

# Machine Learning and optimization Project

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## 1 Question 1

In the first part of the problem our main motive is to compare different approaches of modelling such as different kernels, different GP configurations(different lengthscale and different variance). For the comparison we have used different train sets and test sets to evaluate the performances of each modeling approach. The measure of performances can be done by the use of RMSE, R2 score, MNLL, Std RMSE and as we know the best combinations from all is that which have the  $r^2$  value very near to 1 . In our sampling we have used 7 different kernels with lengthscales are 1, 0.1 ,10. And we also observed that with the increase in the number of points errors such as RMSE, MNLL and Std RMSE decreases for most of combinations but this is also increase for very few cases in which kernels not nicely fit to our problem.

kernel name	pts	ls	var	R2 score	RMSE	MNLL	Std RMSE
RBF	500	0.1	0.1	0.84283	0.68791	0.10725	0.02935
RBF	1000	0.1	0.1	0.86679	0.65473	0.10707	0.04700
RBF	500	0.1	1.0	0.87642	0.64487	0.11213	0.08539
RBF	1000	0.1	1.0	0.86914	0.64779	0.09686	0.04042
RBF	500	0.1	10.0	0.83817	0.73330	0.10363	0.08562
RBF	1000	0.1	10.0	0.87773	0.62982	0.08651	0.01935
RBF	500	1.0	0.1	0.85124	0.68034	0.10533	0.07726
RBF	1000	1.0	0.1	0.88125	0.60208	0.09464	0.02572
RBF	500	1.0	1.0	0.85462	0.67836	0.10975	0.08118
RBF	1000	1.0	1.0	0.88768	0.59401	0.09479	0.04439
RBF	500	1.0	10.0	0.85299	0.66042	0.10038	0.05158
RBF	1000	1.0	10.0	0.86256	0.66650	0.09453	0.05881
RBF	500	10.0	0.1	0.85599	0.65100	0.09348	0.06703
RBF	1000	10.0	0.1	0.88294	0.60353	0.09154	0.02451
RBF	500	10.0	1.0	0.83700	0.72030	0.09499	0.06603
RBF	1000	10.0	1.0	0.88938	0.59334	0.09290	0.04248
RBF	500	10.0	10.0	0.85359	0.70931	0.08560	0.04297
RBF	1000	10.0	10.0	0.88089	0.61582	0.09105	0.03352

Error observed using RBF kernels with different combination(length scale and variance), R2 score, RMSE, MNLL and standard RMSE are used. For error quantification best results are highlighted.

In this table we observe that RBF is fairly a good kernel for this problem. We choose 500 and 1000 sample points to start with and divide it into 80-20 percent. We also have a very similar result on varying the length scale and variance, hence not much is achieved while changing the parameters over a factor of 10, However we are using m.optimize, hence it automatically adjusts the values and much effect of the parameters cant be observed. Overall, if more samples are considered, RBF could reach to a very good fit, but will be costly. A GPU will be needed each time to fit it.

kernel name	pts	ls	var	R2 score	RMSE	MNLL	Std RMSE
Exp	500	0.1	0.1	0.82431	0.71470	0.28748	0.04010
Exp	1000	0.1	0.1	0.88872	0.60506	0.30230	0.03777
Exp	500	0.1	1.0	0.87777	0.64489	0.29223	0.05768
Exp	1000	0.1	1.0	0.88079	0.61486	0.30018	0.03161
Exp	500	0.1	10.0	0.84547	0.69000	0.29714	0.04264
Exp	1000	0.1	10.0	0.90946	0.52262	0.30433	0.03619
Exp	500	1.0	0.1	0.88900	0.59132	0.30543	0.05930
Exp	1000	1.0	0.1	0.89097	0.58174	0.30392	0.04903
Exp	500	1.0	1.0	0.86709	0.62865	0.30971	0.06908
Exp	1000	1.0	1.0	0.88941	0.60661	0.30046	0.04704
Exp	500	1.0	10.0	0.86992	0.64896	0.29768	0.04262
Exp	1000	1.0	10.0	0.89503	0.59042	0.30361	0.03667
Exp	500	10.0	0.1	0.87024	0.62915	0.29696	0.04428
Exp	1000	10.0	0.1	0.90925	0.54663	0.30159	0.01673
Exp	500	10.0	1.0	0.85649	0.65917	0.29600	0.04515
Exp	1000	10.0	1.0	0.87394	0.62449	0.29330	0.03062
Exp	500	10.0	10.0	0.84426	0.70316	0.29287	0.06494
Exp	1000	10.0	10.0	0.89711	0.57742	0.29386	0.02796

Error observed using Exponential kernels with different combination(lengthscale and variance), R2 score, RMSE, MNLL and standard RMSE are used. For error quantification best results are highlighted.

Exponential kernel gives better results than the RBF kernel, we are judging better results by R2 score, which is the most recognized error estimate for regression problems. There is no desired value of R2 score to be reached but a score closer to one gives the user a confidence that his fit is good. This case also has the same effects of parameters as the RBF case.

kernel name	pts	ls	var	R2 score	RMSE	MNLL	Std RMSE
Mat32	500	0.1	0.1	0.86166	0.65756	0.21210	0.04351
Mat32	1000	0.1	0.1	0.88871	0.60455	0.19457	0.02393
Mat32	500	0.1	1.0	0.86305	0.65934	0.21744	0.06009
Mat32	1000	0.1	1.0	0.90046	0.56331	0.20948	0.02700
Mat32	500	0.1	10.0	0.86772	0.62160	0.21194	0.06963
Mat32	1000	0.1	10.0	0.90556	0.56019	0.21430	0.03279
Mat32	500	1.0	0.1	0.83532	0.72865	0.19824	0.09471
Mat32	1000	1.0	0.1	0.90164	0.55424	0.22347	0.06132
Mat32	500	1.0	1.0	0.85627	0.64921	0.19143	0.04993
Mat32	1000	1.0	1.0	0.89432	0.58666	0.20902	0.05284
Mat32	500	1.0	10.0	0.87433	0.63001	0.21923	0.04802
Mat32	1000	1.0	10.0	0.87292	0.64179	0.20135	0.03977
Mat32	500	10.0	0.1	0.86575	0.63491	0.21152	0.08523
Mat32	1000	10.0	0.1	0.89049	0.58283	0.22233	0.03749
Mat32	500	10.0	1.0	0.86069	0.64932	0.21969	0.05768
Mat32	1000	10.0	1.0	0.88311	0.62394	0.20971	0.04286
Mat32	500	10.0	10.0	0.83698	0.70185	0.20869	0.03379
Mat32	1000	10.0	10.0	0.89391	0.58531	0.20781	0.05013

Error observed using RBF kernels with different combination(lengthscale and variance), Matern32 score, RMSE, MNLL and standard RMSE are used. For error quantification best results are highlighted.

Matern32 kernel gives good values of fit at low length scale combined with a high variance, the standard root mean square error also follows the desired property that it should be less than the RMSE. We also have a property that fit on 1000 points is better than the fit on 500 points, which means the choice of the kernel is suitable and the fit is extremely good at most of the places. However there is not a sharp rise in the R2 score when points are doubled, it means there are some areas where data is not approximated well.

kernel name	pts	ls	var	R2 score	RMSE	MNLL	Std RMSE
Mat52	500	0.1	0.1	0.85883	0.66092	0.17642	0.06594
Mat52	1000	0.1	0.1	0.90758	0.56094	0.18016	0.06769
Mat52	500	0.1	1.0	0.85830	0.65612	0.16428	0.02897
Mat52	1000	0.1	1.0	0.88556	0.61102	0.16301	0.02219
Mat52	500	0.1	10.0	0.85859	0.68046	0.15526	0.07536
Mat52	1000	0.1	10.0	0.88699	0.59882	0.15444	0.03674
Mat52	500	1.0	0.1	0.87779	0.62298	0.17951	0.06358
Mat52	1000	1.0	0.1	0.86939	0.64044	0.17554	0.03485
Mat52	500	1.0	1.0	0.88054	0.58881	0.18552	0.11465
Mat52	1000	1.0	1.0	0.90714	0.55446	0.17467	0.02174
Mat52	500	1.0	10.0	0.86197	0.66137	0.19046	0.03779
Mat52	1000	1.0	10.0	0.88754	0.58193	0.16701	0.03415
Mat52	500	10.0	0.1	0.83404	0.71988	0.16444	0.06412
Mat52	1000	10.0	0.1	0.89584	0.57779	0.16668	0.02818
Mat52	500	10.0	1.0	0.85539	0.66901	0.18099	0.02863
Mat52	1000	10.0	1.0	0.89045	0.58911	0.17434	0.03218
Mat52	500	10.0	10.0	0.85185	0.68602	0.17482	0.11884
Mat52	1000	10.0	10.0	0.89983	0.57698	0.17536	0.03322

Error observed using Matern52 kernels with different combination(lengthscale and variance), R2 score, RMSE, MNLL and standard RMSE are used. For error quantification best results are highlighted.

Matern52 shows a remarkable difference with the Matern32, that is the results are best when both the lengthscale and variance is low. This means less peaks are required by the second order differentiable function to approximate the booster function whereas more peaks are required by the first order differentiable function to fit the data.

kernel name	pts	ls	var	R2 score	RMSE	MNLL	Std RMSE
Exp+M32	500	0.1	0.1	0.87786	0.62810	0.25175	0.06096
Exp+M32	1000	0.1	0.1	0.87846	0.63743	0.27642	0.02544
Exp+M32	500	0.1	1.0	0.86321	0.66816	0.27566	0.03040
Exp+M32	1000	0.1	1.0	0.89669	0.58483	0.27844	0.07460
Exp+M32	500	0.1	10.0	0.88650	0.62016	0.26595	0.02690
Exp+M32	1000	0.1	10.0	0.87976	0.59945	0.28732	0.04420
Exp+M32	500	1.0	0.1	0.87247	0.64634	0.28153	0.05008
Exp+M32	1000	1.0	0.1	0.90047	0.56983	0.29635	0.03777
Exp+M32	500	1.0	1.0	0.88732	0.59734	0.29494	0.04516
Exp+M32	1000	1.0	1.0	0.90639	0.54002	0.30186	0.02720
Exp+M32	500	1.0	10.0	0.84619	0.68768	0.28074	0.03885
Exp+M32	1000	1.0	10.0	0.88921	0.59995	0.28687	0.02503
Exp+M32	500	10.0	0.1	0.86520	0.66791	0.24997	0.03580
Exp+M32	1000	10.0	0.1	0.89966	0.55933	0.22547	0.04413
Exp+M32	500	10.0	1.0	0.84432	0.69011	0.22758	0.05412
Exp+M32	1000	10.0	1.0	0.87878	0.63902	0.22672	0.02939
Exp+M32	500	10.0	10.0	0.85890	0.66873	0.21989	0.08071
Exp+M32	1000	10.0	10.0	0.91559	0.53117	0.22687	0.04395

Error observed using Exponential+M32 kernels with different combination(lengthscale and variance), R2 score, RMSE, MNLL and standard RMSE are used. For error quantification best results are highlighted.

We now try a guess to add the Exponential kernel and the Matern32 function, as we observed we need a high variance to fit the data, and we get the same result. A high lengthscale is also needed in this case because of the exponential function.

kernel name	pts	ls	var	R2 score	RMSE	MNLL	Std RMSE
M52*RBF	500	0.1	0.1	0.84811	0.67704	0.18697	0.06817
M52*RBF	1000	0.1	0.1	0.88086	0.61822	0.17519	0.05866
M52*RBF	500	0.1	1.0	0.84911	0.68811	0.17345	0.05219
M52*RBF	1000	0.1	1.0	0.86920	0.66004	0.15261	0.02731
M52*RBF	500	0.1	10.0	0.88082	0.60672	0.17307	0.06903
M52*RBF	1000	0.1	10.0	0.89026	0.60922	0.16295	0.03251
M52*RBF	500	1.0	0.1	0.87882	0.63020	0.18200	0.04477
M52*RBF	1000	1.0	0.1	0.90353	0.56771	0.17681	0.03259
M52*RBF	500	1.0	1.0	0.86653	0.65585	0.17483	0.02630
M52*RBF	1000	1.0	1.0	0.90669	0.54171	0.17949	0.05095
M52*RBF	500	1.0	10.0	0.89088	0.59123	0.17907	0.04817
M52*RBF	1000	1.0	10.0	0.90452	0.54962	0.16507	0.04630
M52*RBF	500	10.0	0.1	0.86159	0.66368	0.18149	0.05352
M52*RBF	1000	10.0	0.1	0.89130	0.59609	0.16376	0.01426
M52*RBF	500	10.0	1.0	0.86956	0.64317	0.17958	0.08067
M52*RBF	1000	10.0	1.0	0.87805	0.62143	0.17710	0.06333
M52*RBF	500	10.0	10.0	0.86213	0.66745	0.15652	0.07453
M52*RBF	1000	10.0	10.0	0.89591	0.58045	0.17955	0.02549

Error observed using M52\*RBF kernels with different combination(lengthscale and variance), R2 score, RMSE, MNLL and standard RMSE are used. For error quantification best results are highlighted.

We now try a new kernel Matern52 product with RBF, as we can make a guess that low variance as compared to the Matern32 value should be good with this, it comes out to be true. Very good values of R2 score are observed in general.

kernel name	pts	ls	var	R2 score	RMSE	MNLL	Std RMSE
Exp+RBF	500	0.1	0.1	0.85159	0.67709	0.27678	0.04326
Exp+RBF	1000	0.1	0.1	0.90152	0.55204	0.29381	0.03203
Exp+RBF	500	0.1	1.0	0.86841	0.64169	0.29044	0.04605
Exp+RBF	1000	0.1	1.0	0.88193	0.59507	0.29184	0.04891
Exp+RBF	500	0.1	10.0	0.86999	0.61748	0.29482	0.03867
Exp+RBF	1000	0.1	10.0	0.89485	0.59442	0.29006	0.04349
Exp+RBF	500	1.0	0.1	0.89710	0.57461	0.28661	0.04112
Exp+RBF	1000	1.0	0.1	0.88224	0.61559	0.29722	0.01925
Exp+RBF	500	1.0	1.0	0.87219	0.65022	0.26917	0.05402
Exp+RBF	1000	1.0	1.0	0.88494	0.60293	0.29361	0.01369
Exp+RBF	500	1.0	10.0	0.88073	0.59334	0.28472	0.05993
Exp+RBF	1000	1.0	10.0	0.89834	0.57735	0.28273	0.04122
Exp+RBF	500	10.0	0.1	0.87260	0.63284	0.27844	0.07450
Exp+RBF	1000	10.0	0.1	0.89014	0.59406	0.28919	0.05952
Exp+RBF	500	10.0	1.0	0.84972	0.66180	0.27939	0.05610
Exp+RBF	1000	10.0	1.0	0.88655	0.60151	0.28508	0.04149
Exp+RBF	500	10.0	10.0	0.83283	0.69272	0.28705	0.03904
Exp+RBF	1000	10.0	10.0	0.88838	0.60101	0.28705	0.03641

Error observed using Exponential+RBF kernels with different combination(lengthscale and variance), R2 score, RMSE, MNLL and standard RMSE are used. For error quantification best results are highlighted.

We now try a new kernel exponential addition with RBF, as we can make a guess that low variance as compared to the Matern32 value should be good with this, it comes out to be true. Very good values of R2 score are observed in general.



kernel name	pts	ls	var	R2 score	RMSE	MNLL	Std RMSE
RBF	1000	10.0	1.0	0.88938	0.59334	0.09290	0.04248
Exp	1000	10.0	0.1	0.90925	0.54663	0.30159	0.01673
Mat32	1000	0.1	10.0	0.90556	0.56019	0.21430	0.03279
Mat52	1000	0.1	0.1	0.90758	0.56094	0.18016	0.06769
M52*RBF	1000	1.0	10.0	0.90452	0.54962	0.16507	0.04630
Exp+M32	1000	10.0	10.0	0.91559	0.53117	0.22687	0.04395
Exp+RBF	1000	0.1	0.1	0.90152	0.55204	0.29381	0.03203

The best from the table is Exp+M32

This table shows all the best possible combinations of above kernels and from that we observed that the best configurations are lengthscale and variance is 10 for Exp+M32.

## 2 Part 2 BO

In this part we have to optimize the booster function to calculate its optima, optimum values of booster function are tuff to calculate because the function is a black box function and is not easy to compute, only selected values are tranfered to the function to calculate the value over them as explicit calculation at all points is not possible. We use 5 acquisition function of Bayesian optimisation to calculate the optimum values of the function. Acquisition functions are mathematical techniques that guide how the parameter space should be explored during Bayesian optimization. They use the predicted mean and predicted variance generated by the Gaussian process model. The predicted variance is very close to zero at or very near to an existing result. The first three tables of Probability improvement, UCB, direct approach are not considered constraints and rest two cases consider constraints.

iter	x1	x2	x3	x4	y
10	0.288	0.016	0.322	0.891	4.536
20	0.727	0.513	0.164	0.957	4.820
30	0.357	0.936	0.403	0.962	5.114
40	0.425	0.869	0.176	0.711	5.102
50	0.468	0.751	0.086	0.775	5.208
60	0.486	0.670	0.337	0.973	5.038

EI

The first approach we use is the Expected Improvement approach, it is one of the most used approaches of Bayesian optimization to calculate the optima. We perform the calculation on 20 points and add upto 60 points in the sample space. The results seem to converge near 5 and indicate the convergence. The convergence plots of part 2 can be found with the attached file and they show convergence.

iter	x1	x2	x3	x4	y
10	0.336	0.713	0.107	0.779	5.181
20	0.227	0.657	0.167	0.746	5.083
30	0.426	0.949	0.323	0.948	5.212
40	0.427	0.250	0.163	0.986	5.099
50	0.879	0.966	0.069	0.778	5.055
60	0.189	0.413	0.273	0.915	5.265

PI

The second approach we use is the probability improvement, In this case also, the convergence value is near to the one in case of EI, which solidifies our belief that the results are robust.

iter	x1	x2	x3	x4	y
10	0.215	0.332	0.120	0.756	5.196
20	0.157	0.659	0.268	0.906	5.175
30	0.221	0.344	0.366	0.811	4.897
40	0.314	0.674	0.234	0.917	5.324
50	0.218	0.418	0.194	0.999	5.480
60	0.985	0.998	0.114	0.974	5.143

UCB

The third approach we use is the UCB, In this case also, the convergence value is near to the one in case of EI, which solidifies our belief that the results are robust.

iter	x1	x2	x3	x4	y
10	0.262	0.283	0.118	0.889	5.367
20	0.217	0.413	0.202	0.907	5.353
30	0.483	0.779	0.135	0.772	5.210
40	0.374	0.675	0.253	0.911	5.254
50	0.180	0.211	0.181	0.786	5.193
60	0.171	0.468	0.177	0.784	5.157

Direct approach

The fourth approach we use is the direct approach, In this case also, the convergence value is near to the one in case of EI, which solidifies our belief that the results are robust.

iter	x1	x2	x3	x4	y
10	0.328	0.615	0.402	1.000	5.093
20	0.264	0.389	0.152	0.995	5.503
30	0.801	0.889	0.081	0.904	5.236
40	0.433	0.920	0.121	0.909	5.383
50	0.597	0.882	0.261	0.967	5.201
60	0.220	0.161	0.026	0.935	5.140

POF The fifth approach we use is POF, In this case also, the convergence value is near to the one in case of EI, which solidifies our belief that the results are robust.