Predictability on Performance of Surrogate-assisted Evolutionary Algorithm According to Problem Dimension

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ABSTRACT

As the demand for computationally expensive optimization has increased, so has the interest in surrogate-assisted evolutionary algorithms (SAEAs). However, if a fitness landscape is approximated using only a surrogate model, thereby replacing a fitness function, it is possible for a solution to evolve toward a false optimum based on the surrogate model. Therefore, many conventional studies have been carried out in which the real fitness function and surrogate model are dealt with simultaneously. Nevertheless, such an approach leaves much to be desired because studies should be performed for real fitness function evaluation and surrogate model-aware search mechanisms. In this study, we discovered that the approximation error of the surrogate model at low dimensions has a significant relationship with the performance of SAEAs at high dimensions for three binary encoding problems and three real encoding problems. Therefore, if the approximate error is sufficiently small in the low dimension, then high GA performance can be obtained even when the real fitness function is not used, because a high-quality surrogate model can be obtained in the high dimension.

CCS CONCEPTS

• **Computing methodologies → Genetic algorithms**; *Machine learning*;

KEYWORDS

Surrogate-assisted evolutionary algorithm, genetic algorithm, machine learning

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1 INTRODUCTION

A majority of problems in the real-world have no analytical fitness function by which to accurately calculate the fitness value of a chromosome [2]. In this case, if the respective fitness evaluation is highly time consuming when obtaining fitness through experiment or by computational simulation, surrogate-assisted evolutionary algorithms (SAEAs) should be considered to reduce the computation time. However, if a fitness landscape is approximated using only a surrogate model, it is possible for the solution to evolve toward a false optimum based on the surrogate model [1]. Therefore, many studies have been carried out in which a surrogate model and a real fitness function are dealt with simultaneously. In this paper, we discovered that, for the same type of problem, the approximation error of the surrogate model at low dimensions has a significant relationship with the performance of SAEAs at high dimensions. Therefore, because a high quality surrogate model can be obtained in a high dimension if the approximation error is sufficiently small in the low dimension, the SAEAs can achieve high performance even when a real fitness function is not used. This paper is an extension of [3] in which an *NK* landscape problem (k=12) is added to previous binary encoding problems (One-max, *NK* landscape (k=2) problem), and in which additional experiments have been carried out for three real encoding problems (Minimum-sum, Rastrigin, Rosenbrock problem).

2 APPROXIMATE MODELS

The algorithms used to make a model are linear regression (LR), support vector regression (SVR), and deep neural networks (DNN). In our experiments, "LinearRegression" and "SMOreg" algorithm of WEKA[1] was used. TensorFlow[2] was used to make a neural network model.

3 PROBLEMS

Experiments targeting three problems each of the binary encoding and real encoding, respectively, were performed. In the case of real encoding problems, the value range of the gene was set at [-5, 5]. For the binary encoding and real encoding problems, computational budgets of 50 and 1,000 generations were used, respectively. The one-max problem is to maximize the number of genes each of which has a value of 1. An *NK* landscape model was constructed to define a fitness function with various dimensions and epistasis. The fitness function is tuned by two parameters n and k, where n defines the dimensions of the problem space, and k determines the degree of epistasis between the genes making up chromosomes. In our experiment, we used *NK* landscape with k of 2 and one with k of 12. The minimum sum problem is to minimize the value of genes in chromosome. The Rastrigin function is a non-convex function and a non-linear multimodal function. Because of the large search space and many local optima, it is somewhat difficult to find a global optimum. The global optimum is $f(0,\ldots,0)=-330$. Since the Rosenbrock function is a non-convex function, a global optimum exists in a parabolic-shaped flat valley. Finding the valley is simple,

[1] https://www.cs.waikato.ac.nz/ml/weka
[2] https://www.tensorflow.org

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but convergence to the global optimum is somewhat difficult. The global optimum is f(0,…,0)=390.

4 RESULTS AND ANALYSIS

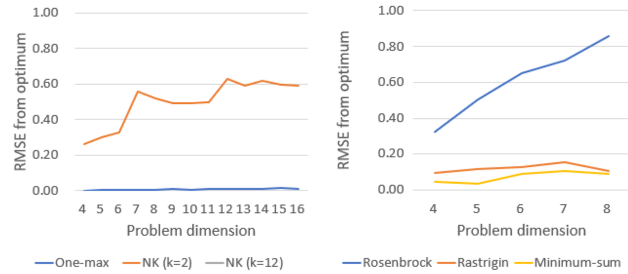
All of the binary encoding problems used tournament selection and one-point crossover. Bitwise mutation was used with probability of 0.7, and a generational genetic algorithm was used. The population size and the number of generations was 50. All of the real encoding problems used tournament selection and extended box crossover. Gaussian mutation was used with a probability of 0.5, and a generational genetic algorithm was used. The population size was 300 and the number of generations was 1,000.

At low dimensions ($n \leq 16$), the root mean square error (RMSE) between the value predicted by the approximate model and the actual fitness was calculated. The results are shown in Figure 1.[3] For the binary encoding problems, the approximation error was obtained by using all solutions, and for the real encoding problems, the approximation error was obtained by arbitrarily extracting 30,000 solutions. Based on these findings, it was determined that, in the binary encoding problems, the approximation error of the One-max problem was smallest, followed by that of the *NK* landscape (k=2) and *NK* landscape (k=12) problems, in that order. In the real encoding problems, the approximation error of the minimum-sum was smallest, followed by that of the Rastrigin and Rosenbrock problems, in that order. At high dimensions ($n>16$), a surrogate model was created by arbitrarily extracting 10,000 solutions for the binary encoding and real encoding problems, and the performance of the GA that used the surrogate model was compared to the performance of the GA that solved the objective function directly. The performance of the approximated and calculated objective functions was evaluated using an average value with n = 50. The value of the difference between the GA performance obtained by the objective function and the one obtained by the SVR model at high dimensions is shown in Figure 2. The performance of the approximated and calculated objective functions is shown in Table 1. Based on these findings, it was confirmed the difference in performance was small with regard to the order of the approximation error when the dimension was low.

5 CONCLUSION

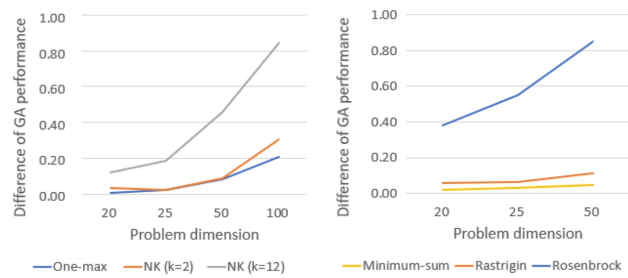
Many surrogate-assisted evolutionary algorithms deal with a real fitness function and a surrogate model together instead of replacing the fitness function with the surrogate model. However, they leave much to be desired, because a large number of real fitness function evaluations must still be performed. In this paper, we conducted experiments for three binary encoding problems and three real encoding problems. From the results, it was determined that the approximation error of the surrogate model at low dimensions has a significant relationship with the performance of SAEAs at high dimensions. The three binary encoding problems and the minimum-sum problem showed small approximation errors at low dimensions, and because the performance of the SAEAs at high dimensions was high, the fitness function could only be replaced by the surrogate model. However, the Rastrigin and Rosenbrock problems demonstrated large approximation errors at low dimensions. Because the performance of the SAEAs at high dimensions was poor when the fitness function was replaced by only the surrogate model, the solution evolved toward a false optimum. In future research, additional experiments will be conducted on highly time-consuming real-world problems.

[3] SVR was adopted as a representative. Because of the space limit of this paper, we could not show all results of algorithms we tested.



(a) Binary encoding problem (b) Real encoding problem

Figure 1: Normalized approximation error of SVR model at low dimensions ($n \leq 16$).



(a) Binary encoding problem (b) Real encoding problem

Figure 2: The normalized value of difference between GA performance obtained by objective function and one obtained by SVR model at high dimensions ($n>16$).

Table 1: Comparison of performance

Problem (size: *n* or *n*, *k*)	Obj function Ave/SD	SVR Ave/SD	DNN Ave/SD	LR Ave/SD
One-max(20)	19.86/0.35	19.94/0.24	19.98/0.14	19.86/0.35
One-max(25)	24.54/0.61	24.82/0.39	24.76/048	24.54/0.61
One-max(50)	44.40/1.73	45.38/1.67	45.58/1.53	44.40/1.73
One-max(100)	77.68/3.07	80.18/2.53	79.22/3.19	77.68/3.07
***NK*(20, 2)**	13.78/0.73	13.39/0.52	14.38/0.53	13.41/0.61
***NK*(25, 2)**	17.04/0.77	17.27/0.72	17.76/0.52	17.25/0.67
***NK*(50, 2)**	32.68/1.36	31.63/1.36	33.03/1.24	31.06/1.21
***NK*(100, 2)**	60.30/1.76	56.66/2.11	59.17/2.30	56.82/2.15
***NK*(20, 12)**	13.79/0.68	12.33/1.02	11.68/1.25	12.23/1.12
***NK*(25, 12)**	17.04/0.78	14.83/1.17	14.54/1.10	14.82/1.34
***NK*(50, 12)**	32.20/0.86	27.71/1.23	27.50/1.56	27.97/1.52
***NK*(100, 12)**	61.60/0.95	53.47/1.28	53.19/2.57	53.60/1.68
Minimum(20)	-100.00/0.00	-99.00/0.64	-100.00/0.00	-100.00/0.00
Minimum(25)	-125.00/0.00	-123.31/0.77	-125.00/0.00	-125.00/0.00
Minimum(50)	-249.97/0.42	-242.46/1.46	-243.14/1.53	-249.86/0.42
Rastrigin(20)	-308.19/7.41	-25.81/32.51	-126.35/47.94	-13.58/30.97
Rastrigin(25)	-294.54/9.25	31.57/57.10	-65.27/41.14	51.95/49.27
Rastrigin(50)	-161.08/25.92	403.11/70.48	208.99/60.73	403.90/59.58
Rosenbrock(20)	448.3/25.7	19134.2/7962.9	1934.2/519.1	22436.9/6307.1
Rosenbrock(25)	483.7/25.5	27446.2/6340.4	5914.1/2298.6	28276.5/6989.2
Rosenbrock(50)	670.1/32.1	42669.5/18195.8	11203.0/4327.5	39542.5/11757.6

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