Assignment 2 – k-nearest neighbours and k-fold cross validation

In this lab, the goal is the implement kNN model and perform 5-fold cross validation to choose the best k-NN model.

The kNN model is achieved by calculating the Euclidean distance between the test point and all the other points, then picking out k numbers of nearest point, and find the average of the corresponding target values.

Cross validation method is built based on the kNN model where the training data set is split into 5 parts, taking 4 sets as new training set and 1 for test. The kNN model is run through all 5 combinations and the average training error for all combinations is calculated to be the cross-validation error.

Plots of training error and the cross-validation error for all k-NN models:

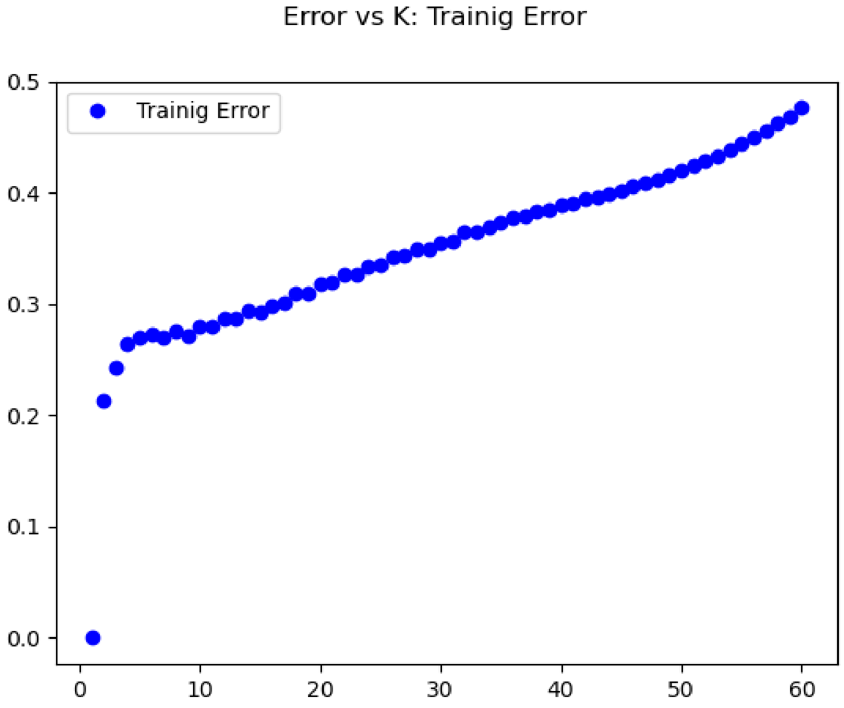


Figure 1: Training error vs k

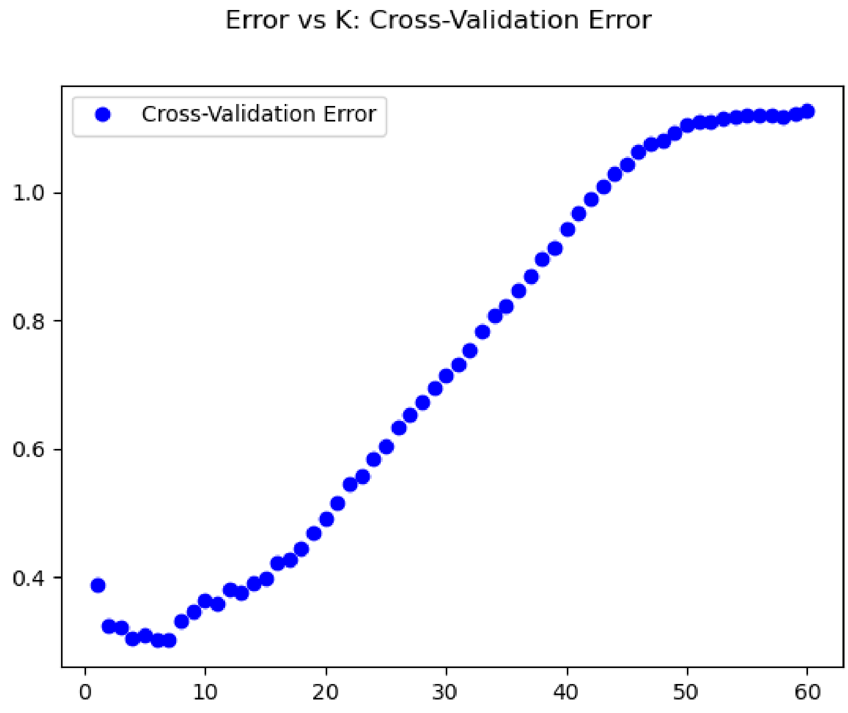


Figure 2: Cross-Validation Error vs K

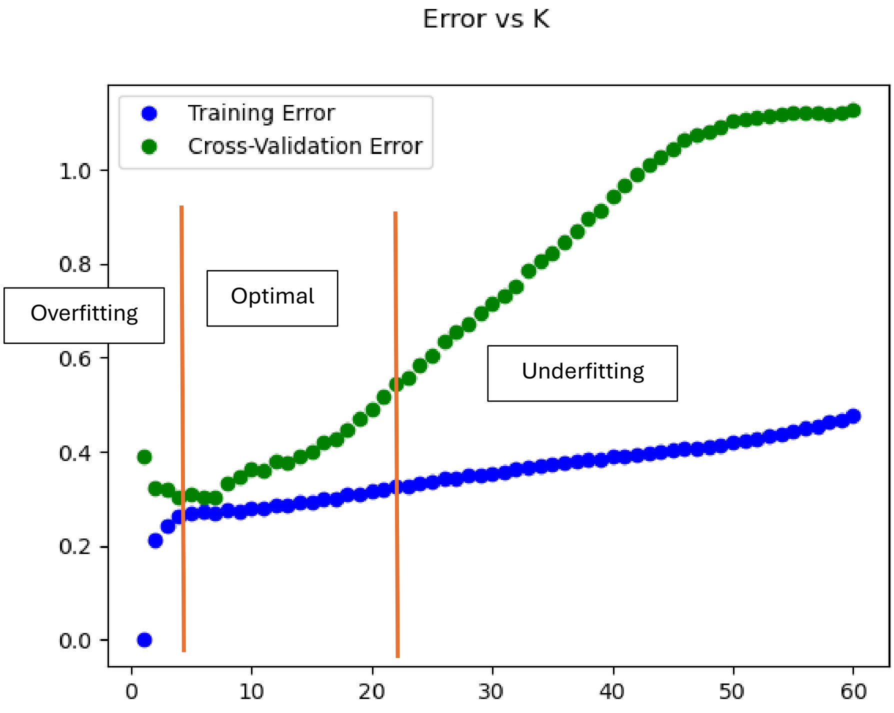
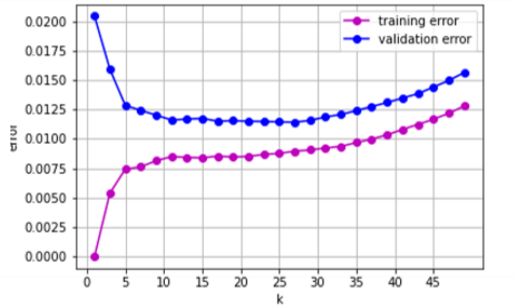


Figure 3: Training Error & Cross-Validation Error vs K

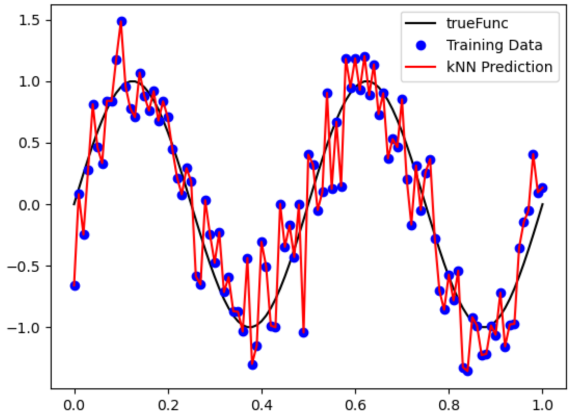
Figure 3 shows the comparison between the training error and the validation error. In the lecture, the error trends should have been shown as figure 4. In comparison to figure 3, the training error follows the exact trend. For the cross-validation error, the trend is slightly off as the slope increases relatively more rapidly. However, the trend is still acceptable as the rising trend follows the expected values.



(b) $1 \leq k \leq 49$.

Figure 4: Lecture Example on Error Comparison

Identify k values for underfitting, overfitting, region of optimal capacity:



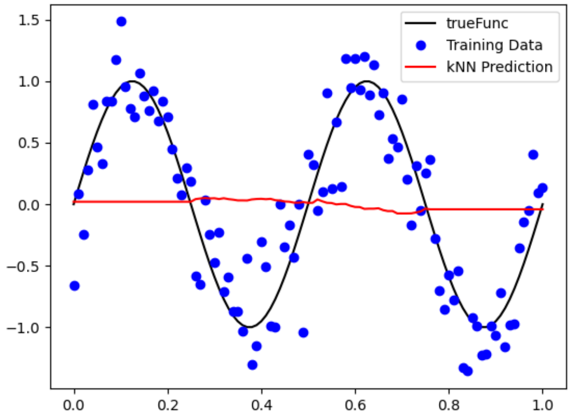


Figure 5: K = 1, Overfitting

Figure 6: k = 50, Underfitting

* The “training data” label should be “test data”

Figure 3 also depicts the three regions of model fitting. The beginning of the converging trend between training error and cross-validation error can be identified as the overfitting region. This region can be roughly identified from $1 \leq k \leq 4$. By picking $k = 1$, and plot the prediction model with 1NN prediction model, figure 5 shows the overfitting of the model. Additionally, the overfitting of the model can be depicted by the “fuzzy” trend in the prediction model as it overcompensates for every single test points. Figure 6 is a great example of underfitting, with $k = 50$, locating in the underfitting region in figure 3. The prediction model in figure 6 failed to capture any trend that the test set possesses as it does not have the capacity to do such. The underfitting region can be roughly identified around $22 \leq k \leq 60$. The starting point of the underfitting region is not quite accurate as there is no significant change or threshold in the uprising trend.

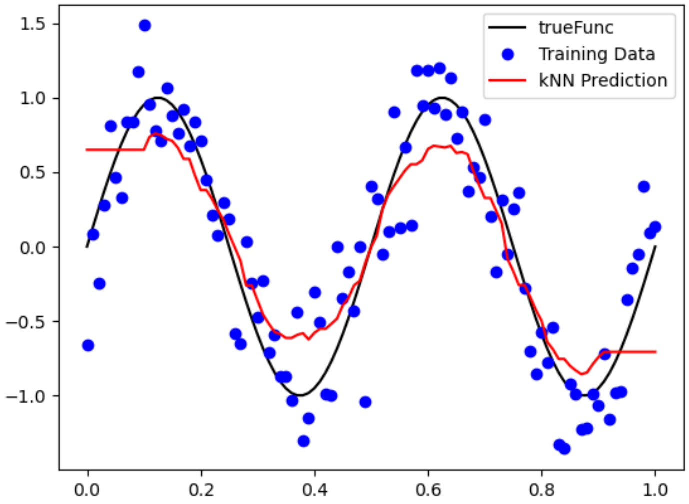


Figure 7: k = 20, Optimal Capacity

* The "training data" label should be "test data"

The optimal capacity is located between $4 \leq k \leq 22$ from figure 3. Figure 7 is plotted with kNN where $k = 20$. It is identifiable that the prediction model is able to capture the general trend presented by the test set and it sticks quite close to the true function.

k	Training Error	Cross-Validation Error
1	0	0.388736637
2	0.212587084	0.324139225
3	0.243156848	0.321459716
4	0.263938216	0.303941702
5	0.269442196	0.310970292
6	0.272885461	0.301482272
7	0.269586102	0.30332941
8	0.274867613	0.331910193
9	0.271726328	0.345730078
10	0.279589701	0.362735111
11	0.280224343	0.359301325
12	0.286453203	0.380431578
13	0.287561928	0.376012238
14	0.294150336	0.391959891
15	0.292626507	0.399290667
16	0.298214347	0.421636596
17	0.300569438	0.428784879
18	0.309027219	0.44578767

19	0.309244678	0.469197156
20	0.317489012	0.491872144
21	0.319286122	0.516287381
22	0.32680958	0.545398063
23	0.326751893	0.558520575
24	0.334186472	0.585085422
25	0.335211958	0.604994863
26	0.342738372	0.635014805
27	0.343629364	0.654644681
28	0.348789961	0.673450132
29	0.349648223	0.696230791
30	0.354195428	0.71484126
31	0.356552942	0.732246283
32	0.364537132	0.753871932
33	0.365488549	0.784624546
34	0.369743328	0.807725472
35	0.373260483	0.821985559
36	0.37789315	0.847421557
37	0.379414711	0.86914684
38	0.383887751	0.895904394
39	0.384325359	0.914878022
40	0.388833187	0.942227409
41	0.390495433	0.967460322
42	0.394451649	0.989802041
43	0.395503371	1.009647557
44	0.399322071	1.028759883
45	0.402128611	1.043554324
46	0.405670228	1.064278027
47	0.40852264	1.075445398
48	0.411718286	1.081461518
49	0.415231129	1.092434795
50	0.419673354	1.105681752
51	0.42412163	1.109491771
52	0.428321573	1.111090721
53	0.433472674	1.115476079
54	0.438622837	1.118114367
55	0.444037507	1.119935637
56	0.450222341	1.120223897
57	0.455542047	1.12122262
58	0.462981145	1.116624899
59	0.4689268	1.122493313
60	0.476220652	1.126610178

Table 1: k vs training error vs cross-validation error

Best model:

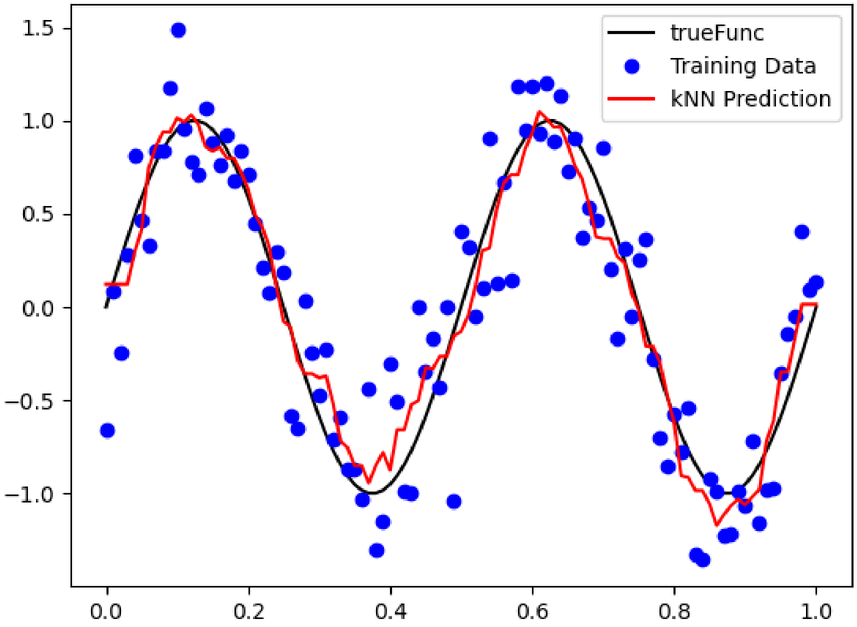


Figure 6: Best kNN model prediction - Test Set Performance

* The “training data” label should be “test data”

The best k-value is determined by locating the minimum cross-validation error in the training set. Looking at table 1 and using the argmin() function, it is determined that the best kNN prediction model occurs when $k = 6$. This k hyperparameter value is located correctly in the optimal capacity. The test error (RMSE) is calculated to be 0.30087546405653753.

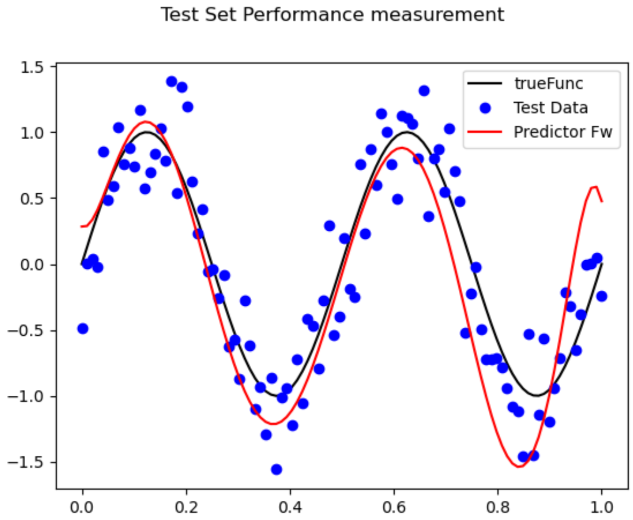


Figure 7: Assignment 1 - Optimal Model performance in test data

$$\begin{aligned} f(x) = {} & [-0.1143765] + [-0.62578146]x + [84.10397188]x^2 + [-740.2899919]x^3 + [2334.17849351]x^4 \\ & + [-3407.55041947]x^5 + [2480.14060814]x^6 + [-1081.13405016]x^7 \\ & + [537.35399237]x^8 + [-206.34937555]x^9 \end{aligned}$$

Figure 9 shows the best prediction model from of assignment 1 where a least squares linear regression formula was used. The best prediction function is written as above. The prediction model has a test error (RMSE) of 0.3949494709298686.

kNN, k = 6	Least squares linear regression
0.30087546405653753	0.3949494709298686

By comparing the test errors from both model, it is obvious that kNN with k = 6 has a lower test error. In terms of actual fitting, figure 9 (least squares) definitely has a smoother fitting than figure 8 (kNN). However, the kNN fitting in figure 8 shows a closer fit to the true function than least squares model. Therefore, it is confident to say that in this case, the kNN model with k = 6 is a better prediction model than the least squares linear regression mode.