Offspring Generation Method using Delaunay Triangulation for Real-Coded Genetic Algorithms

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Abstract. To design crossover operators with high search ability in real-coded Genetic Algorithms, it will be efficient to utilize both information regarding the parent distribution and the landscape of the objective function. Here, we propose a new offspring generation method using Delaunay triangulation. The proposed method can concentrate offspring in regions with a satisfactory evaluation value, inheriting the parent distribution. Through numerical examples, the proposed method was shown to be capable of deriving the optimum with a smaller population size and lower number of evaluations than Simplex Crossover, which uses only information of the parent distribution.

1 Introduction

Genetic Algorithms (GAs) are optimization methods that simulate the heredity and evolution of living organisms. Real-Coded GA (RCGA), which uses real number vector representation of chromosomes, is utilized for global optimization of nonlinear functions. In RCGAs, offspring can be generated by dealing directly with the parent distribution in design space. Various crossover operators have been proposed in RCGAs some of which have also been shown to have efficient search ability[1–5]. A well-known set of guidelines for design of these crossover operators is the functional specialization hypothesis[6]. In this hypothesis, it is important that a crossover operator generates offspring with the same distribution as the parents. Then, a generation alternation model changes the distribution and evolves the population. Based on this hypothesis, it is commonly believed that crossover operators with high search ability can be designed easily in RCGAs. In addition, the offspring generation that correctly inherits the parent distribution is an important design guideline in Probabilistic Model-Building GA (PMBGA)[7, 8].

On the other hand, some of offspring generation methods with higher search ability in real-coded PMBGAs estimate the parent distribution using the joint normal kernels distribution or the histogram distribution[9–11]. These methods implicitly construct the probabilistic model similar to the landscape of the objective function. Therefore, in RCGAs as in real-coded PMBGAs, crossover operators with higher search ability can be designed by utilizing not only the parent distribution but also the landscape of the objective function. In Simplex Crossover (SPX)[4, 5], which is one of the crossover operators for RCGAs, offspring generation range is first defined from the parent distribution. Then, large numbers of offspring are generated uniformly within the defined range. In the offspring generation of SPX, it is possible that the search ability will be increased by concentrating offspring in regions with a satisfactory evaluation value within the defined region.

From these backgrounds, in this paper, to concentrate offspring in regions with a satisfactory evaluation value, we propose a new offspring generation method using the Delaunay triangulation. The next section first presents an outline of the Delaunay triangulation. Then, we discuss the details of SPX, which forms the foundation of the proposed method. Finally, we describe the proposed offspring generation method in detail. In the numerical examples in this paper, the effectiveness of the proposed method is discussed by comparison with the search ability of SPX.

2 Voronoi Diagram and Delaunay Triangulation

2.1 Voronoi Diagram

The Voronoi diagram[12] decides how to divide the space between the region of each point and its boundary as in Equation 1, when a point set $P = \{\boldsymbol{p}_1, \boldsymbol{p}_2, \boldsymbol{p}_3, ..., \boldsymbol{p}_m\}$ is given in an n-dimensional space. In Equation 1, $d(\boldsymbol{p}_i, \boldsymbol{p}_j)$ expresses the distance function between $\boldsymbol{p}_i$ and $\boldsymbol{p}_j$. Generally, the Euclid distance is used as the distance function.

$$V(\boldsymbol{p}_i) = \{\boldsymbol{p} | \boldsymbol{p} \in \mathrm{R}^n, d(\boldsymbol{p}, \boldsymbol{p}_i) < d(\boldsymbol{p}, \boldsymbol{p}_j), j \neq i\} \tag{1}$$

Fig. 1 shows an example of the Voronoi diagram with 8 points in a 2-dimensional space. Each point that generates the Voronoi diagram is called a Voronoi generator, and each region divided by Voronoi generators is known as a Voronoi region. The region $V(\boldsymbol{p}_i)$ that includes the point $\boldsymbol{p}_i$ shows that, at any arbitrary location in the regions, the point $\boldsymbol{p}_i$ is the closest point in the point set.

2.2 Delaunay Triangulation

The Delaunay triangulation can be created by connecting neighboring Voronoi generators in a Voronoi diagram. Fig. 2 shows an example of the Delaunay triangulation created from the Voronoi diagram shown in Fig. 1. Each triangle that consists of $(n+1)$ Voronoi generators in an n-dimensional space is called a Delaunay triangle. One of the typical applications that can create the Voronoi diagram and the Delaunay triangulation is Qhull[13, 14]. In this study, Qhull was used for creating the Delaunay triangulation.

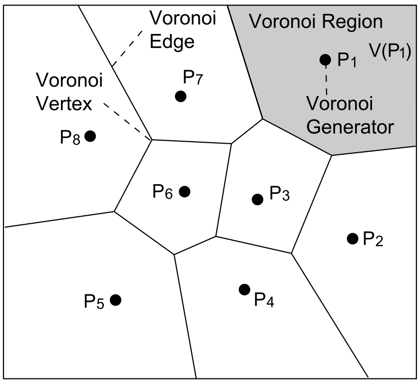

Fig. 1. Voronoi diagram

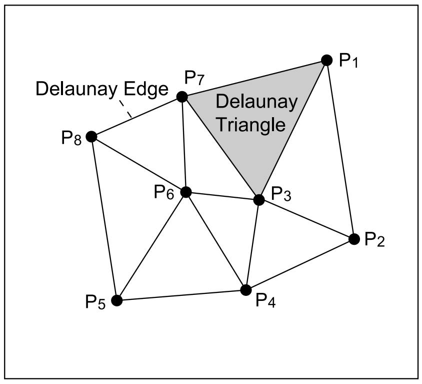

Fig. 2. Delaunay triangulation

3 Simplex Crossover

Simplex Crossover (SPX) is a typical crossover based on the functional specialization hypothesis. In an n-dimensional design space, SPX generates offspring as follows:

1. Select $(n+1)$ parents $\boldsymbol{P}_0, \boldsymbol{P}_1, \ldots, \boldsymbol{P}_n$ from the population by random sampling.
2. Calculate their center of mass $\boldsymbol{G}$ as
$$\boldsymbol{G} = \frac{1}{n+1}\sum_{i=0}^{n}\boldsymbol{P}_i \tag{2}$$
3. Calculate $\boldsymbol{x}_k$ and $\boldsymbol{C}_k$, respectively, as
$$\boldsymbol{x}_k = \boldsymbol{G} + \epsilon(\boldsymbol{P}_k - \boldsymbol{G}) \qquad (k = 0, \ldots, n) \tag{3}$$
$$\boldsymbol{C}_k = \begin{cases} \boldsymbol{0} & (k = 0) \\ \boldsymbol{r}_{k-1} - \boldsymbol{x}_k + \boldsymbol{C}_{k-1} & (k = 1, \ldots, n) \end{cases} \tag{4}$$
$$\boldsymbol{r}_k = (u(0,1))^{\frac{1}{k+1}} \qquad (k = 0, \ldots, n-1) \tag{5}$$
where ϵ is the expansion rate, a control parameter of SPX and $u(0,1)$ is uniform random number $\in$ [0,1].
4. Generate offspring $\boldsymbol{C}$ as
$$\boldsymbol{C} = \boldsymbol{x}_n + \boldsymbol{C}_n \tag{6}$$

Fig. 3 shows the offspring generation range in SPX. Generally, SPX generates large numbers of offspring, which are distributed uniformly on the gray range in Fig. 3. Then, a generation alternation model chooses a few better offspring and substitutes them into the population. ϵ is the expansion rate and a positive parameter of SPX. The expansion rate has a marked effect on the search of SPX. However, SPX also recommends the value $\epsilon_{spx} = \sqrt{n+2}$, which is based on the functional specialization hypothesis[5].

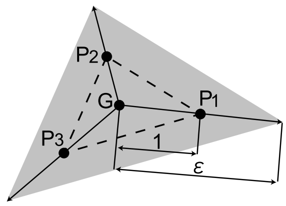

Fig. 3. Offspring generation range in SPX

4 Offspring Generation Method using Delaunay Triangulation

SPX and other crossover operators based on the functional specialization hypothesis generate offspring with the same distribution as the parents. On the other hand, crossover operators with higher search ability can be designed by utilizing not only the parent distribution but also the landscape of the objective function. Therefore, in this paper, a new offspring generation method using the Delaunay triangulation is proposed. The proposed method enables the generation and concentration of offspring in regions with a satisfactory evaluation value, inheriting the parent distribution.

4.1 Procedure of Offspring Generation using Delaunay Triangulation

Fig. 4 shows an overview of the proposed method. In an n-dimensional design space, the proposed method generates N_{off} offspring from $(n+1)$ parents as follows:

1. Select $(n+1)$ parents $\boldsymbol{P}_0, \boldsymbol{P}_1, \ldots, \boldsymbol{P}_n$ from the population by random sampling.
2. Using SPX, first $(N_{off} \times R_{spx})$ offspring are generated.
3. Repeat the following items $N_{delaunay}$ times.
4. Create the Delaunay triangulation from the offspring coordinates.
5. Evaluate offspring and calculate the evaluation value of each Delaunay triangle. In this item, offspring evaluated in the past should not be re-evaluated. The evaluation value of a triangle is the summation of the evaluation value of the offspring, which form its triangle.
6. Select $(N_{off} \times (1 - R_{spx})/N_{delaunay})$ Delaunay triangles in decreasing order of evaluation value of triangles and generate offspring on the center of mass of each triangle.

The important parameters of the proposed method are the expansion rate ϵ of SPX that defines the offspring generation range, the R_{spx} that determines the number of first offspring generated by SPX, and the $N_{delaunay}$ that determines

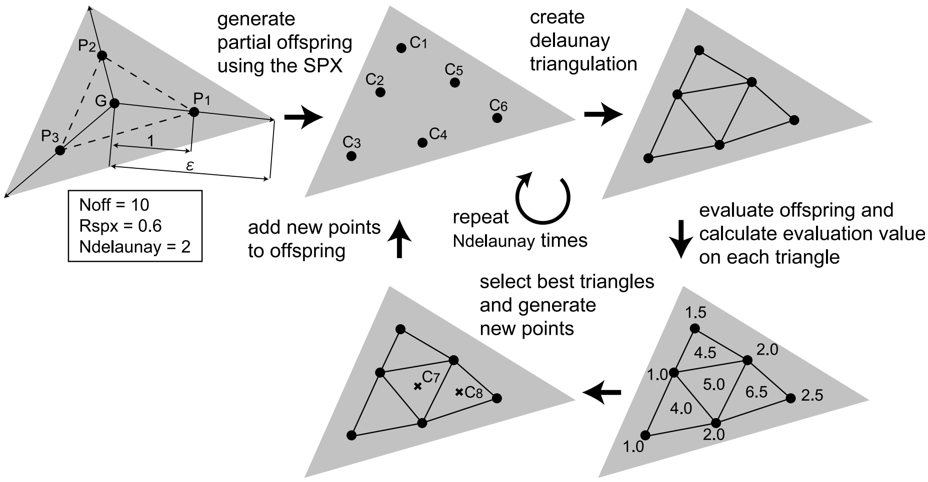

Fig. 4. Offspring generation procedure in the proposed method

the number of iterations of offspring generation using the Delaunay triangulation. The number of evaluations for each generation alternation in the proposed method is N_{off}, which is the same number in the offspring generation of the original SPX.

4.2 Offspring Distributions

Fig. 5 shows the offspring distributions when 500 offspring ($N_{off} = 500$) are generated from 3 parents ($n + 1$) in 2-dimensional design space ($n = 2$) of 3 test functions. The expansion rate ϵ is 1.0. Then, offspring are generated within the 3 parents. In addition, R_{spx} is defined as 0.5 and $N_{delaunay}$ is also defined as 2. Therefore, the first 250 offspring ($N_{off} \times R_{spx}$) are generated by SPX and the last 250 offspring are generated by 2 Delaunay triangulations. Each triangulation generates 125 offspring ($N_{off} \times (1 - R_{spx})/N_{delaunay}$). The number of generators that is the same as the number of generated offspring is 250 in the first triangulation and 375 in the second triangulation.

As shown in Fig. 5, the distributions of all offspring are different according to the landscape of each objective function. However, the distributions of the first 250 offspring generated by SPX are uniform and the same regardless of the landscape of each objective function. On the other hand, the last 250 offspring generated by the Delaunay triangulations are concentrated in regions with a satisfactory evaluation value. In particular, the last 125 offspring generated by the second Delaunay triangulation are concentrated more in regions with better evaluation value. Therefore, $N_{delaunay}$ can control the concentration level of offspring.

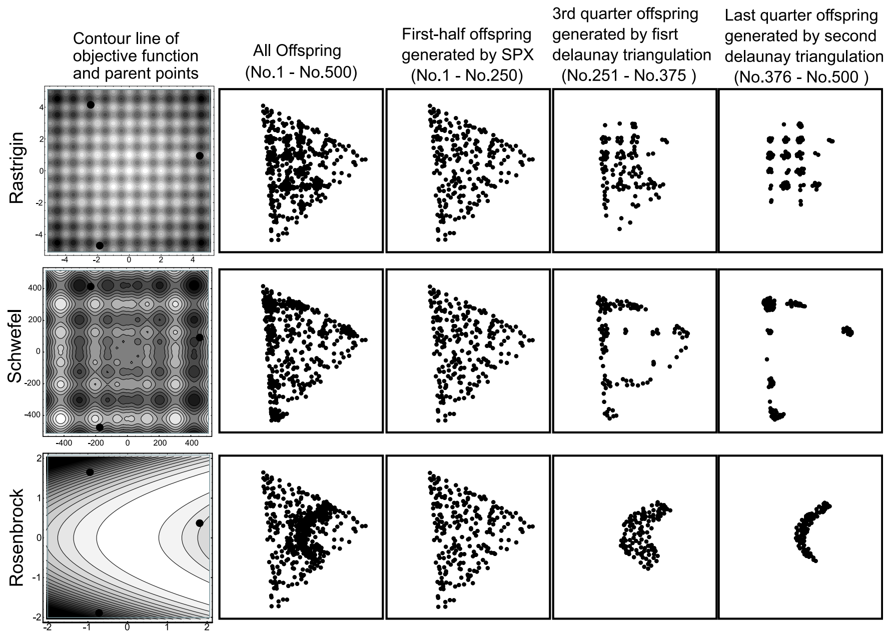

Fig. 5. Distributions of offspring generated by the proposed method

5 Numerical Examples

As described in Subsection 4.1, the three parameters, ϵ, R_{spx}, and $N_{delaunay}$, have marked effects on offspring generation in the proposed method. In these parameters, the expansion rate ϵ that is used for generating offspring in SPX is the most important because it defines the offspring generation range. As explained in Section 3, SPX recommends the value $\epsilon_{spx} = \sqrt{n+2}$, which is based on the functional specialization hypothesis. However, ϵ_{spx} designates that offspring are generated using a uniform distribution. Therefore, ϵ_{spx} is not effective in the proposed method. In the numerical examples described in this paper, we first discuss the most appropriate expansion rate, ϵ, in the proposed method. Then, the effectiveness of the proposed method is clarified through comparison of its search ability with that of SPX.

5.1 Target Problems

In these numerical examples, Sphere, Rosenbrock, Ill-Scaled Rosenbrock, and Ridge functions shown in Equation 7-10 are used as single-peak test functions. Of these functions, the Rosenbrock, Ill-Scaled Rosenbrock, and Ridge functions have correlations among design variables. The Ill-Scaled Rosenbrock function also has a non-uniform scale on the coordinate system. On the other hand, Rastrigin, Griewank, and Schwefel functions shown in Equation 11-13 are used as multi-peak test functions. In addition, the Rotated Rastrigin function, which is obtained by rotating each coordinate axis of the Rastrigin function by $(\pi/3)$, and the Rastrigin-2.0 function, which is obtained by translating each coordinate axis with 2.0, are also used. Of these functions, the Rotated Rastrigin and Griewank functions have correlations among design variables. In the Schwefel function, local optima exist separately on the edge of the design space. Therefore, to maintain the diversity of the population, a larger population size is generally required as compared with other functions. In all functions, the region with an evaluation value of less than 1.0×10^{-6} is considered optimal.

$$F_{Sphere}(x) = \sum_{i=1}^{n} \left(x_i\right)^2 \qquad (-5.12 \le x_i \le 5.12) \quad (7)$$
$$F_{Rosenbrock}(x) = \sum_{i=2}^{n} \left(100(x_1 - x_i^2)^2 + (1 - x_i)^2\right) \qquad (-2.048 \le x_i \le 2.048) \quad (8)$$
$$F_{Ill-Scaled-Rosenbrock}(x) = \sum_{i=2}^{n} \left(100(x_1 - (ix_i)^2)^2 + (1 - ix_i)^2\right) \qquad (-2.048/i \le x_i \le 2.048/i) \quad (9)$$
$$F_{Ridge}(x) = \sum_{i=1}^{n} \left(\sum_{j=1}^{i} x_j\right)^2 \qquad (-64 \le x_i \le 64) \quad (10)$$
$$F_{Rastrigin}(x) = 10n + \sum_{i=1}^{n} \left(x_i^2 - 10\cos(2\pi x_i)\right) \qquad (-5.12 \le x_i \le 5.12) \quad (11)$$
$$F_{Griewank}(x) = 1 + \sum_{i=1}^{n} \frac{x_i^2}{4000} - \prod_{i=1}^{n} \left(\cos\left(\frac{x_i}{\sqrt{i}}\right)\right) \qquad (-512 \le x_i \le 512) \quad (12)$$
$$F_{Schwefel}(x) = 418.9828873n + \sum_{i=1}^{n} x_i \sin\left(\sqrt{|x_i|}\right) \qquad (-512 \le x_i \le 512) \quad (13)$$

5.2 Experimental Methodology

The generation alternation model in these numerical examples is the Minimal Generation Gap (MGG)[15]. The MGG model has desirable convergence properties for maintaining the diversity of the population, and shows better performance than other conventional models. However, MGG was designed with the number of parents set to 2. Therefore, we extended MGG as follows:

1. In an n-dimensional design space, select $(n + 1)$ parents from the population by random sampling.
2. Generate N_{off} offspring by applying the proposed method or SPX.
3. Select 2 parents from the $(n+1)$ parents by random sampling without replacement.
4. Substitute the best individual and another randomly selected individual with rank-based roulette-wheel selection among the 2 parents selected in Item 3 and the offspring into the population.

No mutation method is applied. The initial population is generated randomly within the domain of definition with a uniform distribution. However, no explicit treatment of the domain of definition is considered during the GA search in all test functions except the Schwefel function, in which there are better regions than optimum outside the domain of definition. Therefore, in the offspring generation using SPX in the Schwefel function, when an offspring is generated outside the domain of definition, it is re-generated until it is located inside the domain of definition.

5.3 Discussion of the Expansion Rate

In this example, we discuss the appropriate expansion rate in the proposed method. Experimental conditions are defined as follows:

Table 1. Number of times that the optimum was achieved (single-peak functions)

Expansion Rate	$\epsilon_{spx} \times 1.0$				$\epsilon_{spx} \times 1.5$				$\epsilon_{spx} \times 2.0$				$\epsilon_{spx} \times 2.5$			
Number of Dimensions	2	4	6	8	2	4	6	8	2	4	6	8	2	4	6	8
Sphere	20	20	19	18	20	20	20	20	20	20	20	20	20	20	20	20
Rosenbrock	11	0	0	0	20	20	20	3	20	20	20	20	20	20	20	20
Ill-Scaled Rosenbrock	13	1	0	0	20	20	20	4	20	20	20	20	20	20	20	20
Ridge	20	20	16	1	20	20	20	20	20	20	20	20	20	20	20	20

Table 2. Number of times that the optimum was achieved (multi-peak functions)

Expansion Rate	$\epsilon_{spx} \times 1.0$				$\epsilon_{spx} \times 1.5$				$\epsilon_{spx} \times 2.0$				$\epsilon_{spx} \times 2.5$			
Number of Dimensions	2	4	6	8	2	4	6	8	2	4	6	8	2	4	6	8
Rastrigin	20	19	18	19	20	20	20	19	20	20	20	20	20	20	20	20
Rotated Rastrigin	20	19	18	19	20	20	20	20	20	20	20	20	20	20	20	20
Rastrigin-2.0	20	6	1	0	20	20	14	16	20	20	20	20	20	20	20	20
Griewank	17	7	8	5	20	16	17	19	20	19	20	20	20	0	20	20
Schwefel	5	2	0	0	15	5	2	2	19	15	18	17	18	19	3	0

– Number of dimensions (n): 2, 4, 6, 8
– Population size:
  $n \times 10$ (all single-peak functions and the Schwefel function),
  $n \times 25$ (all multi-peak functions except the Schwefel function)
– Number of offspring (N_{off}): $n \times 10$
– Number of trials: 20. Maximum number of evaluations: 2.0×10^6
– Parameters of the proposed method: $R_{spx} = 0.5$, $N_{delaunay} = 2$

Tables 1 and 2 show the number of times that the optimum was achieved in the proposed method when the expansion rate ϵ is defined as $\epsilon_{spx} \times 1.0$ to $\epsilon_{spx} \times 2.5$. The $\epsilon_{spx} = \sqrt{n+2}$ is the recommended value of SPX. Table 1 shows that the proposed method whose ϵ is defined as greater than $\epsilon_{spx} \times 2.0$ can perform an effective search in single-peak functions. In addition, the proposed method can derive the optimum regardless of the correlations among design variables and the scale of the coordinate system. Table 2 also shows that the proposed method whose ϵ is defined as greater than $\epsilon_{spx} \times 2.0$ can perform effective searches in multi-peak functions. However, in the higher-dimensional Schwefel function and the 4-dimensional Griewank function, the proposed method whose ϵ is defined as $\epsilon_{spx} \times 2.5$ cannot derive the optimum, because the population cannot converge on the optimum or a certain local optimum. Therefore, the most appropriate expansion rate is $\epsilon_{spx} \times 2.0$ in the proposed method.

5.4 Comparison of the Searching Abilities between the Offspring Generation Method using Delaunay Triangulation and SPX

Through the comparison of searching abilities between the proposed method and SPX, we discuss the effectiveness of the proposed method. The number of dimensions (n) is

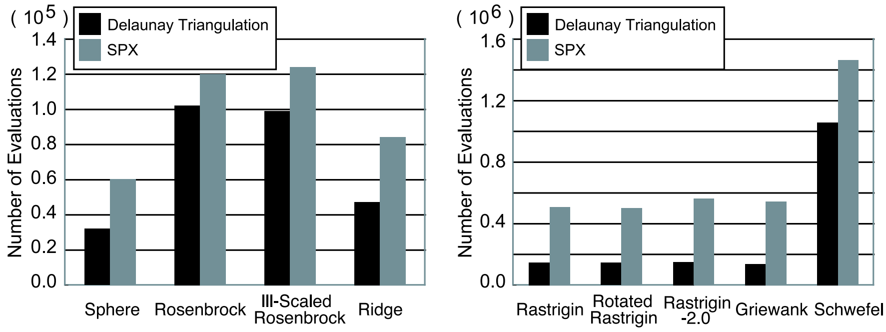

Fig. 6. Average number of evaluations when the optimum was achieved in the proposed method and SPX

8 and other experimental conditions are same as the previous ones. However, to derive the same number of times that the optimum is achieved with the proposed method in SPX, the population size of SPX is defined as 120 ($n \times 15$) in single-peak functions, 200 ($n \times 25$) in multi-peak functions except the Schwefel function and 880 ($n \times 110$) in the Schwefel function. These sizes are larger than the population sizes of the proposed method. With regard to the expansion rate, $\epsilon_{spx} = \sqrt{n+2}$ is applied in SPX and $\epsilon_{spx} \times 2$ is applied in the proposed method. In this example, the average number of evaluations when the optimum is achieved is compared.

Fig. 6 shows the average number of evaluations when the optimum was achieved in both methods. The number of times that the optimum was achieved in both methods was 17 in the Schwefel function and 20 in other functions. As shown in Fig. 6, in all test functions, the proposed method can derive the optimum with a lower number of evaluations than SPX. Especially, with the exception of the Schwefel function, the proposed method requires only about the one-third or one-quarter number of evaluations in multi-peak functions.

These results indicated that the proposed method has the following features. First, the proposed method can derive the optimum with a smaller population size than SPX. This feature is due to concentration of offspring in regions with a satisfactory evaluation value in the proposed method. In addition, as the proposed method requires a smaller population size than SPX, the optimum can be derived with a lower number of evaluations by converging the population earlier than SPX, combining local optima in the design space.

6 Conclusions and Future Work

The crossover operators based on the functional specialization hypothesis generally use only the information of the parent distribution and generate offspring with the same distribution as the parents. On the other hand, we feel that crossover operators with better search ability can be designed by utilizing not only the parent distribution but also the landscape of the objective function. Therefore, we proposed a new offspring generation method using the Delaunay triangulation. In the proposed method, the Delaunay triangulation is used with SPX. Then, the proposed method enables offspring to be concentrated in regions with a satisfactory evaluation value, inheriting the parent distribution. Comparison of search ability between the proposed method and SPX indicated that the proposed method can derive the optimum with smaller population size and lower number of evaluations than SPX.

In future work, we will apply the proposed method to higher-dimensional functions. As Qhull uses a large amount of memory, the proposed method cannot create the Delaunay triangulation with about 100 generators in more than 10-dimensional design space. Therefore, some processes that remove unneeded generators before the Delaunay triangulation creation will be added to the proposed method.

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