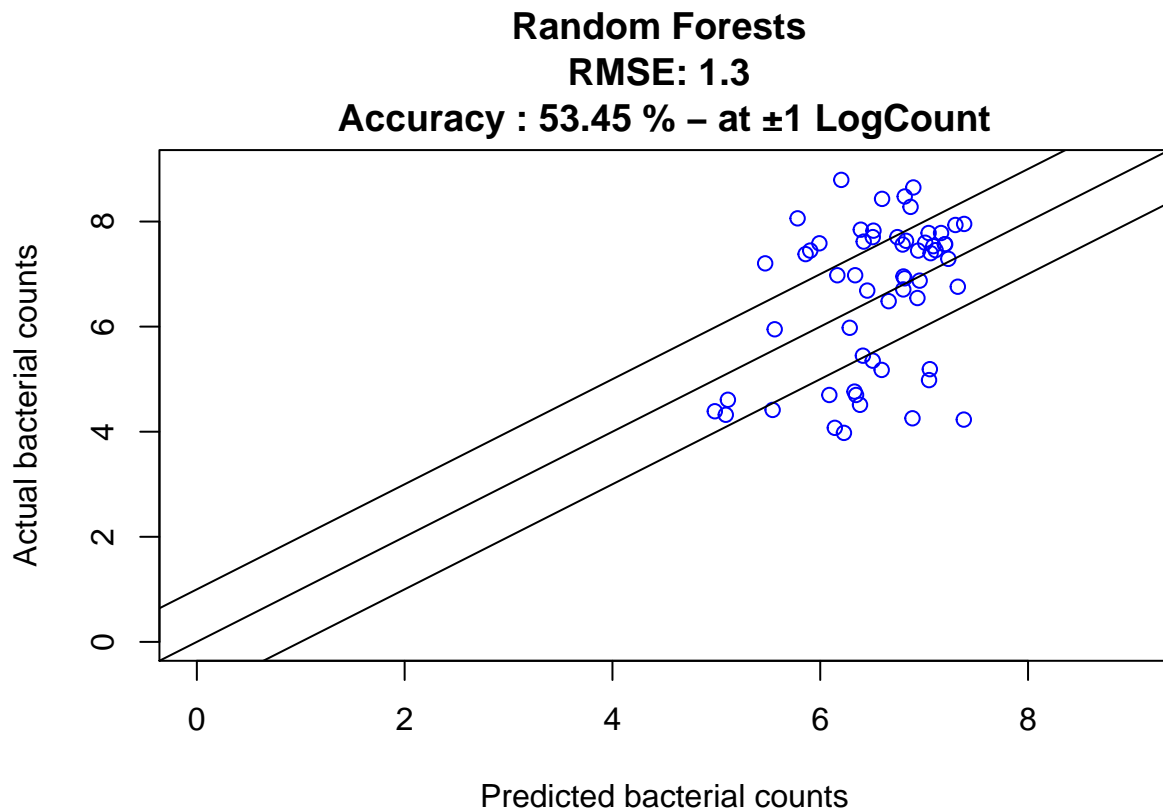
## Total Viable Counts distribution - Linear Regression



## Random Forest for Total Viable Counts

```
## Random Forest
##
## 140 samples
## 87 predictor
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 125, 124, 126, 127, 127, 126, ...
## Resampling results across tuning parameters:
##
##   mtry  RMSE      Rsquared  MAE
##   2     1.149203  0.2290469  0.9365817
##   44    1.132156  0.2439037  0.9343094
##   87    1.127967  0.2516282  0.9388954
##
## RMSE was used to select the optimal model using the smallest value.
## The final value used for the model was mtry = 87.
```

## Total Viable Counts distribution - Random Forests

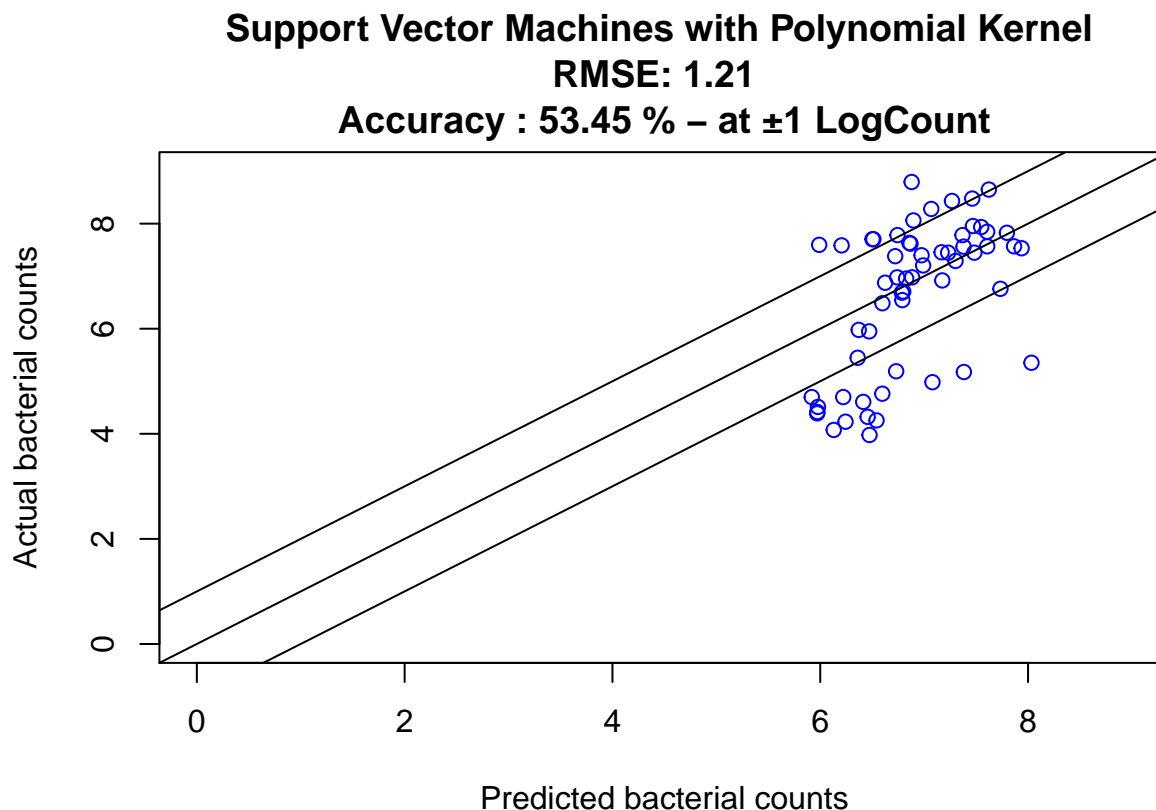


## Support Vector Machines with Polynomial Kernel for Total Viable Counts

```
## Support Vector Machines with Polynomial Kernel
##
## 140 samples
## 87 predictor
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 125, 126, 126, 127, 126, 127, ...
## Resampling results across tuning parameters:
##
## degree scale C      RMSE      Rsquared  MAE
## 1       0.001 0.25  1.306246  0.1424302 1.0315745
## 1       0.001 0.50  1.293355  0.1451438 1.0230369
## 1       0.001 1.00  1.276397  0.1605745 1.0111579
## 1       0.010 0.25  1.247781  0.1799142 0.9936865
## 1       0.010 0.50  1.232637  0.1803201 0.9786634
## 1       0.010 1.00  1.215038  0.2097056 0.9693145
## 1       0.100 0.25  1.166124  0.2554735 0.9283953
## 1       0.100 0.50  1.115263  0.3014314 0.8899613
```

##	1	0.100	1.00	1.060336	0.3547220	0.8483706
##	2	0.001	0.25	1.277966	0.1571411	1.0145764
##	2	0.001	0.50	1.257731	0.1826859	0.9966802
##	2	0.001	1.00	1.239065	0.1899285	0.9835172
##	2	0.010	0.25	1.317651	0.2102557	1.0310033
##	2	0.010	0.50	1.328532	0.2056404	1.0275893
##	2	0.010	1.00	1.366823	0.2039065	1.0423103
##	2	0.100	0.25	1.393003	0.2151160	1.0418781
##	2	0.100	0.50	1.418304	0.2114329	1.0520162
##	2	0.100	1.00	1.458741	0.2205167	1.0834204
##	3	0.001	0.25	1.258093	0.1694985	0.9954683
##	3	0.001	0.50	1.243575	0.1964172	0.9856855
##	3	0.001	1.00	1.240786	0.2117537	0.9906919
##	3	0.010	0.25	1.293126	0.2085688	0.9817202
##	3	0.010	0.50	1.385919	0.2260791	0.9962888
##	3	0.010	1.00	1.523964	0.2389240	1.0284305
##	3	0.100	0.25	3.763051	0.1575650	1.8359804
##	3	0.100	0.50	3.446561	0.1667429	1.8483165
##	3	0.100	1.00	2.769581	0.1814648	1.9017701
##						
##	RMSE was used to select the optimal model using the smallest value.					
##	The final values used for the model were degree = 1, scale = 0.1 and C = 1.					

## Total Viable Counts distribution - Support Vector Machines with Polynomial Kernel

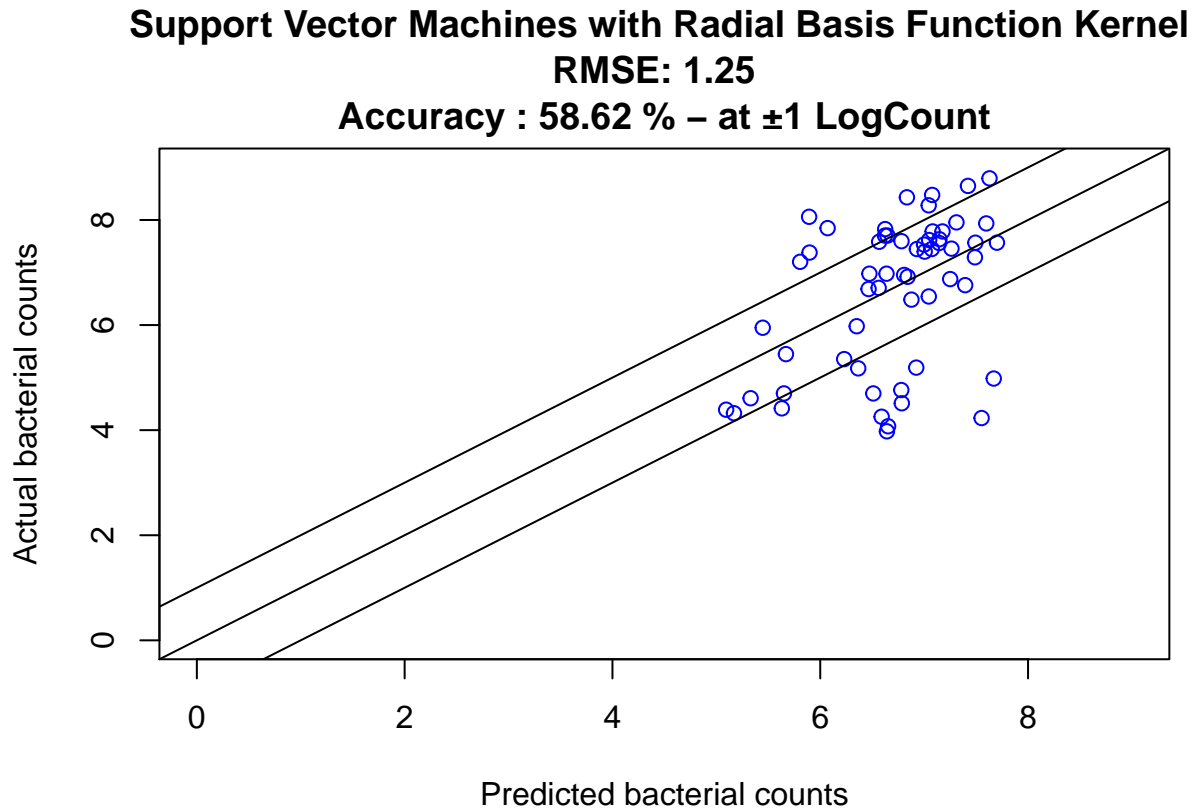


## Support Vector Machines with Radial Basis Function Kernel for Total Viable Counts

```
## Support Vector Machines with Radial Basis Function Kernel
##
## 140 samples
## 87 predictor
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 127, 125, 125, 126, 127, 126, ...
## Resampling results across tuning parameters:
##
##  C      RMSE      Rsquared  MAE
##  0.25  1.178506  0.2203075  0.9403277
##  0.50  1.158531  0.2413842  0.9252186
##  1.00  1.129424  0.2687901  0.9035943
##
## Tuning parameter 'sigma' was held constant at a value of 0.01845421
## RMSE was used to select the optimal model using the smallest value.
```

```
## The final values used for the model were sigma = 0.01845421 and C = 1.
```

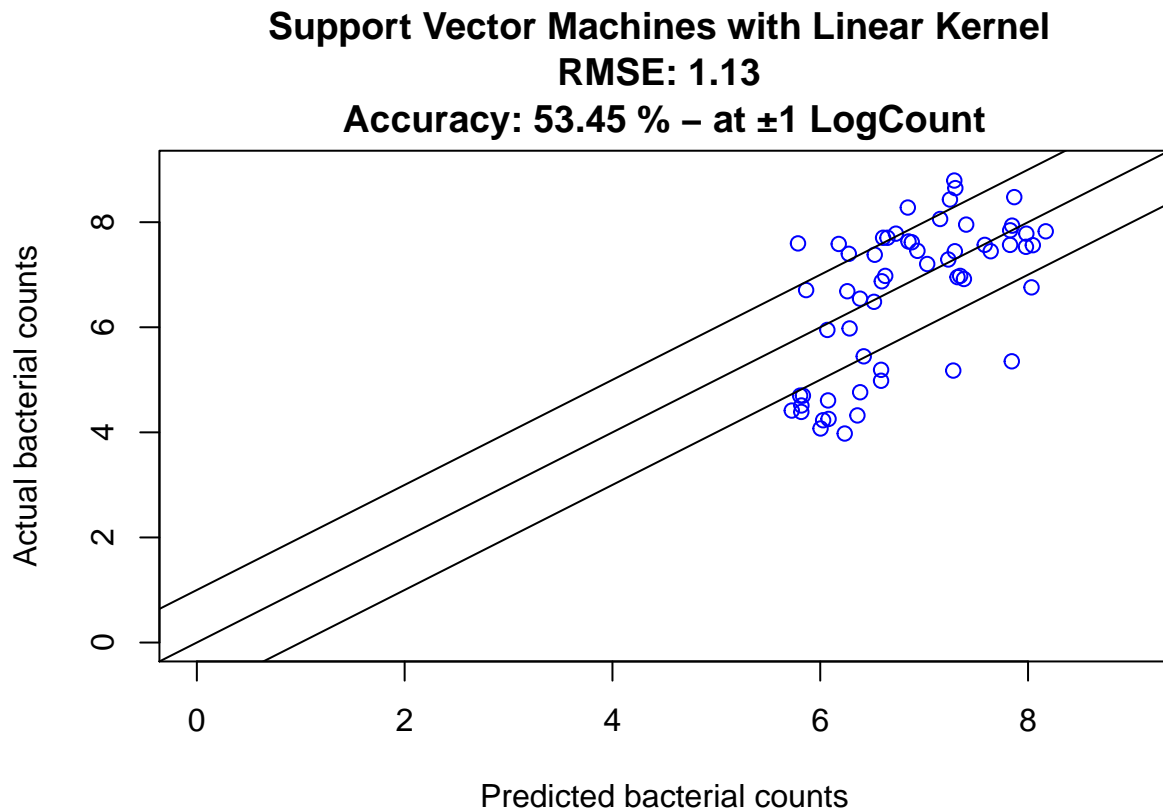
## Total Viable Counts distribution - Support Vector Machines with Radial Basis Function Kernel



## Support Vector Machines with Linear Kernel for Total Viable Counts

```
## Support Vector Machines with Linear Kernel
##
## 140 samples
## 87 predictor
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 126, 127, 125, 126, 126, 127, ...
## Resampling results:
##
##   RMSE      Rsquared   MAE
## 1.000353  0.4169443  0.8116841
##
## Tuning parameter 'C' was held constant at a value of 1
```

## Total Viable Counts distribution - Support Vector Machines with Linear Kernel

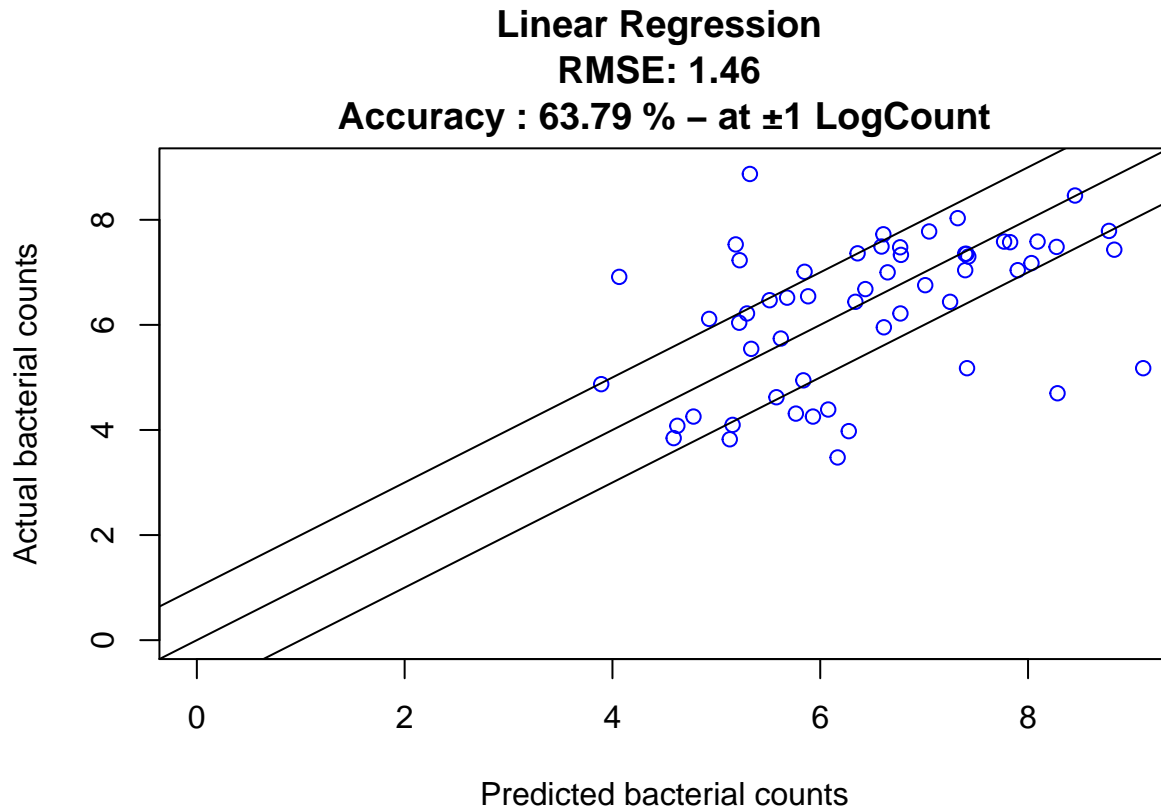


## Linear Regression for Pseudomonas count

```
## Linear Regression
##
## 140 samples
## 98 predictor
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 127, 124, 126, 127, 125, 126, ...
## Resampling results:
##
##   RMSE    Rsquared   MAE
##  2.31028  0.2564407  1.744293
##
## Tuning parameter 'intercept' was held constant at a value of TRUE
```



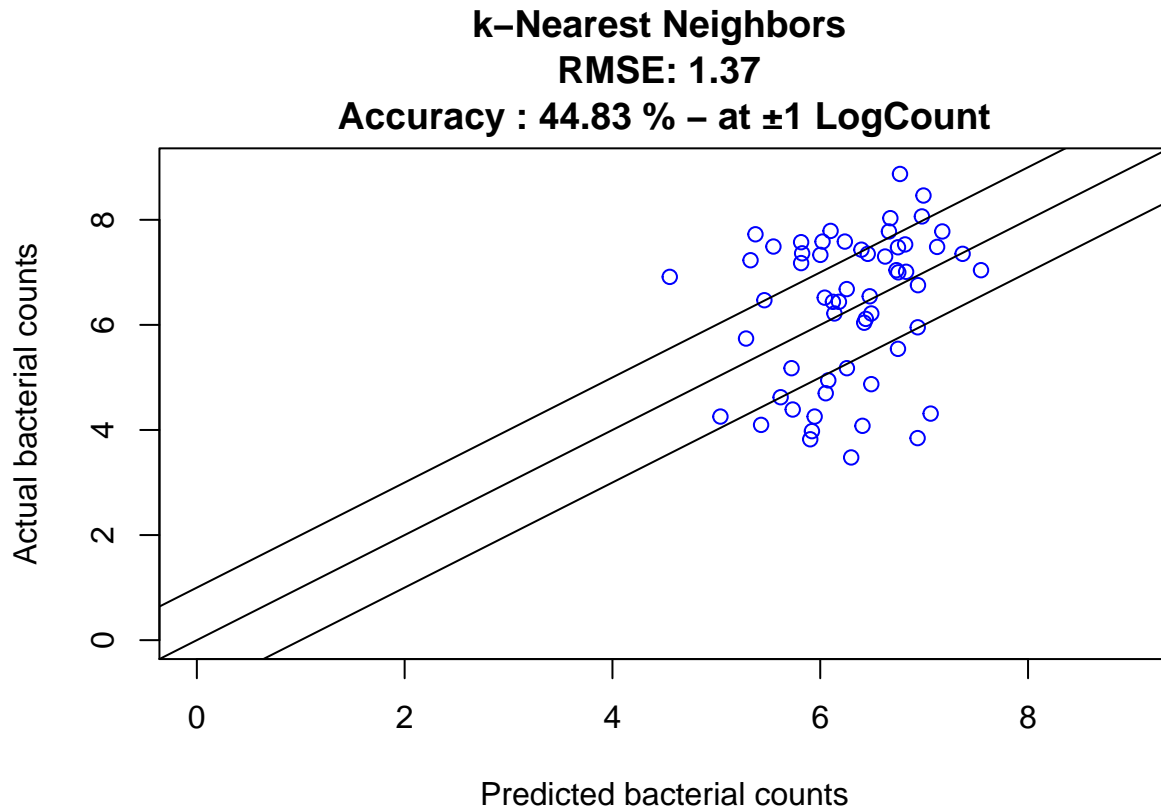
## Pseudomonas count distribution - Linear Regression



## k-Nearest Neighbors for Pseudomonas count

```
## k-Nearest Neighbors
##
## 140 samples
## 98 predictor
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 126, 126, 125, 125, 126, 126, ...
## Resampling results across tuning parameters:
##
##  k  RMSE      Rsquared  MAE
##  5  1.437180  0.1444040  1.180251
##  7  1.396105  0.1673076  1.174195
##  9  1.421391  0.1364347  1.219741
##
## RMSE was used to select the optimal model using the smallest value.
## The final value used for the model was k = 7.
```

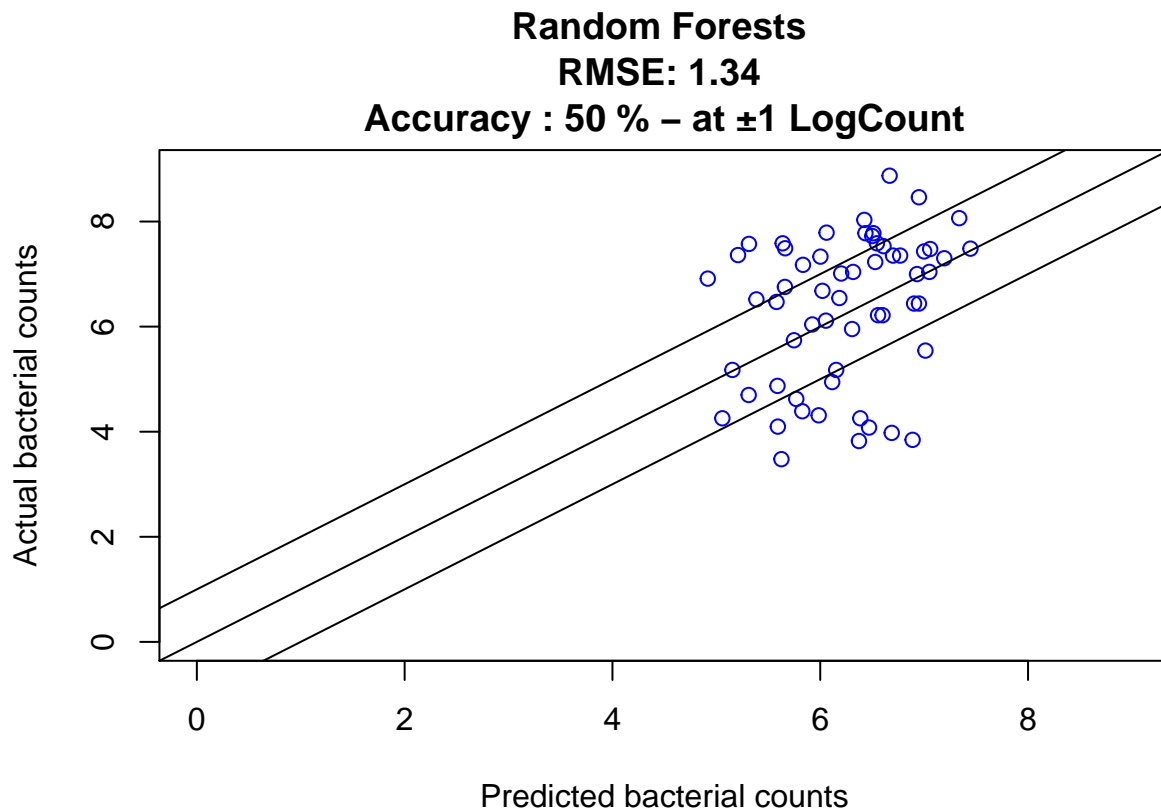
## Pseudomonas count distribution - k-Nearest Neighbors



## Random Forests for Pseudomonas count

```
## Random Forest
##
## 140 samples
## 98 predictor
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 126, 125, 125, 126, 128, 126, ...
## Resampling results across tuning parameters:
##
##  mtry  RMSE      Rsquared  MAE
##    2    1.308829  0.2888134  1.076976
##   50    1.280621  0.3197117  1.053160
##   98    1.284983  0.3135855  1.059817
##
## RMSE was used to select the optimal model using the smallest value.
## The final value used for the model was mtry = 50.
```

## Pseudomonas count distribution - Random Forests



## Support Vector Machines with Polynomial Kernel for Pseudomonas count

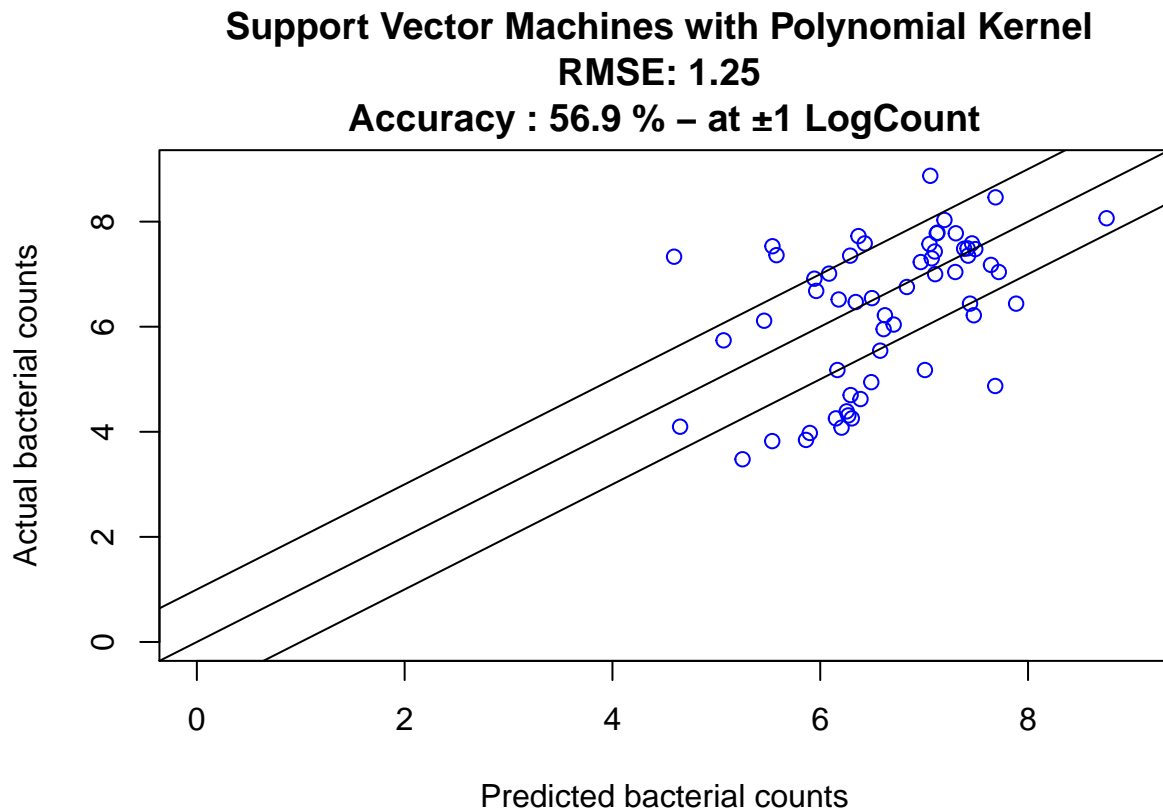
```
## Support Vector Machines with Polynomial Kernel
##
## 140 samples
## 98 predictor
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 126, 127, 128, 125, 124, 125, ...
## Resampling results across tuning parameters:
##
## degree scale C      RMSE      Rsquared  MAE
## 1      0.001 0.25  1.459750  0.1380977 1.1946343
## 1      0.001 0.50  1.444866  0.1428607 1.1832152
## 1      0.001 1.00  1.423784  0.1562445 1.1656968
## 1      0.010 0.25  1.398572  0.1811840 1.1411336
## 1      0.010 0.50  1.366719  0.2098208 1.1201395
## 1      0.010 1.00  1.335950  0.2309229 1.1036692
## 1      0.100 0.25  1.273949  0.2867240 1.0646266
## 1      0.100 0.50  1.207687  0.3596532 0.9959901
```

```

## 1      0.100  1.00  1.149015  0.4320187  0.9416107
## 2      0.001  0.25  1.435521  0.1524355  1.1672221
## 2      0.001  0.50  1.419882  0.1741607  1.1438058
## 2      0.001  1.00  1.400194  0.2018573  1.1242823
## 2      0.010  0.25  1.377706  0.2321406  1.1062694
## 2      0.010  0.50  1.363287  0.2440428  1.0963755
## 2      0.010  1.00  1.364725  0.2327690  1.0873932
## 2      0.100  0.25  1.446703  0.2819263  1.0767714
## 2      0.100  0.50  1.495325  0.2918589  1.0982055
## 2      0.100  1.00  1.491639  0.3164031  1.1035568
## 3      0.001  0.25  1.422841  0.1722414  1.1462753
## 3      0.001  0.50  1.402159  0.2016791  1.1270315
## 3      0.001  1.00  1.375570  0.2194981  1.1131028
## 3      0.010  0.25  1.412612  0.2247790  1.1233675
## 3      0.010  0.50  1.447197  0.2475521  1.1589851
## 3      0.010  1.00  1.520506  0.2650465  1.1927783
## 3      0.100  0.25  2.573459  0.2703094  1.6418631
## 3      0.100  0.50  3.905923  0.2340753  2.0826941
## 3      0.100  1.00  5.723412  0.1558691  2.7354258
##
## RMSE was used to select the optimal model using the smallest value.
## The final values used for the model were degree = 1, scale = 0.1 and C = 1.

```

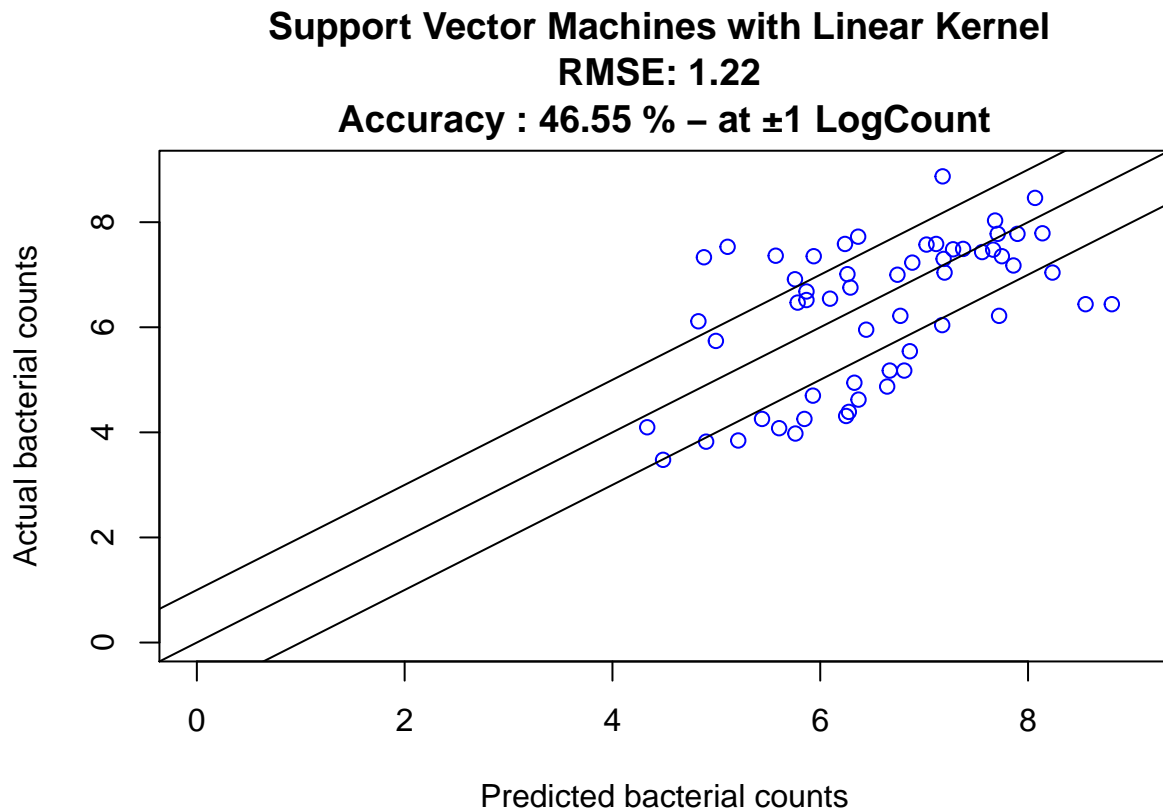
## Pseudomonas count distribution - Support Vector Machines with Polynomial Kernel



## Support Vector Machines with Linear Kernel for Pseudomonas count

```
## Support Vector Machines with Linear Kernel
##
## 140 samples
## 98 predictor
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 125, 126, 127, 127, 125, 127, ...
## Resampling results:
##
##   RMSE      Rsquared   MAE
## 1.009994  0.5395713  0.8397219
##
## 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
##
## 140 samples
## 98 predictor
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 128, 125, 126, 126, 127, 124, ...
## Resampling results across tuning parameters:
##
##  C      RMSE      Rsquared    MAE
##  0.25  1.312389  0.2523271  1.0639887
##  0.50  1.283796  0.2825282  1.0249203
##  1.00  1.237863  0.3344892  0.9884672
##
## Tuning parameter 'sigma' was held constant at a value of 0.01745488
## RMSE was used to select the optimal model using the smallest value.
```

## The final values used for the model were  $\sigma = 0.01745488$  and  $C = 1$ .

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

