A PRELIMINARY STUDY ON DISCRETIZED BBOB PROBLEMS

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This problem set is constructed by discretizing the well-known Black-Box Optimization Benchmark noiseless (BBOB-noiseless) [1] as the original BBOB-noiseless focuses on continuous *minimization* problems. The original BBOB-noiseless problem set contains 24 specifically designed noise-free-problems which can be classified into five categories with respect to their properties e.g. degree of conditioning and structural characteristics [1]. Each of these problem challenges a search algorithm from unique perspectives and is capable of suggesting the effectiveness of an algorithm in handling similar problems. More details regarding definition and property of these problems can be found in [1]. The utilized discretization method in our study is proposed in and implemented by [2]. More concrete explanations can be found in [3].

An independent preliminary study is carried out to identify the capability of all the implemented surrogate models (see Table 1) in fitting the created discretized BBOB problems. The first five problems (P1 to P5) are not taken into considerations for the reason that they are separable functions, which means the search process on these problems can be simply reduced to multiple one-dimensional search procedures [1]. Thus, our interest is on the other 19 non-separable functions (P6 to P24) that are more complex and more difficult to solve. For each function between F9 to F24, 500 data samples (input solutions and their output, i.e., values of objective function for these solutions) are generated by performing Latin hyper cube sampling. The data samples are later utilized to test the performance (using R^2 score) of surrogate models through a 5-fold cross-validation. The whole procedure is then repeated twice with different data samples to obtain more reliable outcomes. R^2 score is chosen since it is independent from the scale of problems.

Through the proportion of explained variance, R^2 score can suggest goodness of fit of a surrogate model and, as a result, a measure of how well the model is likely to predict unseen landscape of a problem. Generally speaking, the closer the score is to one, the better the surrogate model performs. A heat map is shown in Figure 1 describing the results (mean R^2 score over three repetitions of 5-fold cross-validation) obtained by each surrogate model on 19 discretized BBOB functions. The purple cells are cases where surrogate models obtained a mean R^2 score larger than 0. The raw scores are given in Table. 1. It is possible to roughly categorize the discretized BBOB problems into three groups based on the wellness of fitting of the implemented surrogates:

Good (G) Most of the surrogates obtained R^2 scores greater than 0.5 on **problems 6, 7, 8, 10, 11, 13, 15 and 20**, which suggests that these models can extrapolate unseen landscapes of problems from available data samples.

Moderate (M) Most of the surrogates obtained R^2 scores that are greater than 0 but less than 0.5 on **problems 12, 14, 17, 18 and 24**, whereas the other models only got negative scores. It means that surrogate are capable of explaining some landscapes of the problems.

Bad (B) It seems to be very hard for surrogate models to interpolate **problems 9, 16, 19, 21, 22, 23** as nearly all models acquired negative R^2 scores. Considering the modality of problems, except for the problem 9 which is uni-modal, the other 5 are all multi-modal problems.

The Selected Problems

Given the results of preliminary study, all the six *bad* problems are chosen since it is important to study the performance of a surrogate assisted algorithm (SAMA-DiEGO) if its back-end surrogate(s) struggle with interpolating problems. Moreover, nine out of thirteen *simple* and *moderate* problems are randomly sampled into the test problems. The full list of fifteen test problems are given below, the capital letter G, M, B is the wellness of fitting as described in previous section.

Table 1: R^2 scores obtained by 31 surrogate models on discretized BBOB problems. Each score is the average of 15 scores gathered from three repetitions of a 5-fold cross-validation. The full names of abbreviations in *Specification* column can be found in Appendix.

Model Family	ID	Specification	P6	P7	P8	P9	P10	P11	P12	P13	P14
Kriging	1	Constant + SGC	0.866	0.902	0.765	-0.071	0.899	0.922	0.294	0.919	0.532
	2	Linear + SGC	0.840	0.902	0.799	-0.092	0.897	0.925	0.218	0.912	0.520
	3	Constant + Matern52	0.867	0.900	0.790	-0.104	0.896	0.929	0.169	0.915	0.478
	4	Constant + Matern32	0.866	0.887	0.829	-0.100	0.894	0.942	0.165	0.907	0.495
	5	Linear + Matern52	0.815	0.897	0.814	-0.042	0.888	0.932	0.161	0.904	0.403
	6	Linear + OUP	0.812	0.699	0.894	-0.048	0.733	0.941	0.249	0.829	0.421
	7	Quadratic + OUP	0.777	0.868	0.736	-1.560	0.880	0.900	-0.417	0.894	0.007
	8	Constant + OUP	0.826	0.714	0.897	-0.069	0.743	0.942	0.308	0.831	0.420
	9	Linear + Gower	0.801	0.669	0.892	-0.427	0.705	0.937	0.147	0.822	0.247
	10	Linear + Matern32	0.818	0.885	0.817	-0.062	0.891	0.939	0.139	0.891	0.403
	11	Constant + Gower	0.815	0.681	0.895	-0.357	0.712	0.939	0.196	0.826	0.256
	12	Quadratic + Gower	0.752	0.860	0.720	-1.903	0.860	0.882	-1.041	0.867	-0.284
	13	Quadratic + Matern52	0.632	0.789	0.349	-3.092	0.804	0.801	-1.207	0.817	-0.708
	14	Quadratic + Matern32	0.647	0.799	0.473	-2.213	0.838	0.839	-0.958	0.860	-0.361
	15	Quadratic + SGC	0.611	0.782	0.317	-3.114	0.797	0.822	-1.644	0.805	-0.759
RBF Interpolation	1	Thin Plate Spline	0.881	0.863	0.714	-0.050	0.846	0.904	0.389	0.908	0.594
	2	Multiquadric	0.863	0.767	0.699	0.037	0.731	0.857	0.406	0.864	0.544
	3	Linear	0.863	0.767	0.699	0.037	0.731	0.857	0.406	0.864	0.544
	4	Cubic	0.866	0.881	0.624	-0.472	0.895	0.921	0.249	0.867	0.511
	5	Polyharmonic spline 4	0.815	0.893	0.565	-0.916	0.895	0.894	-0.206	0.904	0.246
	6	Invmultiquadric	0.808	0.567	0.669	0.023	0.491	0.758	0.289	0.778	0.358
	7	Invquadric	0.807	0.567	0.669	0.023	0.491	0.758	0.288	0.778	0.358
	8	Gaussian function	0.807	0.567	0.669	0.023	0.491	0.758	0.288	0.778	0.358
	9	Polyharmonic spline 5	-0.391	-51.558	-8.708	-14.586	-5.401	-1367661.901	-187.263	-6.520	-7.458
SVM Regression	1	poly 2	0.811	0.765	0.671	-0.084	0.666	0.720	0.407	0.804	0.495
	2	linear	0.797	0.556	0.666	0.019	0.510	0.745	0.327	0.774	0.396
	3	poly 2	0.739	0.696	0.653	-0.488	0.503	0.526	0.050	0.706	0.177
	4	rbf	0.726	0.642	0.630	0.069	0.574	0.640	0.321	0.755	0.436
	5	poly 5	0.392	0.298	0.499	-0.797	-0.539	-0.305	-0.116	0.234	-0.611
	6	sigmoid	-0.116	-0.665	-1.020	-0.215	-0.877	-0.933	-0.421	-0.247	-0.446
Random Forest Regression		100 decision trees	0.611	0.441	0.764	-0.035	0.354	0.672	0.106	0.549	0.298

Model Family	ID	Specification	P15	P16	P17	P18	P19	P20	P21	P22	P23	P24
Kriging	1	Constant + SGC	0.846	-0.170	0.684	0.672	-0.148	0.900	-0.047	-0.141	-0.168	0.290
	2	Linear + SGC	0.852	-0.169	0.683	0.691	-0.136	0.912	-0.026	-0.105	-0.215	0.141
	3	Constant + Matern52	0.846	-0.120	0.653	0.664	-0.092	0.913	-0.128	-0.225	-0.110	0.080
	4	Constant + Matern32	0.844	-0.099	0.622	0.682	-0.069	0.928	-0.097	-0.205	-0.118	0.161
	5	Linear + Matern52	0.845	-0.179	0.585	0.643	-0.042	0.891	-0.125	-0.021	-0.209	0.045
	6	Linear + OUP	0.844	-0.167	0.639	0.679	-0.103	0.937	0.038	0.022	-0.180	0.036
	7	Quadratic + OUP	0.758	-2.440	0.126	0.393	-1.821	0.845	-1.494	-1.527	-2.619	-0.079
	8	Constant + OUP	0.836	-0.089	0.632	0.684	-0.074	0.939	0.003	-0.035	-0.117	0.106
	9	Linear + Gower	0.822	-0.723	0.527	0.636	-0.414	0.938	-0.377	-0.393	-0.728	-0.143
	10	Linear + Matern32	0.847	-0.169	0.614	0.677	-0.090	0.928	-0.063	0.015	-0.199	0.010
	11	Constant + Gower	0.823	-0.669	0.543	0.648	-0.376	0.939	-0.334	-0.379	-0.666	-0.070
	12	Quadratic + Gower	0.721	-3.351	0.005	0.252	-2.514	0.858	-1.919	-1.985	-3.215	-0.347
	13	Quadratic + Matern52	0.647	-4.310	-0.289	0.062	-3.474	0.747	-3.007	-2.895	-5.388	-1.269
	14	Quadratic + Matern32	0.604	-3.276	-0.220	0.203	-2.698	0.780	-2.131	-2.396	-4.103	-0.782
	15	Quadratic + SGC	0.611	-4.069	-0.258	0.136	-3.263	0.756	-3.243	-3.209	-4.585	-0.748
RBF Interpolation	1	Thin Plate Spline	0.844	-0.324	0.619	0.695	-0.168	0.845	0.012	0.043	-0.393	0.392
	2	Multiquadric	0.799	-0.141	0.587	0.646	-0.047	0.794	0.100	0.144	-0.189	0.314
	3	Linear	0.799	-0.141	0.587	0.646	-0.046	0.794	0.100	0.144	-0.189	0.314
	4	Cubic	0.833	-0.683	0.544	0.685	-0.731	0.833	-0.249	-0.367	-0.810	-0.022
	5	Polyharmonic spline 4	0.801	-1.668	0.363	0.529	-1.367	0.867	-0.838	-0.988	-1.823	0.005
	6	Invmultiquadric	0.702	-0.076	0.441	0.485	-0.035	0.711	0.054	0.120	-0.108	0.089
	7	Invquadric	0.702	-0.076	0.441	0.485	-0.035	0.711	0.053	0.120	-0.108	0.089
	8	Gaussian function	0.702	-0.076	0.441	0.485	-0.035	0.711	0.053	0.120	-0.108	0.089
	9	Polyharmonic spline 5	-1.898	-146231.756	-19.007	-3.038	-169.010	-5.618	-357.175	-1057.016	-26.085	-116.984
SVM Regression	1	poly 2	0.766	-0.242	0.452	0.527	-0.099	0.726	0.069	0.151	-0.317	0.345
	2	linear	0.707	-0.074	0.472	0.501	-0.016	0.699	0.056	0.166	-0.137	0.054
	3	poly 2	0.666	-0.752	0.094	0.211	-0.554	0.606	-0.289	-0.372	-0.823	0.318
	4	rbf	0.652	-0.077	0.416	0.496	0.016	0.683	0.139	0.157	-0.097	0.260
	5	poly 5	0.222	-0.859	-1.182	-0.989	-1.551	-0.051	-1.016	-1.207	-1.236	0.118
	6	sigmoid	-0.159	-0.154	-1.272	-1.198	-0.242	-0.642	-0.303	-0.523	-0.091	-0.075
Random Forest Regression		100 decision trees	0.482	-0.133	0.268	0.336	-0.035	0.724	-0.021	-0.056	-0.092	0.055

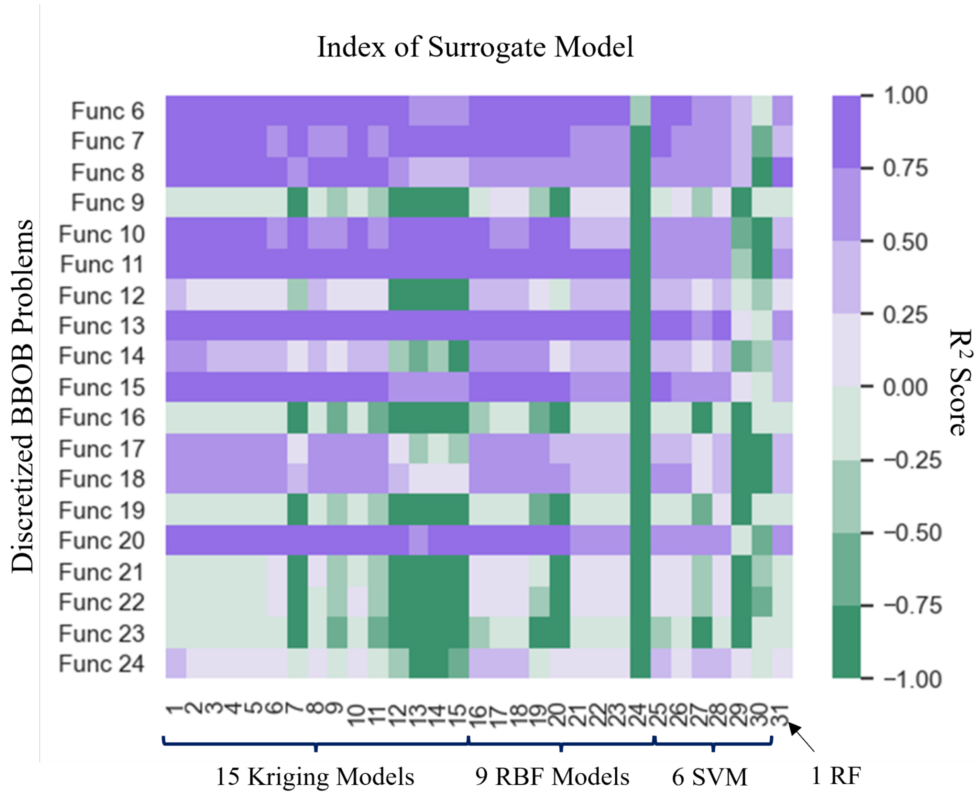

Figure 1: The heat map of R^2 scores of 31 surrogate models obtained on 19 discretized BBOB functions using 500 data samples. Notably, all scores that are less than -1 are raised to -1 for nicer visualization.

Problem 6 (G) : Attractive Sector Function

Problem 7 (G) : Step Ellipsoidal Function

Problem 8 (G) : Rosenbrock Function

Problem 9 (B) : Rosenbrock Function, rotated

Problem 11 (G) : Discus Function

Problem 13 (G) : Sharp Ridge Function

Problem 15 (G) : Rastrigin Function

Problem 16 (B) : Weierstrass Function

Problem 18 (M) : Schaffers F7 Function, moderately ill-conditioned

Problem 19 (B) : Composite Griewank-Rosenbrock Function F8F2

Problem 20 (G) : Schwefel Function

Problem 21 (B) : Gallagher's Gaussian 101-me Peaks Function

Problem 22 (B) : Gallagher's Gaussian 21-hi Peaks Function

Problem 23 (B) : Katsuura Function

Problem 24 (M) : Lunacek bi-Rastrigin Function

More descriptions on the definitions and properties of these functions can be found in [1].

Implemented Surrogate Models

Four categories of surrogate models (RBF, Kriging, SVM and RF) are considered in SAMA-DiEGO. The surrogate pool contains 31 models in total, i.e., nine RBF interpolation models, fifteen (5×3) Kriging models, six SVM regression models and one RF model:

RBF A total of nine Euclidean-distance-based radial basis functions ($\varphi(\| \cdot \|)$ are considered in this research. Suppose using $d_{ij} = \|\vec{x_i} - \vec{x_j}\|_2$ to shortly describe the Euclidean distance between two data samples in the search space $\mathcal{S}$, i.e., $\vec{x_i}, \vec{x_j} \in \mathcal{S}$. The definitions of nine radial basis functions can be therefore written in Table 2. Moreover, only linear tail $p(\vec{x}) = \sum_{z_t \in \vec{x}} \mu_t \cdot z_t + 1$ is considered in the experiments.

Kriging Five correlation functions together with three types of basic functions are adopted in SAMA-DiEGO. A summary of these functions are given in Table 3. More details regarding the implementations are introduced in [4].

SVM and RF The implemented SVM and RF in SAMA-DiEGO are mostly based on the scikit-learn [5] package. The six kernels defined on two example data samples x_i, x_j for $\epsilon-$SVM regression are shown in Table 4, where $\langle \ , \ \rangle$ is the inner product of two samples, γ and r are two hyper-parameters and d is the degree of polynomial kernel. Three degrees, 2, 3 and 5 are considered for the polynomial kernels of SVM regression in SAMA-DiEGO. The γ and r along with other hyperparameters are set using their default values in scikit-learn.

With respect to random forest, the default implementation and hyper-parameters provided by scikit-learn are used. Note that starting from 0.22, scikit-learn ensembles 100 decision trees in one random forest regression instead of 10 in previous versions and our implementation is based on the 0.24.2 version.

Table 2: Specifications of the nine radial basis functions in SAMA-DiEGO. Specifically, $\log(d_{ij})$ will programmatically return 1 if $d_{ij} = 0$.

Name	Definition (φ)
Linear	d_{ij}
Cubic	$d_{ij} \cdot d_{ij} \cdot d_{ij}$
Thin plate spline	$d_{ij} \cdot d_{ij} \cdot \log(d_{ij})$
Polyharmonic spline 4	$d_{ij} \cdot d_{ij} \cdot d_{ij} \cdot d_{ij} \cdot \log(d_{ij})$
Polyharmonic spline 5	$d_{ij} \cdot d_{ij} \cdot d_{ij} \cdot d_{ij} \cdot d_{ij}$
Multiquadric	$\sqrt{1 + (d_{ij} \cdot d_{ij})}$
Gaussian function	$exp(-d_{ij} \cdot d_{ij})$
Invmultiquadric	$1/\sqrt{1 + d_{ij} \cdot d_{ij}}$
Invquadric	$1/(1 + d_{ij} \cdot d_{ij})$

References

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Table 3: Three basic functions and five correlation functions used for Kriging interpolation.

Correlation Functions $C\left(\vec{x}^{(i)}, \vec{x}^{(j)}\right)$
Ornstein–Uhlenbeck Process (OUP)
Squared Gaussian Correlation (SGC)
Matérn Correlation 3/2 (Matern32)
Matérn Correlation 5/2 (Matern52)
Gower Distance (Gower)

Basic Functions $\xi_i(\vec{x})$	Specification
Constant	1
Linear	x_i
Quadratic	$x_i \cdot x_i$

Table 4: The four types of SVM kernels in SAMA-DiEGO.

Kernel Name (API)	Definition
linear	$\langle \vec{x_i}, \vec{x_j} \rangle$
poly	$(\gamma \langle \vec{x_i}, \vec{x_j} \rangle + r)^d$
rbf	$\exp(-\gamma \|\vec{x_i} - \vec{x_j}\|^2)$
sigmoid	$\tanh(\gamma \langle \vec{x_i}, \vec{x_j} \rangle + r)$

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