ASSIGNMENT 1

CS5691 Pattern Recognition and Machine Learning

CS5691 Assignemnt 1

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1 Task 1

1.1 Mathematical Formulation

The data for univariate polynomial regression is obtained by raising it to the required degree. In case of univariate polynomial regression of degree d, the dependent variable, of size $(d, 1)$ is assumed to have the form

$$\vec{y}_{n\times1} = \phi_{n\times d} W_{d\times1} \tag{1}$$

The weights corresponding to a given degree is then calculated by using the closed form solution for univariate polynomial regression:

$$W = (\phi^T\phi + \lambda I)^{-1}\phi^T\vec{y} \tag{2}$$

Where, λI is the regularization term.

1.2 Training and Validation Accuracies

In order to pick the parameters that best fit the dataset, a grid search was performed on the dataset. Prior to this, the dataset was split into training set, validation set and the testing set, in the ratio 70:10 (from the training data) :30. The results obtained is as follows:

Degree	λ	**Train Error**	**Validation Error**
6	0.0	0.044889	0.159636
3	0.0	0.672882	1.001484
9	0.5	0.750020	1.469413
2	0.0	1.014199	1.883134
9	1.0	1.040132	1.929033
9	2.0	1.354363	2.165779
9	10.0	2.281929	1.857270
9	50.0	3.342110	1.447933
9	100.0	3.782560	1.380623
9	0.0	5.063475	92.085167

Table 1: Results obtained for Task 1, with sample size of 10

Regularization was only applied in case of degree 9.

Degree	λ	**Train Error**	**Validation Error**
6	0.0	0.094536	0.094379
9	0.0	0.093581	0.100752
9	0.5	0.134226	0.152565
9	1.0	0.186479	0.209008
9	2.0	0.289107	0.311716
9	10.0	0.766298	0.776521
3	0.0	0.934079	0.862605

2	0.0	1.591842	1.421021
9	50.0	1.620063	1.707757
9	100.0	2.138200	2.310223

Table 2: Results obtained for Task 1, with sample size of 200

From the table above, we see that the best fit for the data is obtained for degree: 6 and $\lambda : 0$.

1.3 Model Fits

1.3.1 Sample Size: 10

The polynomial models and the corresponding fits obtained for sample size of 10 are as follows:

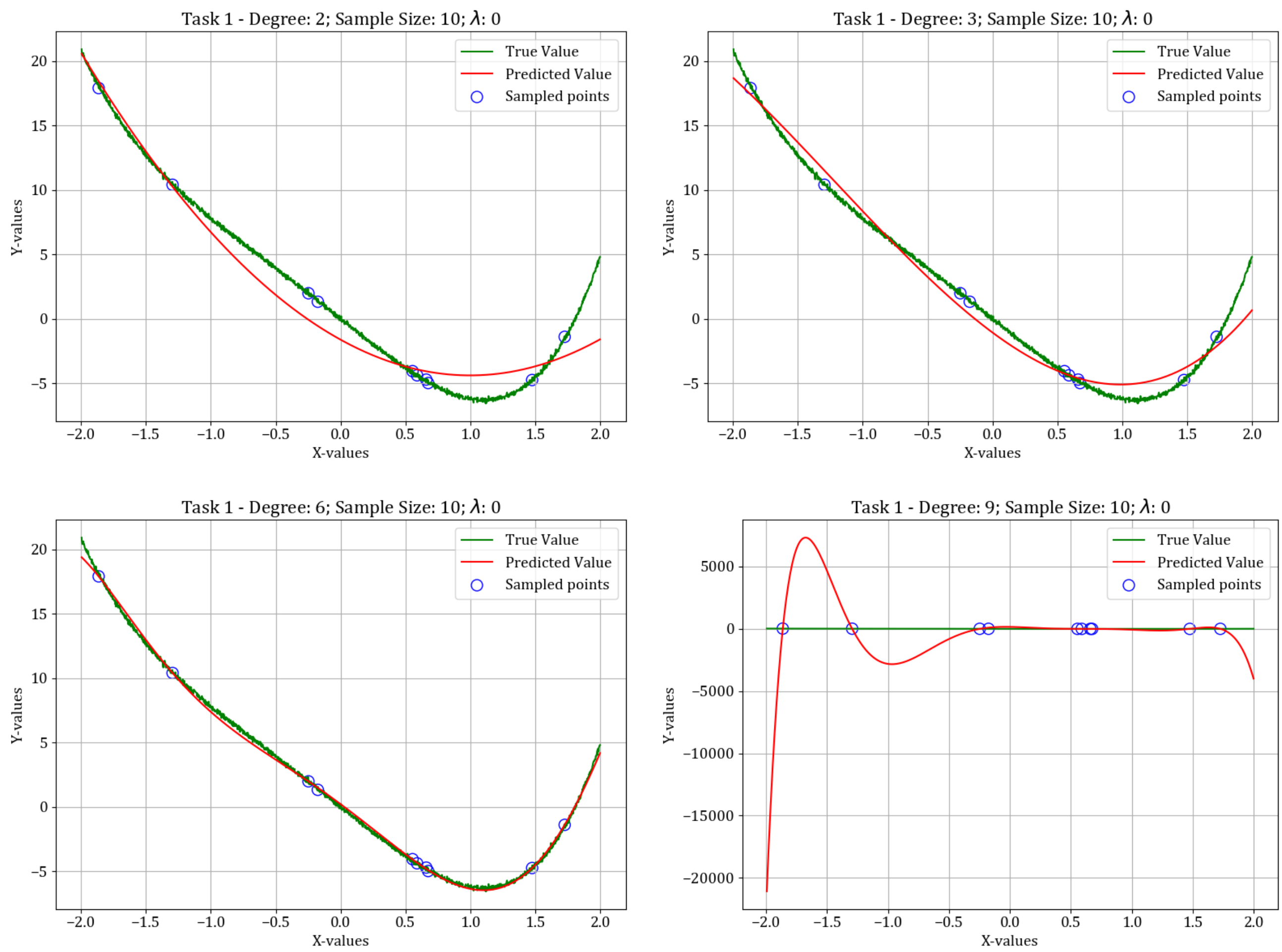


Figure 1: Task 1 - Polynomial fits, Sample size: 10

1.3.2 Sample Size: 200

The polynomial models and the corresponding fits obtained for sample size of 200 are as follows:

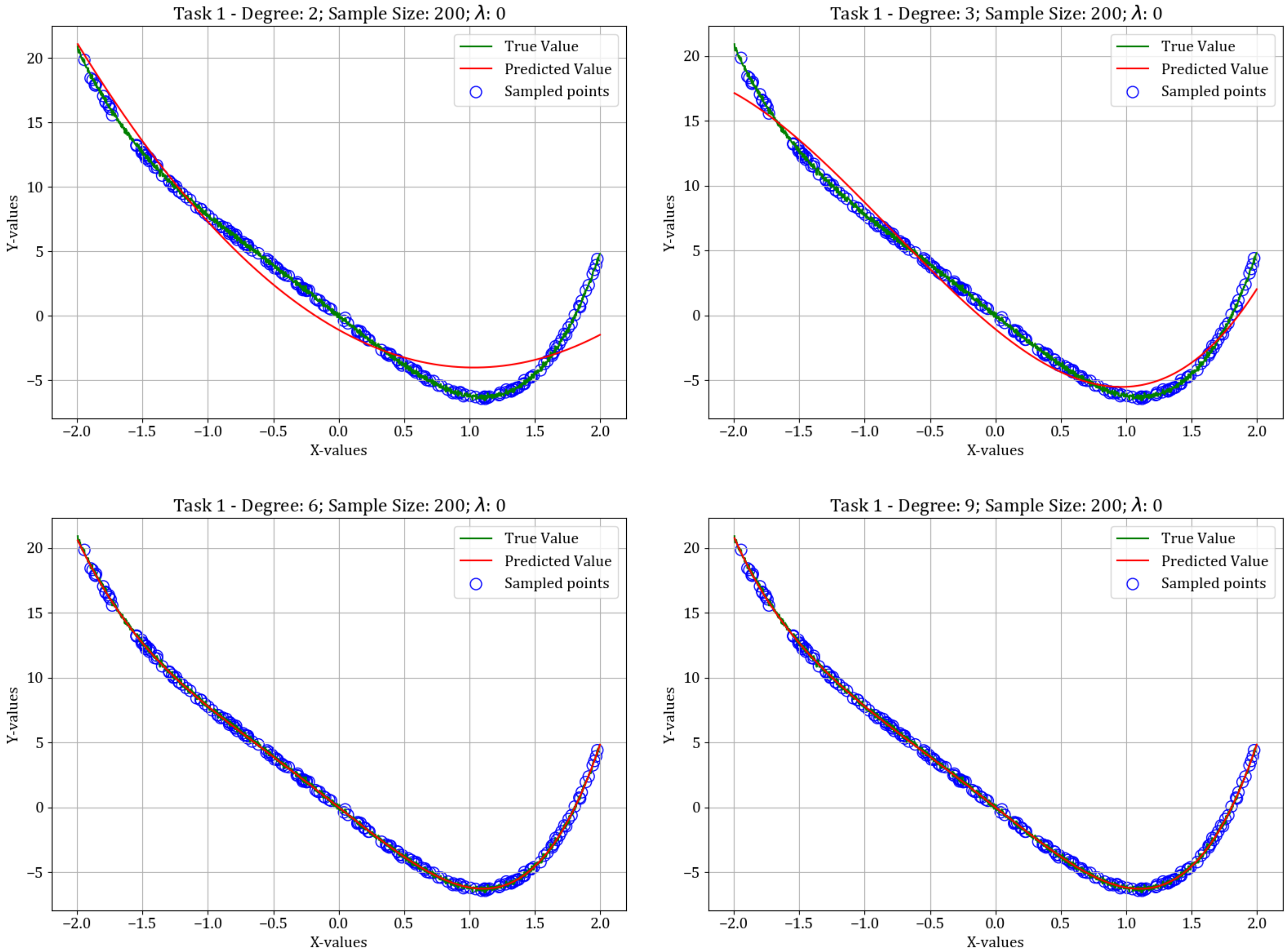
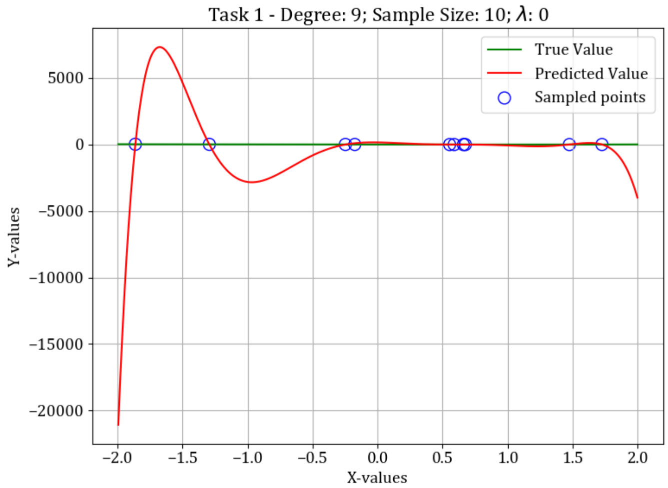
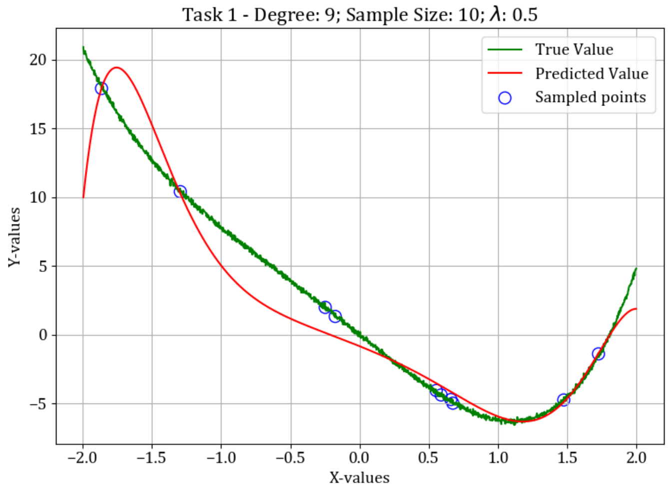


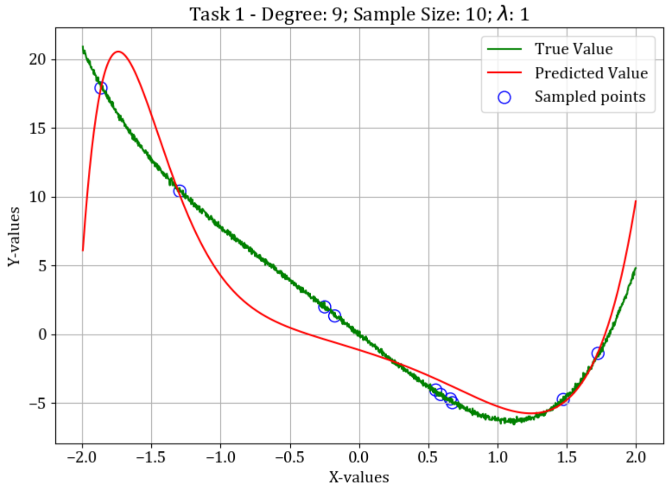
Figure 2: Task 1 - Polynomial fits, Sample size: 200

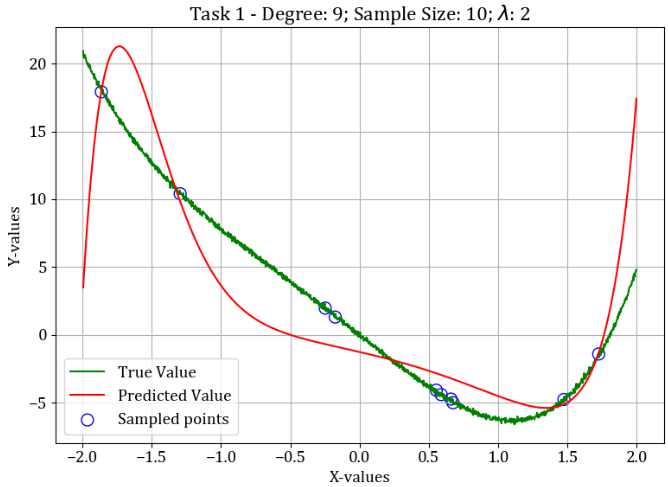
1.3.3 Effects of Regularization

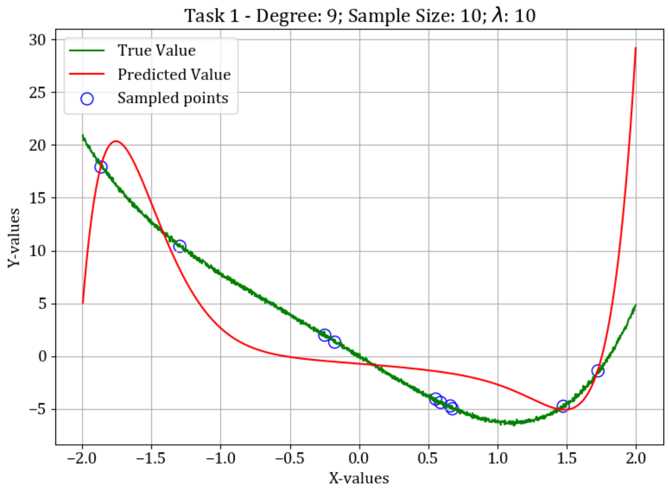
The polynomial models and the corresponding fits obtained for sample size of 10, across different λ values are as follows:

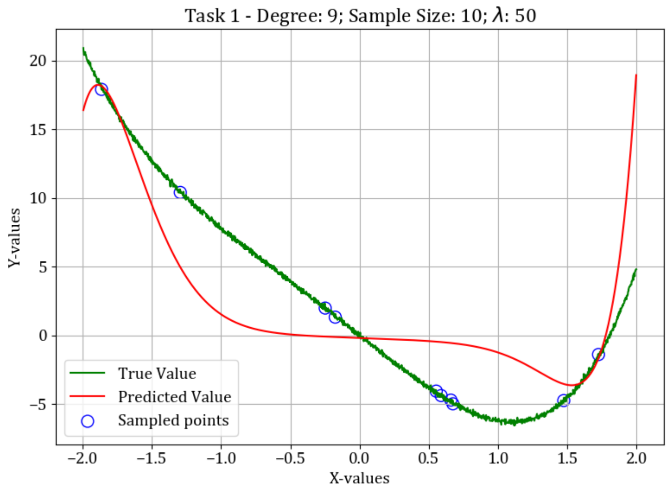

Task 1 - Degree: 9; Sample Size: 10; λ: 0
True Value
Predicted Value
Sampled points
X-values
Y-values

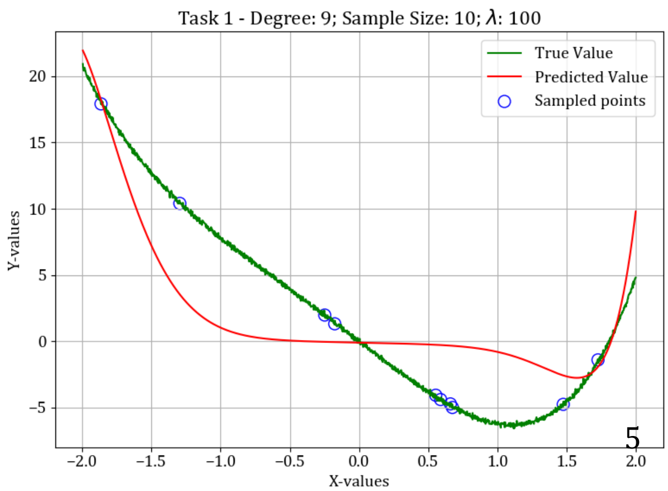

Task 1 - Degree: 9; Sample Size: 10; λ: 0.5
True Value
Predicted Value
Sampled points
X-values
Y-values


Task 1 - Degree: 9; Sample Size: 10; λ: 1
True Value
Predicted Value
Sampled points
X-values
Y-values


Task 1 - Degree: 9; Sample Size: 10; λ: 2
True Value
Predicted Value
Sampled points
X-values
Y-values


Task 1 - Degree: 9; Sample Size: 10; λ: 10
True Value
Predicted Value
Sampled points
X-values
Y-values


Task 1 - Degree: 9; Sample Size: 10; λ: 50
True Value
Predicted Value
Sampled points
X-values
Y-values


Task 1 - Degree: 9; Sample Size: 10; λ: 100
True Value
Predicted Value
Sampled points
X-values
Y-values

1.4 Best Model

The best fit, $d : 6$ and $\lambda : 0$ is visualized as follows:

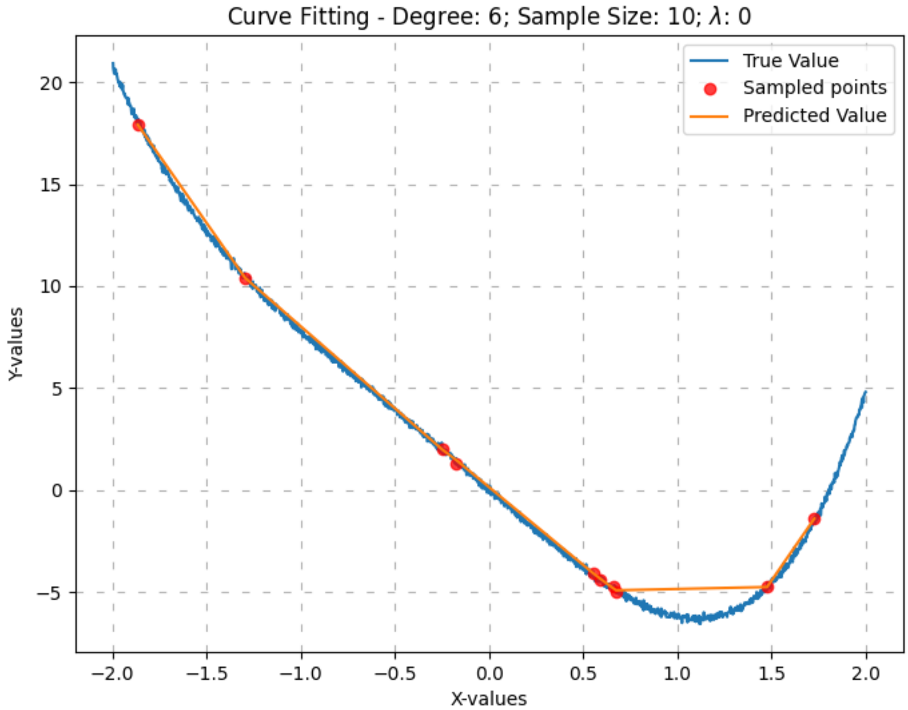


Figure 3: Task 1 - Best fit, Sample size: 10

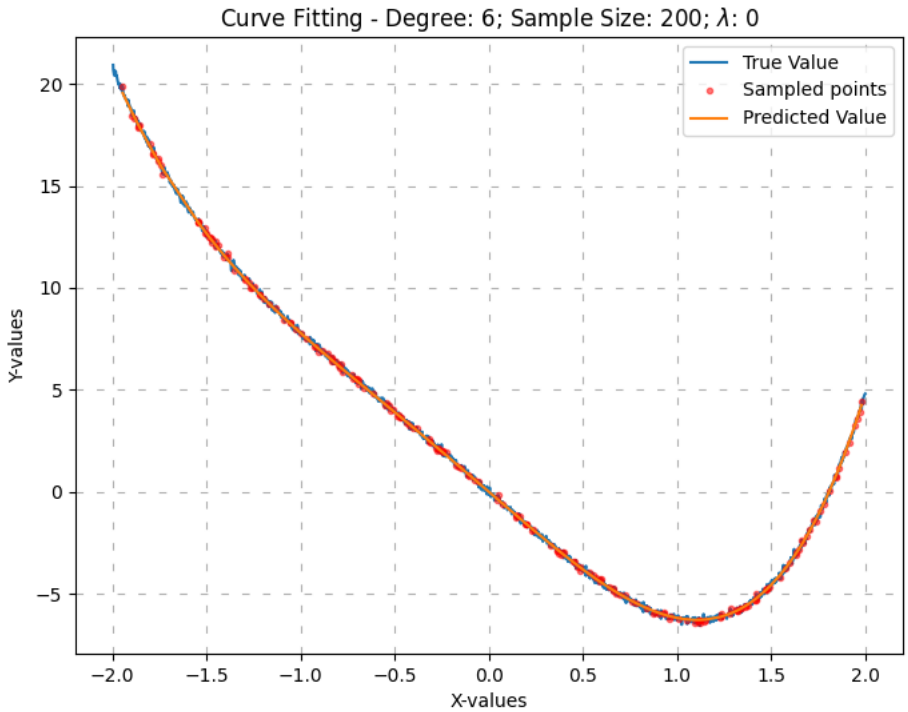


Figure 4: Task 1 - Best fit, Sample size: 200

The final training and testing error obtained is as follows:

- Training Error: 0.09974659089780814
- Testing Error: 0.09793071099285168

2 Task 2

2.1 Polynomial Regression for bivariate data

The second dataset is a bivariate data with 2000 examples. We assume that the target variable is of the form:

$$y = \sum_{i=0} \omega_i \phi_i(x_1, x_2) + \epsilon \tag{3}$$

Where ω_i are the parameters to be found through regression, $\phi_i(x_1, x_2)$ is a polynomial in x_1 and x_2 and ϵ is the normally distributed error.

A breakdown of the steps undertaken is:

- The function `create_phi` generates the design matrix $\phi(x_1, x_2)$ for the required degree of complexity.
- The design matrix is passed to the function `regularized_pseudo_inv`, which generates the Moore-Penrose inverse of the given design matrix (X) and specified value of regularization parameter lambda (λ).

$$(X^T X + \lambda I)^{-1} X^T \tag{4}$$

- The function `opt_regularized_param` is then used to obtain optimum values of $\vec{\omega}$

$$\vec{\omega} = [(X^T X + \lambda I)^{-1} X^T] y \tag{5}$$

  Where y is the output as defined in the Equation 3.
- The optimum parameter vector thus obtained can be used to predict the variable y for new inputs.

$$y_{prediction} = X\vec{\omega} \tag{6}$$

2.2 Data processing

- The range of variables is same for x_1 and x_2, (i.e.) $(-16, 16)$ hence no scaling is required, there are no null data values.
- The data is first shuffled and then split into Train data, Cross-validation data and Test data. Train data sizes: $50, 200, 500$
- The independent vectors $\vec{x_1}$ and $\vec{x_2}$ are extracted from the datasets and then design matrices $\phi_{n \times m}$ are created using the function `create_phi`. Here, n is the number of samples in the respective sample and m is the number of components for the corresponding degree.

2.3 Degree of complexity 2

With degree of complexity set to 2, for a particular data point,

$$y_i = \omega_0 + \omega_1 x_1 + \omega_2 x_2 + \omega_3 {x_1}^2 + \omega_4 {x_2}^2 + \omega_5 x_1 x_2 \tag{7}$$

2.3.1 Varying λ, Sample size of 50

After the above pre-processing, The optimum parameter $\vec{\omega}$ is obtained for the following lambda values - $[0, 0.5, 1, 2, 10, 50, 100]$. The variation in RMSE across lambda is as follows:

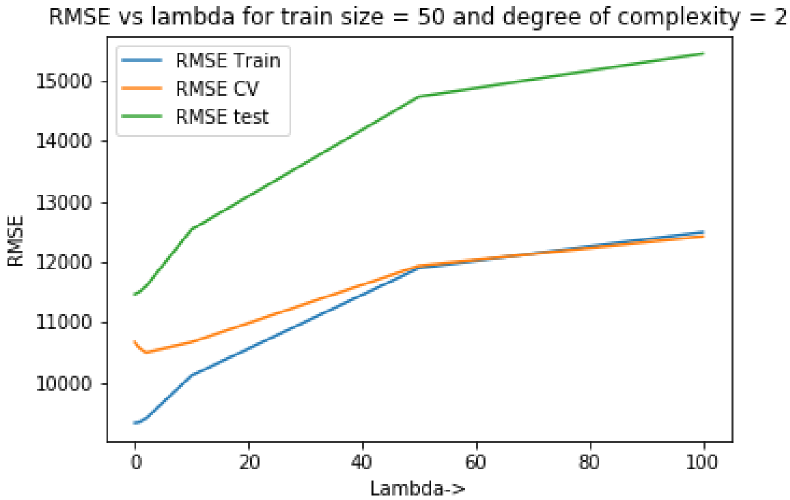


Figure 5: RMSE across λ; Sample size: 50, Degree: 2

Lambda	RMSE Train	RMSE CV	RMSE Test
0	9340.73	10671.59	11468.19
0.5	9346.19	10611.41	11487.13
1	9361.17	10564.66	11516.49
2	9412.58	10503.67	11598.33
10	10120	10672.93	12534.16
50	11897.56	11935.27	14729.56
100	12491.10	12420.38	15443.04

Table 3: Variation in RMSE values with lambda

2.3.2 Varying λ, Sample size of 200

The optimum parameter $\vec{\omega}$ is obtained for the following lambda values - $[0, 0.5, 1, 2, 10, 50, 100]$. The variation in RMSE across lambdas is as follows:

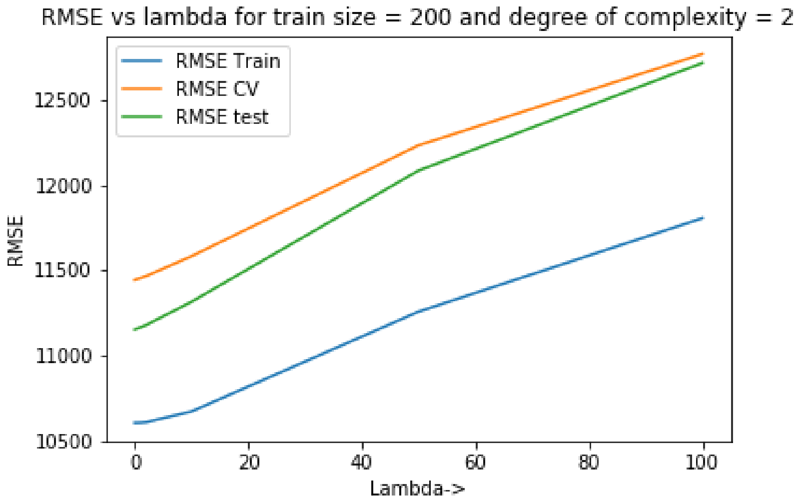


Figure 6: RMSE across λ; Sample size: 200, Degree: 2

Lambda	RMSE Train	RMSE CV	RMSE Test
0	10	10671.59	11468.19
0.5	9346.19	10611.41	11487.13
1	9361.17	10564.66	11516.49
2	9412.58	10503.67	11598.33
50	11897.56	11935.27	14729.56
100	12491.10	12420.38	15443.04

Table 4: Variation in RMSE values with lambda

2.3.3 Varying λ, Sample size of 500

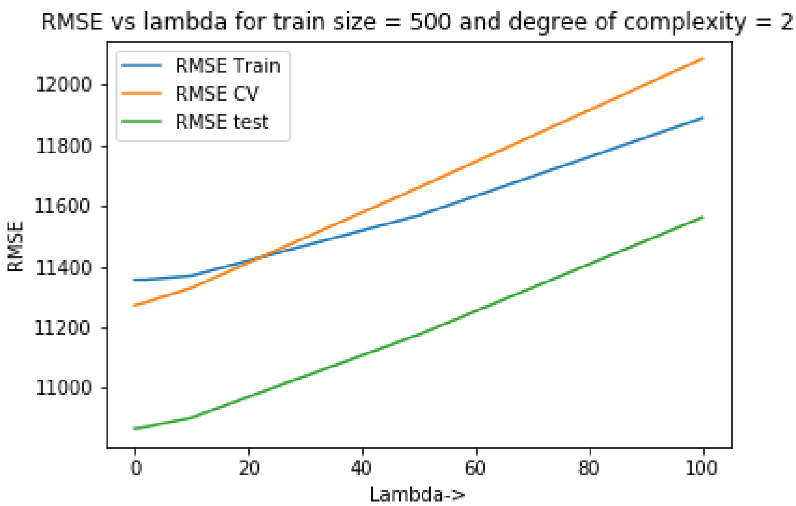


Figure 7: RMSE across λ; Sample size: 500, Degree: 2

2.4 Degree of complexity 3

With degree of complexity set to 3, for a particular data point,

$$y_i = \omega_0 + \omega_1 x_1 + \omega_2 x_2 + \omega_3 {x_1}^2 + \omega_4 {x_2}^2 + \omega_5 x_1.x_2 + \omega_6 {x_1}^3 + \omega_7 {x_2}^3 + \omega_8 {x_2}^2 x_1 + \omega_9 {x_1}^2 x_2 \quad (8)$$

2.4.1 Varying λ, Sample size of 50

After the above pre processing, The optimum parameter $\vec{\omega}$ is obtained for the following lambda values - $[0, 0.5, 1, 2, 10, 50, 100]$. The variation in RMSE across lambdas is as follows:

Lambda	RMSE Train	RMSE CV	RMSE Test
0.0	8407.761210828727	11960.392166857815	12390.588660098681
0.5	8414.299614637861	11743.19358761457	12329.126658336485
1.0	8431.988457444206	11558.772331311482	12293.299535838765
2.0	8491.472017549635	11270.79171291384	12280.362852665143
10.0	9240.199538933726	10757.219031210356	13112.100832682248
50.0	10876.901176573218	12040.04490493105	15628.464519645266
100.0	11379.791399813128	12642.949547533039	16474.271301190667

Table 5: Results obtained for Task 2

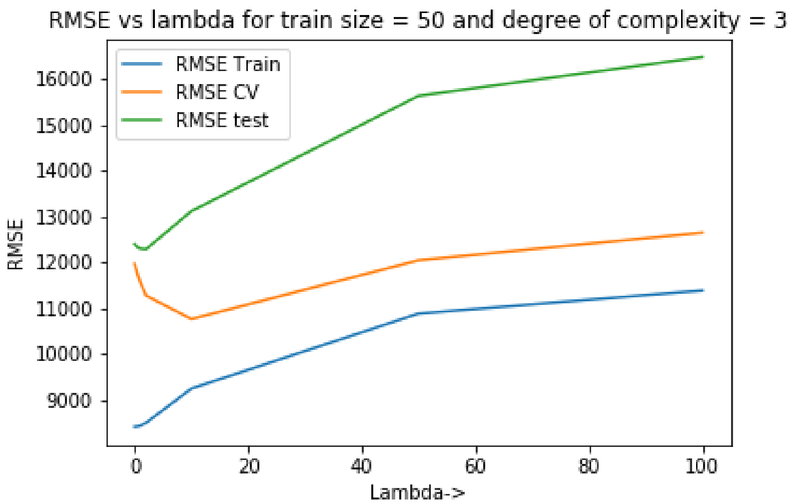


Figure 8: RMSE across λ; Sample size: 50, Degree: 3

2.4.2 Varying λ, Sample size of 200

The obtained results are:

Lambda	RMSE Train	RMSE CV	RMSE Test
0.0	10322.506441224592	11480.65137585371	11540.748956514151
0.5	10322.74337910385	11484.060426748905	11548.276365031981
1.0	10323.437876912261	11487.78843512935	11556.1380959018
2.0	10326.106384432025	11496.129590042878	11572.780261162094
10.0	10392.059429467075	11592.560024074122	11735.150238100397
50.0	10984.962331062083	12191.950852364467	12578.93878751002
100.0	11522.792243145757	12692.364674117875	13234.250404753897

Table 6: Results obtained for Task 2

Scatter plots of the model prediction using the regularization parameter value 0.01:

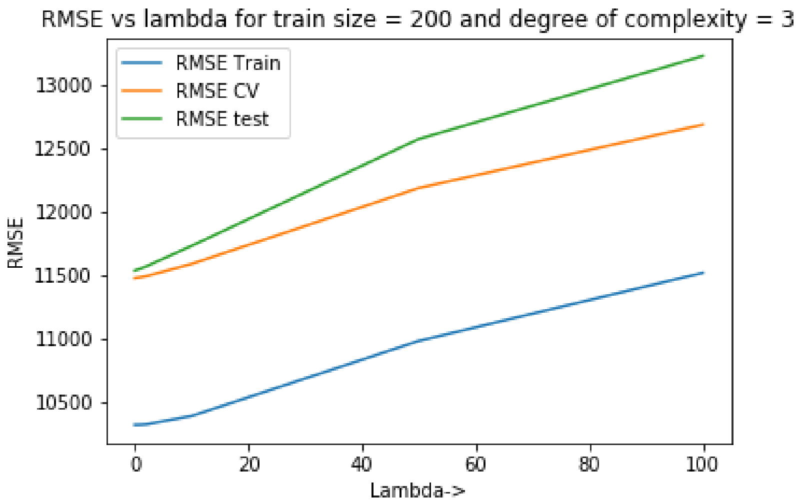


Figure 9: RMSE across λ; Sample size: 200, Degree: 3

2.4.3 Varying λ, Sample size of 500

The optimum parameter $\vec{\omega}$ is obtained for the following lambda values - $[0, 0.5, 1, 2, 10, 50, 100]$. The variation in RMSE across lambdas is as follows:

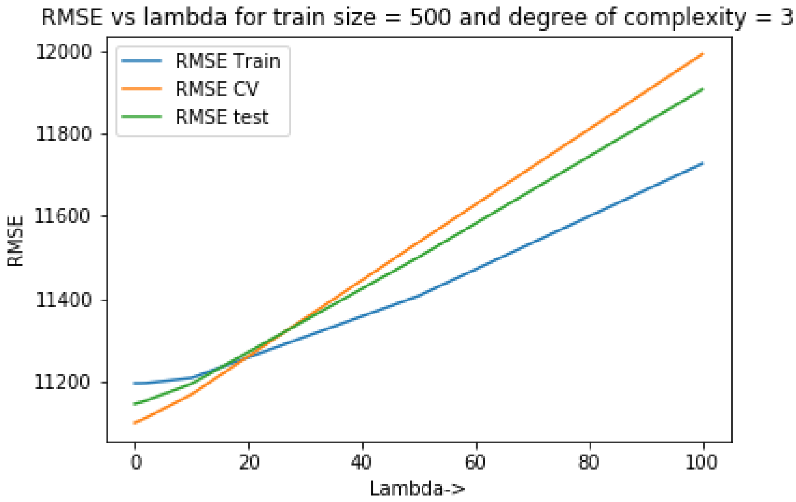


Figure 10: RMSE across λ; Sample size: 500, Degree: 3

2.5 Degree of complexity 6

With the degree of complexity 6,

$$y = \sum {x_1}^{\alpha} * {x_2}^{\beta} \tag{9}$$

Where $0 \leq \alpha + \beta \leq 6$.

2.5.1 Varying λ, Sample size of 50

Lambda	RMSE Train	RMSE CV	RMSE Test
0.0	1.3582344908807028e-07	1.3024937374699014e-07	2.736466435265001e-07
0.5	5.3224862846108924e-05	0.0006389419451237852	0.0011697424661700818
1.0	0.00010241277566647342	0.001259472447857696	0.0022735033897776087
2.0	0.00019571426483158983	0.002466786482370453	0.00436957859101229
10.0	0.0009066540184949185	0.011454915983379615	0.0195422946271592
50.0	0.004319989638299114	0.04968278699370095 4	0.08571221964007386
100.0	0.008418172149435164	0.09086562659012756	0.15931182940985875

Table 7: Results obtained for Task 2

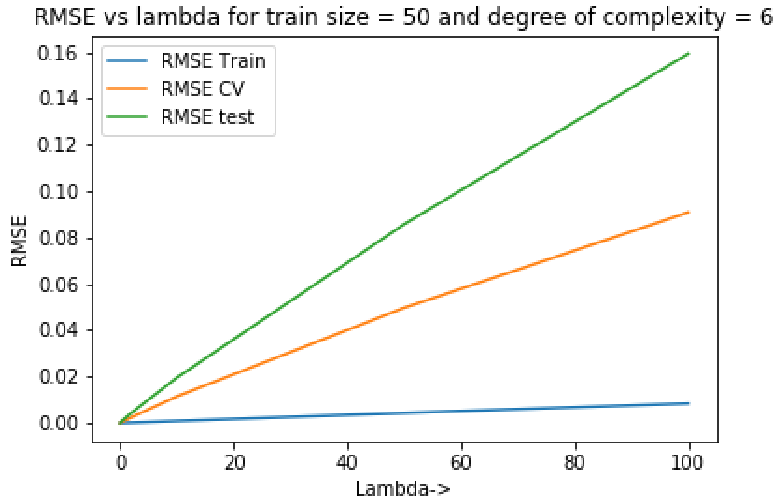


Figure 11: RMSE across λ; Sample size: 50, Degree: 6

2.5.2 Varying λ, Sample size of 200

Lambda	RMSE Train	RMSE CV	RMSE test
0.0	4.145074549079158e-08	4.5876133577776055e-08	4.438277930933977e-08
0.5	7.169634585154078e-06	9.351643870044926e-06	1.2226632701546666e-05
1.0	1.4193629639985923e-05	1.852785190860779e-05	2.42010151174377e-05
2.0	2.789871866381927e-05	3.649449750964621e-05	4.7603283521130243e-05
10.0	0.000128403762827723	0.0001679510933427838	0.000216489022423017
50.0	0.0005954210072570998	0.0007608482959799609	0.0009543646518816395
100.0	0.0011768765498580448	0.0014847238097789764	0.001842159446862891

Table 8: Results obtained for Task 2

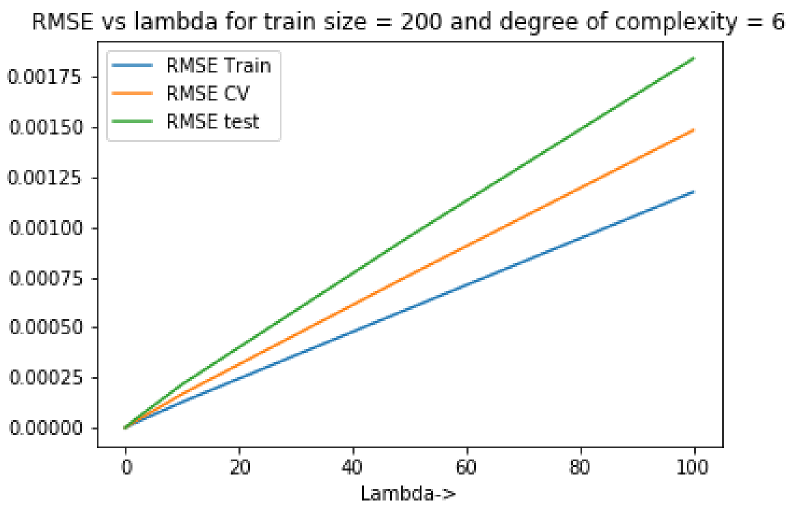


Figure 12: RMSE across λ; Sample size: 200, Degree: 6

2.5.3 Varying λ, Sample size of 500

Lambda	RMSE Train	RMSE CV	RMSE test
0.0	3.540887282123727e-08	3.741549292426492e-08	3.4517606283226707e-08
0.5	2.4891560253931053e-06	2.69805964526573e-06	2.5949552832042936e-06
1.0	4.963649710534798e-06	5.3778590424185165e-06	5.176457054060217e-06
2.0	9.866381792471788e-06	1.069014286492481e-05	1.0291657829414182e-05
10.0	4.744117748092903e-05	5.148944778527705e-05	4.9743962467771885e-05
50.0	0.00021913097081968563	0.00023736669064951702	0.00023193961964998602
100.0	0.00042714320882117563	0.00046046329475841634	0.00045296787349301 64

Table 9: Results obtained for Task 2

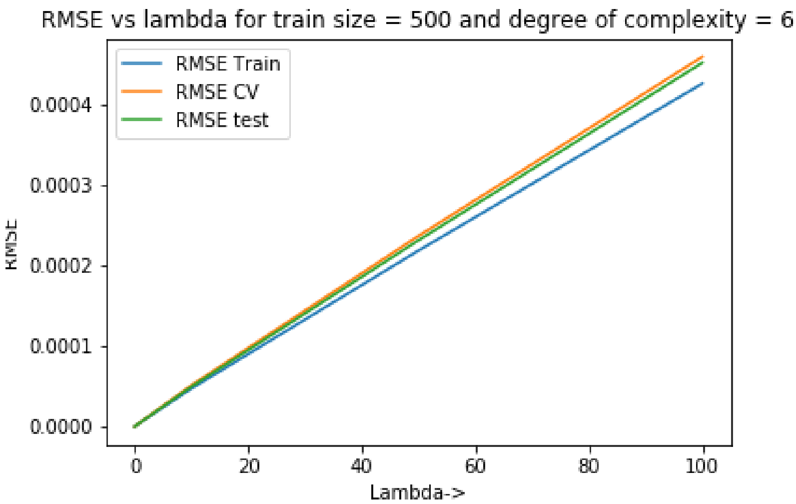


Figure 13: RMSE across λ; Sample size: 500, Degree: 6

2.6 Conclusion

The RMSE values are least over train data, cross-validation data as well as test data for degree of complexity = 6, train data size = 500 and regularization parameter, lambda =0.

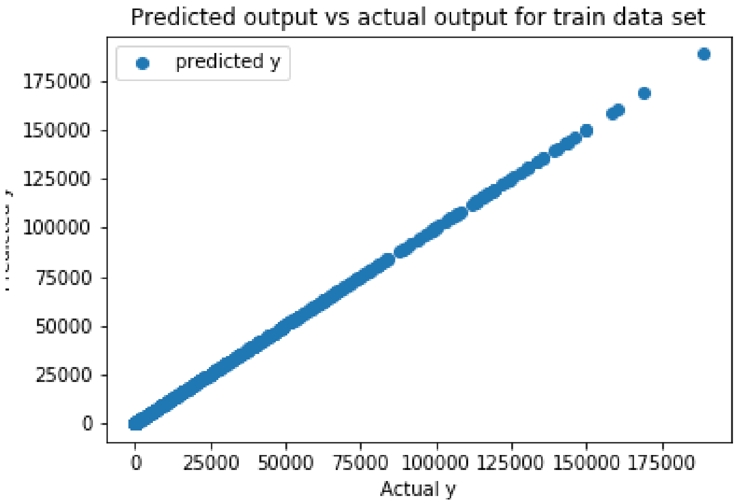


Figure 14: Predicted output, Actual values for Train Data

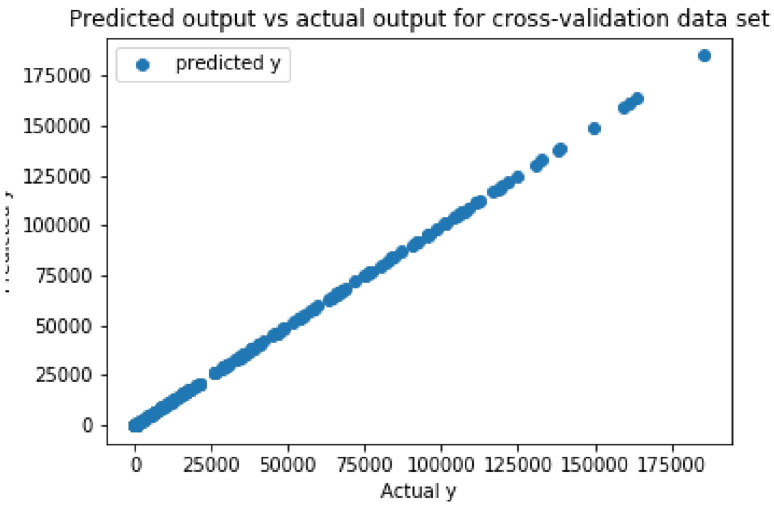


Figure 15: Predicted output, Actual values for CV Data

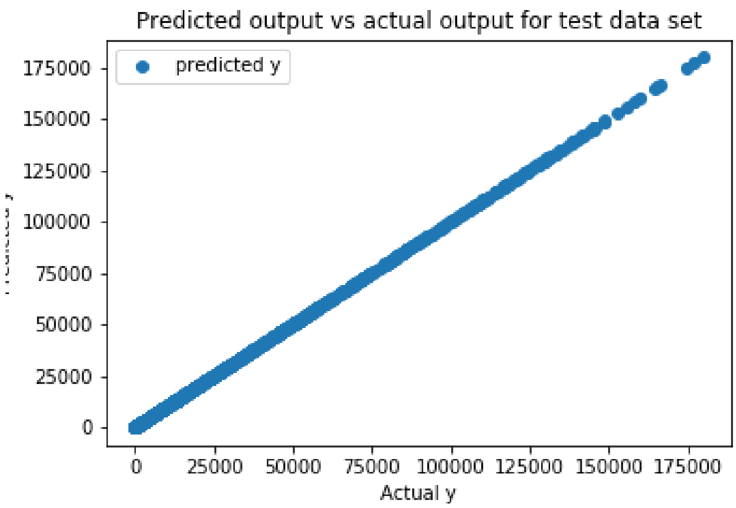


Figure 16: Predicted output, Actual values for Test Data

The surface plots of approximated functions superimposed with the scatter points are generated when the attached python code is run

3 Task 3

Linear regression using Gaussian basis function is given as

$$y(\vec{x}, \vec{w}) = \sum_{i=0}^{D-1} \omega_i \phi_i(\vec{x}) \tag{10}$$

, where D is a hyperparameter. The basis function

$$\phi_i = \exp\left(\frac{-|\vec{x} - \vec{\mu}_i|^2}{\sigma^2}\right) \tag{11}$$

where $i = 1, 2...D - 1$. The μ are the mean vectors for $D - 1$ kernels made from the data set. The value of the mean vectors are found using the KMeans clustering algorithm. In this work, the `sklearn` KMeans function was used. The optimum number of clusters for the dataset 2 - "`function_12d.csv`" was found to be 10 clusters. For the dataset 3 - "`1_bias_clean.csv`", the optimum number of clusters are 9.

3.1 No regularization

The following plots were obtained:

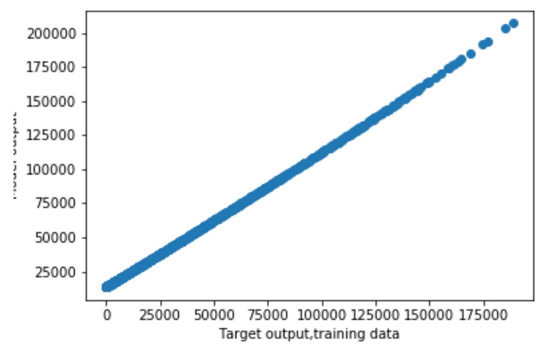


Figure 17: Scatter plot of the target values vs model prediction for Training set of Dataset 2, using linear regression with gaussian basis and no Regularization, $\lambda = 0.01$

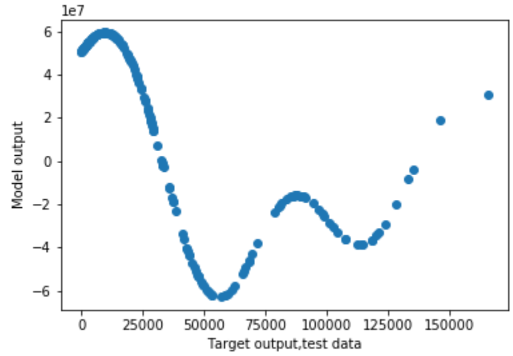


Figure 18: Scatter plot of the target values vs model prediction for Test set of Dataset 2, using linear regression with gaussian basis and no Regularization, $\lambda = 0.01$

3.2 Quadratic Regularization

Optimal parameters using quadratic regularization is given by $\vec{\omega^*}$ = $(\Phi^T\Phi + \lambda I)^{-1}\Phi^T\vec{t}$;

λ is the regularization parameter. The values $0.01, 0.1, 1.0, 5.0, 10.0$ were used to estimate the optimal parameters and the RMSE on the cross-validation set was calculated for each value. The best performing model was selected as the one having least RMSE on CV data

For dataset 2, the RMSE values for the Training, CV and Test data across λ values is:

Lambda	**RMSE Train**	**RMSE CV**	**RMSE Test**
0.01	3059.2231939706166	304419.6502059433	1309688.1097631603
0.1	2967.5181829927037	1260.488802049498	41195.93571016699
1.0	2990.3948869258456	1425.9232970077237	39596.78510421749
5.0	3013.546633117982	1503.9615829712025	39006.81341800579
10.0	3036.360553338793	1541.3504903884834	38684.11470986189

Table 10: Results obtained for Task 3

Scatter plots of the model prediction using the regularization parameter value 0.01:

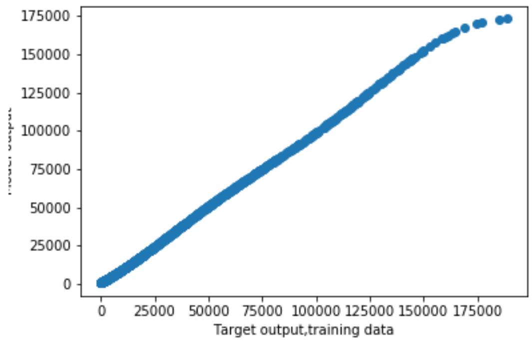


Figure 19: Scatter plot of the target values vs model prediction for Training set of Dataset 2, using linear regression with gaussian basis and quadratic Regularization, $\lambda = 0.01$

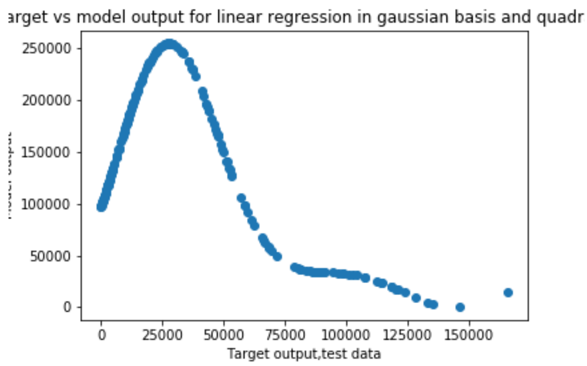


Figure 20: Scatter plot of the target values vs model prediction for Test set of Dataset 2, using linear regression with gaussian basis and quadratic Regularization, $\lambda = 0.01$

For dataset 3, the following RMSE table was obtained:

Lambda	RMSE Train	RMSE CV	RMSE Test
0.01	4929.01653053444	414848.3042013735	3312196.0992440097
0.1	4624.091536077471	1669.205290237633	36902.34473960538
1.0	4637.926167783597	2073.9375316355663	39568.04405922714
5.0	4652.374704231647	2257.2672544567195	40450.17809627787
10.0	4667.40003673528	2346.920490034092	40853.959722564214

Table 1: Results obtained for Task 3

The scatter plots of target vs model output for the optimum value of λ is, for "NTmin" output variable

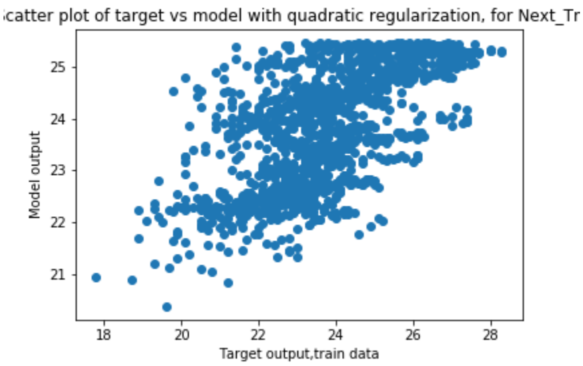


Figure 21: Scatter plot of the target values vs model prediction for Training set of Dataset 3, using linear regression with gaussian basis and quaadratic Regularization, $\lambda = 0.01$ for "NTmin" output variable

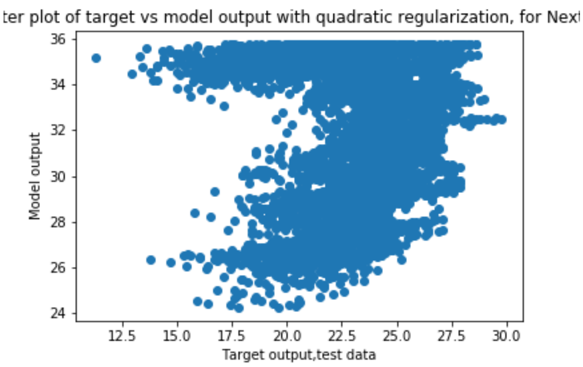


Figure 22: Scatter plot of the target values vs model prediction for Test set of Dataset 2, using linear regression with gaussian basis and quadratic Regularization, $\lambda = 0.01$, for "NTmin" output variable

For "NTmax":

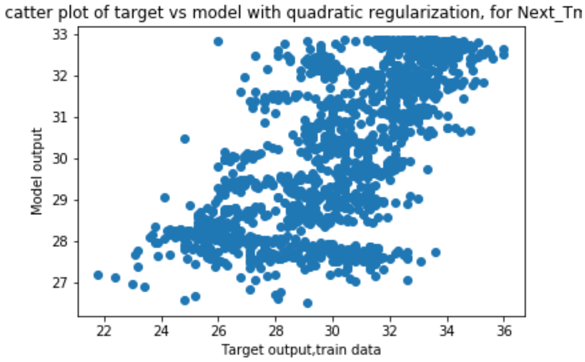


Figure 23: Scatter plot of the target values vs model prediction for Training set of Dataset 3, using linear regression with gaussian basis and quaadratic Regularization, $\lambda = 0.01$ for "NTmax" output variable

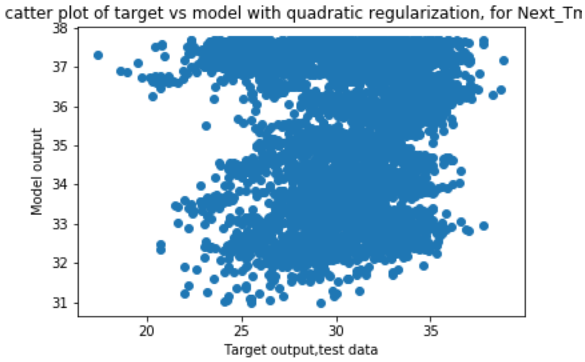


Figure 24: Scatter plot of the target values vs model prediction for Test set of Dataset 2, using linear regression with gaussian basis and quadratic Regularization, $\lambda = 0.01$, for "NTmax" output variable

3.3 Tikhonov Regularization

The Tikhonov regularization term is given by $\vec{\omega^*}$ = $(\Phi * T\Phi + \lambda\tilde{\Phi})^{-1}\Phi^T\vec{t}$. The $\tilde{\Phi}$ term is defined as

$$\tilde{\Phi} = [\tilde{\phi}]_{i,j=1}^{K} \tag{12}$$

where K is the number of clusters and λ is the regularization parameter. The values 0.01,0.1, 1.0,5.0,10.0 were used to estimate the optimal parameters and the RMSE on the cross-validation set was calculated for each value. The best peroming model was selected as the one having least RMSE on CV data

Applying Tikhonov regularization to the bivariate dataset, the optimal value of λ was estimated to be 0.01. The table for the RMSE values for the Training, CV and Test values corresponding to each λ value is

Lambda	RMSE Train	RMSE CV	RMSE test
0.01	78112040.25241715	80416219813.42682	43898825037.538
0.1	78629878.58895023	276304216179.1798	176596027875.55765
1.0	79471104.52781227	357583741029.9827	104372422450.83612
5.0	77593937.82583737	272444591755.6569	174802698267.85687
10.0	77693846.61754198	242869557997.72043	158196054705.92648

Table 1: Results obtained for Task 3

Scatter plots of the model prediction using the regularization parameter value 0.01:

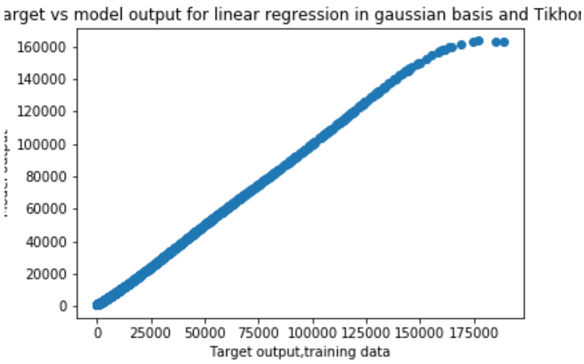


Figure 25: Scatter plot of the target values vs model prediction for Training set of Dataset 2, using linear regression with gaussian basis and Tikhonov Regularization, $\lambda = 0.01$

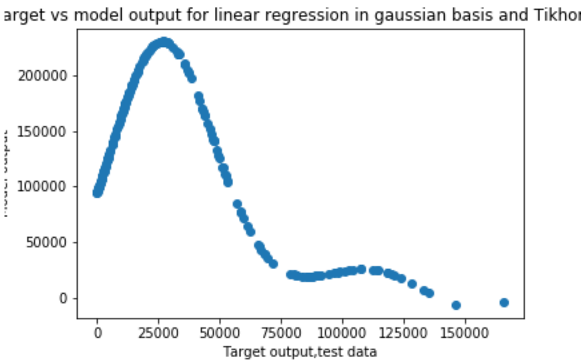


Figure 26: Scatter plot of the target values vs model prediction for Test set of Dataset 2, using linear regression with gaussian basis and Tikhonov Regularization, $\lambda = 0.01$

For Dataset 3, the table for the RMSE values for the Training, CV and Test values corresponding to each λ value corresonding to target variable ”NTmin” is

Lambda	RMSE Train	RMSE CV	RMSE test
0.01	4929.01653053444	414848.3042013735	3312196.0992440097
0.1	4624.091536077471	1669.205290237633	36902.34473960538
1.0	4637.926167783597	2073.9375316355663	39568.04405922714
5.0	4652.374704231647	2257.2672544567195	40450.17809627787
10.0	4667.40003673528	2346.920490034092	40853.959722564214

Table 1: Results obtained for Task 3

the optimal value of λ was estimated to be 0.1 for the target output "NTmin". The scatter plots obtained are Figures 27 and 28

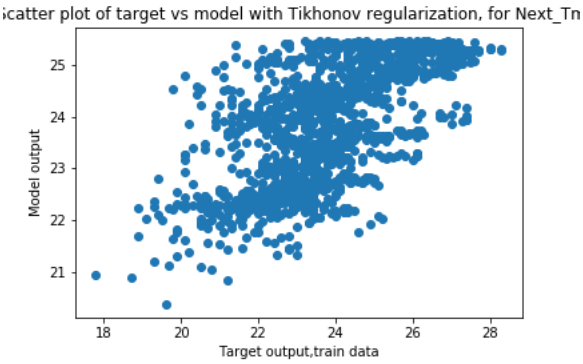


Figure 27: Scatter plot of the target values vs model prediction for Training set of Dataset 3, using linear regression with gaussian basis and Tikhonov Regularization, $\lambda = 0.1$

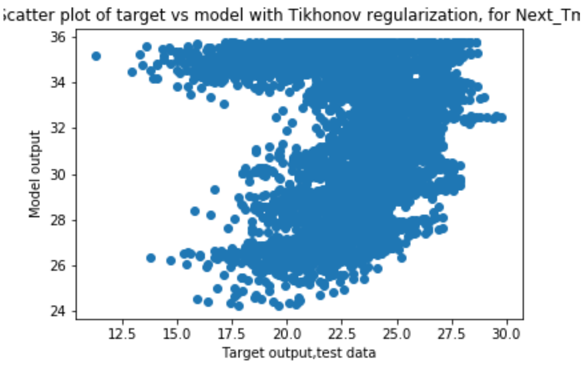


Figure 28: Scatter plot of the target values vs model prediction for Test set of Dataset 3, using linear regression with gaussian basis and Tikhonov Regularization, $\lambda = 0.01$

For the target output "NTmax" the following table of RMSE values for the training, test and CV data was obtained:

Lambda	RMSE Train	RMSE CV	RMSE test
0.01	4929.01653053444	414848.3042013735	3312196.0992440097
0.1	4624.091536077471	1669.205290237633	36902.34473960538
1.0	4637.926167783597	2073.9375316355663	39568.04405922714
5.0	4652.374704231647	2257.2672544567195	40450.17809627787
10.0	4667.40003673528	2346.920490034092	40853.959722564214

Table 1: Results obtained for Task 3

plots were obtained: figures 29 and 30.

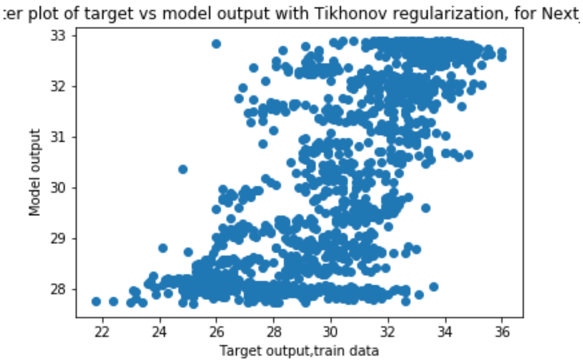


Figure 29: Scatter plot of the target values vs model prediction for Training set of Dataset 3, using linear regression with gaussian basis and Tikhonov Regularization, $\lambda = 0.1$

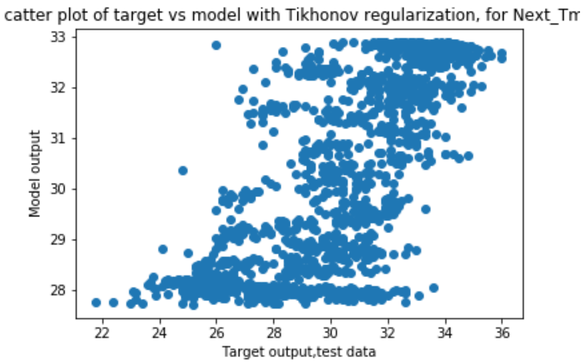


Figure 30: Scatter plot of the target values vs model prediction for Test set of Dataset 3, using linear regression with gaussian basis and Tikhonov Regularization, $\lambda = 0.1$