Theoretical Analysis of the Unimodal Normal Distribution Crossover for Real-coded Genetic Algorithms†

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Real-coded genetic algorithms (RCGAs) attract attention as global optimization methods for nonlinear functions. For RCGAs, there have been proposed many crossover operators so far. Among them, the unimodal normal distribution crossover (UNDX) developed by Ono et al. shows good performance in optimization of multi-modal and highly non-separable fitness functions. However, the performance of the crossover operators have been evaluated only through numerical experiments with some benchmark problems, and clear guidelines to design operators have not been established.

In this paper, first, statistical characteristics of the UNDX is discussed theoretically. The results of the analysis show that the UNDX preserves the statistics of the parent population such as the mean vector and the variance-covariance matrix well. Based on this finding, the authors propose several guidelines to design crossover operators for the RCGAs.

Key Words: real-coded genetic algorithms, function optimization, preservation of statistics, unimodal normal distribution crossover

1. Introduction

In optimization in nonlinear functions in continuous search spaces, global search is needed if the objective function is multi-modal. Genetic Algorithms (GAs)₂,₃) attract attention as effective optimization methods in this field, and especially, real-coded genetic algorithms (RCGAs). GAs utilizing a floating point representation for genetic coding, are expected as promising approaches because they exploit the nature of continuity of the search spaces⁴~⁸).

As crossover operators for the RCGAs, there have been proposed several methods such as crossover operators inherit the parental values in component-wise manner¹³), those yield children as the midpoint or interior division points of the parents⁴~⁷), those yield children by interior/exterior division of parents in component-wise manner⁸). Ono et al. have proposed the Unimodal Normal Distribution Crossover (UNDX). It outperforms other crossover operators in several benchmarking tests, and applied to the design of lens systems successfully¹⁰),¹¹).

However, including the UNDX, crossover operators for RCGAs have been evaluated only through benchmarking tests. Evaluation through benchmarking tests has difficulty that the results depend on the selected test problems, and sometime, due to inadequate selection of test problems, it leads to over estimate of the performance of the RCGAs¹²).

On the other hand, as theoretical studies of the RCGAs, Qi et al.¹³) and Nomura¹⁴) have discussed the distribution of children generated by crossover operations assuming probability distribution of parents. That is, these studies make analysis form a viewpoint of crossover operators as transformation operation of population distribution. While these studies have made analysis of existing crossover operators, they don’t propose any guidelines for designing good operators. In the context of Evolution Strategies (ES), which are evolutionary algorithms similar to GA, Beyer have made theoretical studies on crossover (or recombination) operators¹⁵),¹⁶). However, in the ES, mutation is used as a primary search operator and crossover plays only secondary role. The findings of Beyer’s studies clarified the nature of crossover in this context.

In this paper, first, an overview of the UNDX proposed by Ono et al. is given. Then, theoretical analysis of the UNDX is given from the same viewpoint used by Qi et al. and Nomura. The analytical results show that the UNDX with the parameters recommended by Ono et al. preserves the mean vector and variance-covariance matrix of the population well. Based on this findings, the authors propose some design guidelines for crossover operators for RCGAs.

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2. Unimodal Normal Distribution Crossover

Fig. 1 Unimodal Normal Distribution Crossover (UNDX).

In this section, the Unimodal Normal Distribution Crossover (UNDX) proposed by Ono et al. is described briefly.

2.1 Algorithm of the UNDX

We assume $n$ dimensional real space $\mathbb{R}^n$ as the search space. First, as shown in Fig. 1 (a), Parent 1 ($\mathbf{a}^1 \in \mathbb{R}^n$), and Parent 2 ($\mathbf{a}^2 \in \mathbb{R}^n$) are selected randomly from the population of a genetic algorithm randomly. Let $\mathbf{x}_p$ and $\mathbf{d}$ be the midpoint and difference vector of these parents, respectively:

$$\mathbf{x}_p = \frac{1}{2}(\mathbf{a}^1 + \mathbf{a}^2)$$

$$\mathbf{d} = \mathbf{a}^2 - \mathbf{a}^1$$

In the following, we call the direction expressed by $\mathbf{d}$ ‘the primary search direction’, and the subspace orthogonal to this vector ‘the secondary search space’.

Further, in the UNDX, a third parent $\mathbf{x}_3 \in \mathbb{R}^n$ is picked up randomly also from the population, and let $\mathbf{D}$ be the distance between $\mathbf{v} \mathbf{x}_3$ and the line connecting $\mathbf{x}_1$ and $\mathbf{x}_2$. $\mathbf{D}$ is given by the following equation:

$$\mathbf{D} = |\mathbf{x}_3 - \mathbf{x}_1|$$

$$\times \left(1 - \frac{(\mathbf{x}_3 - \mathbf{x}_1)^T(\mathbf{x}_2 - \mathbf{x}_1)}{|\mathbf{x}_3 - \mathbf{x}_1||\mathbf{x}_2 - \mathbf{x}_1|}\right)^{2/3}$$

Then, as shown in Fig. 1 (b), a child $\mathbf{x}^e$ is yielded by the equation:

$$\mathbf{x}^e = \mathbf{x}_p + \xi \mathbf{d} + \sum_{i=1}^{n-1} \eta_i \mathbf{e}_i \mathbf{D}$$

where $\xi$ is a random number following a normal distribution $N(0, \sigma^2_\xi)$ and $\eta_i$ are $n - 1$ random numbers independently following a normal distribution $N(0, \sigma^2_i)$. The vectors $\mathbf{e}_i, i = 1, \ldots, n-1$ are normalized orthogonal bases that span the secondary search space. In the following, the second term in the RHS of Eq. (4) is called ‘the parallel component’ because it is parallel with the primary search direction, and the third term ‘the normal components’ because they are orthogonal to it.

Ono et al. have recommended the following values for the parameters of the UNDX based on numerical experiments:

$$\sigma^2_\xi = 1/4$$

$$\sigma^2_i = (0.35)^2/n$$

Ono et al. have carried out comparison study of the UNDX with the Blend Crossover (BLX-\alpha) proposed by Eshelman et al. BLX-\alpha is designed for the RCGA taking the continuity of the search space. It yields children by interior or exterior division of the parents in a component-wise manner. Their experiments are carried out by using non-separable or multimodal test functions in the search spaces up to 20 dimension. The results show that the UNDX has similar performance to the BLX-\alpha in multimodal test functions, and outperforms it in the non-separable test function.

2.2 Distribution of Children Obtained by the UNDX

In this section, we show statistical characteristics of the UNDX using a simple examples. The setting of the experiments is as follows:

- Population sizes of parents and children are 1000 respectively.
- Dimension of the search space is 3. The coordinate system of the search space is denoted by $x_1, x_2, x_3$.
- Initial population is generated randomly following the normal distribution of zero mean and the variance-covariance matrix of

$$\Gamma = \begin{bmatrix} \sigma^2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1/\sigma^2 \end{bmatrix}$$

where $\sigma = 5$.

- Recommended parameters for the UNDX is used. No selection operation is introduced, and generation alternation is carried out by replacing simply the parent population by the children yielded by the UNDX.

Calculation for 10 generations is carried out. The results are shown in Figs. 2 and 3. Figure 2 shows the distribution of the individuals in the initial, first and 10th generation. Figure 3 shows the changes of the variance of the population in each dimension. The mean and covariance are almost zero in all the generations, and therefore omitted.

As characteristics of distribution change of population, these figures show that

- The primary search direction of the UNDX tends to be the direction $x_1$ having the broadest distribution.
- The change of the distribution in this direction is small.
The secondary search space tends to be the subspace spanned by $x_2$ and $x_3$. In this subspace, due to the effect of the normal components of the UNDX, the distribution is slowly widen in the direction of $x_2$, and distribution in the direction of $x_3$ become close to that in $x_2$.

That is, the UNDX is a crossover operator that yields children distributed similar to the distribution of the parents.

\[ z^c = z^p + \xi d + \sum_{i=1}^{n-1} \eta_i e_i D \]  

Since random numbers $\xi, \eta$ are independent, we obtain

\[ (z^c)^T = \left( z^p + \xi d + \sum_{i=1}^{n-1} \eta_i e_i D \right)^T = (z^p)^T + \xi (d)^T + \sum_{i=1}^{n-1} \eta_i (e_i D)^T \]

\[ = (z^p)^T x_1 x_2 + 1/2 \left( (z^1)^T x_1 + (z^2)^T x_2 \right) = \bar{z} \]  

3. Theoretical Analysis of UNDX

3.1 A Stochastic Model of Parental Population

So as to examine the statistical characteristics of the UNDX, we assume that the population size of a GA is sufficiently large, and it can be represented by a probability distribution function (p.d.f.). Statistical properties of the parental population are denoted by

- The mean vector of the parental population is given by $\langle x \rangle = \bar{x}$.
- The variance-covariance matrix of the parental population is given by $\langle (x_i - \bar{x}_i)(x_j - \bar{x}_j) \rangle = \gamma_{ij}$.

3.2 Mean of Children

First, we examine the mean vector of the children yielded by the UNDX. In the following $\langle \rangle$ represents expectation over parents $x^1, x^2, x^3$ independently sampled from the parental population, and independent random numbers $\xi, \eta$ used in the UNDX. If we have to express the expectation over particular probabilistic variable explicitly, we write that variable in subscription like $\langle \xi \rangle$ or $\langle \eta \rangle$.

**Theorem 1 (Mean of Children).** The mean vector of the children yielded by the UNDX is equal to the mean of the parental population.

**Proof.** A child is yielded by $x^c = x^p + \xi d + \sum_{i=1}^{n-1} \eta_i e_i D$.
using a parameter value $\sigma^2 = 1/4$. It is the value recommended by Ono et al. shown in Eq. (5). In other words, the parallel component of the UNDX preserves the mean, variance-covariance matrix of the parental population.

### 3.4 Analysis of Normal Components

In the UNDX, the distance $D$ from the third parent $\mathbf{z}^3$ to the primary search line is used so as to decide the magnitude of the normal components. Hence, analysis of the statistics of a child is not easy in a general situation. In this section, we make analysis in the following manner:

- As a simple case, assuming that the parental population is isotropically distributed, we obtain $\langle D^2 \rangle$ analytically.
- As for other cases of parental distribution, we observe the change of $\langle D^2 \rangle$ through numerical computation assuming a typical distribution.

#### 3.4.1 Evaluation of Normal Components

Assuming isotropical distribution as the parental population, we obtain $\langle D^2 \rangle$ analytically. The assumed situation corresponds to the early stage of the search where the initial population is generated randomly.

For analysis, we make the following assumptions:

**Assumption 1.** Parental population is distributed isotropically.

By this assumption, the variance-covariance matrix of parental population is proportional to the identity matrix. It is denoted by $\gamma I$ where $I$ is the $n$ dimensional identity matrix, and $\gamma$ is a positive constant.

**Assumption 2.** The subspace spanned by the selected three parents is not degenerated.

**Theorem 3.** Under the above assumptions,

$$\langle n - 1 \rangle \gamma \leq \langle D^2 \rangle \leq \frac{3}{2} \langle n - 1 \rangle \gamma + \frac{1}{2} \gamma$$

**Proof.** Without loss of generality, we can choose the $n$-th basis of the coordinate system in the direction of the primary search direction. Then, the projection of $\mathbf{z}^3 - \mathbf{z}^p$ onto the secondary search space is to extract the first $n-1$ elements. Hence,

$$D^2 = \sum_{i=1}^{n-1} (x_{3,i} - x_{p,i})^2,$$

where the subscript $i$ represents the $i$-th component. Then,

$$\langle D^2 \rangle = \left\langle \sum_{i=1}^{n-1} (x_{3,i} - x_{p,i})^2 \right\rangle$$

$$= \left\langle \sum_{i=1}^{n-1} (x_{3,i} - \bar{x}_i)^2 \right\rangle + \left\langle \sum_{i=1}^{n-1} (x_{p,i} - \bar{x}_i)^2 \right\rangle$$

$$= (n-1)\gamma + \left\langle \sum_{i=1}^{n-1} (x_{p,i} - \bar{x}_i)^2 \right\rangle_{\mathbf{z}^3, \mathbf{z}^2}$$

$$= (n-1)\gamma + \sum_{i=1}^{n-1} \left( \langle (x_{p,i} - \bar{x}_i)^2 \rangle_{\mathbf{z}^3, \mathbf{z}^2} \right)$$

$$= (n-1)\gamma + \frac{n}{2} \gamma - \left\langle (x_{p,n} - \bar{x}_n)^2 \right\rangle_{\mathbf{z}^3, \mathbf{z}^2}$$

where the second line is obtained using independence of $\mathbf{z}^3, \mathbf{z}^1$ and $\mathbf{z}^2$, the third line is obtained from the isotropic distribution of the $\mathbf{z}^3$. The fifth line is obtained from the
Then, by choosing the parameter value given by this figure, experiment. Setting of the experiment is as follows: non-isotropic parental distribution through numerical experiment. From Eqs. (15) and (16),

\[
(n-1)\gamma \leq \langle D^2 \rangle \leq \frac{3}{2}(n-1)\gamma + \frac{1}{2}\gamma
\]  

As stated in the proof, evaluation of the last term in the Eq. (16) is difficult because the coordinate system is selected depending on the parent \(x^1, x^2\). If it is independent from the selected parents, we obtain an estimation

\[
\langle D^2 \rangle \simeq \frac{3}{2}(n-1)\gamma
\]  

From Eq. (4), the variance of the random number \(\eta\) is given by

\[
\langle (\eta, D)^2 \rangle = \sigma_n^2 \langle D^2 \rangle \simeq \sigma_n^2 \frac{3}{2}(n-1)\gamma
\]

Then, by choosing the parameter value by

\[
\sigma_n^2 = \frac{2}{3} \frac{1}{n-1}
\]  

The magnitude of the variance of the normal components is similar to that of the parental population.

3.4.2 Numerical Experiments

In this section, the distribution of \(D^2\) in the case of non-isotropic parental distribution through numerical experiment. Setting of the experiment is as follows:

- The parental distribution follows the three dimensional normal distribution whose mean is 0, and variance-covariance matrix is given by Eq. (7).

The parameter \(\sigma\) represents the magnitude of asymmetry of the distribution. A case of \(\sigma\) near to 1 represents the early stages of search. On the other hand, larger \(\sigma\) represents a situation of later stage of GA search where the population distributes along the valley of the fitness.

- Three parents are sampled from Eq. (7) independently, and \(D^2\) is calculated.
- With 10001 samples of parents, we obtain the mean and median of the \(D^2\).
- Observe change of the above statistics by changing the value of \(\sigma\) from 1 to 100.

The result of the experiment is shown in Fig. 4. From this figure,

- If the parental distribution is isotropic \((\sigma = 1)\), The mean of \(D^2\) is close to the theoretical estimate

\[
\frac{3}{2}(n-1) \cdot 1 = 3
\]  

\textbf{Fig. 4} Variation of \(D^2\) according to change of \(\sigma^2\).

- If \(\sigma\) gets larger, the mean and the median of \(D^2\) are deviated from each other.
- The mean of \(D^2\) increases almost in proportion to \(\sigma\).
- On the other hand, the median of \(D^2\) stays unchanged.

Let’s discuss the reason of deviation of the mean and the median of \(D^2\). If \(\sigma\) is large, with high probability, the primary search line connecting parent 1 and 2 has the direction of the basis having largest variance \((x_1, \text{the first primary component})\). Then \(D^2\) takes value near to variance of \(x_1\) (the second primary component). However, with low probability, it takes direction far from the first component. In this case, the \(D^2\) takes values near to \((\sigma^2)\) with high probability. Hence, the median of \(D^2\) takes value near to the variance of \(x_2\) on one hand, and on the other hand, the mean takes value between the variances of \(x_1\) and \(x_2\).

Thus, statistically, \(D^2\) takes value between the variance of the first and second primary components of the parental distribution.

3.4.3 Discussion

From Eq. (19), if the distribution of the parental population is isotropic, by selecting \(\sigma_n^2 = 2/3(n-1)\), the magnitude of the normal component of the UNDX become similar to the variance of the parental population. The above numerical experiment shows that in the case of asymmetrical distribution of parental population, the mean or median of the \(D^2\) will be smaller than the magnitude of the first principal component of the parental distribution, and it takes values between it and the magnitude of the second principal component.

The parameter value recommended by Ono et al. is
\[ \sigma^2 = (0.35)^2 / n = 0.1225/n, \]

- The coefficient on the dimension \( n \) has same order \( o(n^{-1}) \) with Eq. (19) and, it cancels the dependency on the dimension appears in the normal components given by Eq. (13).
- The value of parameter 0.1225 is smaller than the value \( 2/3 \) given by Eq. (19). Considering that the parallel component preserves variance-covariance matrix, and the secondary role of the normal components, it will be an adequate choice.

4. Design Guidelines for Crossover for RCGAs

In this section, we propose several design guidelines for crossovers for RCGAs based on the findings obtained in the previous sections.

In GAs, search is accomplished by repetitively applying selection, crossover and mutation operations to the population. The roles of these operators are

**Selection:** To focus search in the promising region by choosing individuals having better fitness values among the population.

**Crossover and Mutation:** Generate novel search points utilizing information of the current population.

The features of the GAs are to accumulate information through the search process into the population, and to utilize it in generation of novel search points in the crossover operation. Generation of search points by crossover is adaptive to the distribution of population, and it is a salient difference from the mutation having perturbation of fixed magnitude. In the following, we focus our discussion on crossover operations.

![Desirable crossover](image)

First, we discuss desirable generation of novel search points by a crossover. If the parental population is given as shown in Fig. 5 (a), it implies that as the consequence of the search carried out so far, the area where the population resides is the promising area to search the optimum. If the crossover generate novel search points narrower than the parental population as shown in Fig. 5(b), it has large risk to miss the optimum. On the other hand, the crossover yield search points in the region wider than the parental population as shown in Fig. 5(b), it will be inefficient. Hence, the adequate generation of novel search points is to generate solutions having a distribution similar to that of the parental distribution as shown in (Fig. 5 (c)).

Hence, we propose a design guideline for crossovers for RCGAs

**Guideline 0:** Children generated by a crossover should have a similar distribution with the parental distribution.

Since the search space is continuous in the RCGAs, statistics such as the mean vector and the variance-covariance matrix will be adequate indexes that characterize the distribution. Then, we can propose a more concrete guideline instead of the Guideline 0.

**Guideline 1 (preservation of statistics):** The children generated by a crossover should preserve the mean vector and variance-covariance matrix of the parental population.

However, only with the ‘preservation of the statistics,’ a nonsense crossover of ‘do nothing’ fulfills it. Crossover operators are required to yield novel search points, and therefore it should be taken into consideration as a design guideline. We add

**Guideline 2 (Diversity of children):** Under the constraint of ‘preservation of statistics,’ crossover operators should generate children having as much diversity as possible.

As a diversity criterion along this guideline, e.g., maximization of entropy of generated children can be used.

The above guidelines assume ideal functional division between selection and crossover. However, in the practical situation, selection operation may carried out inadequately and the optimum may resides outside the region where the population is distributed. Considering such situation, we add a third guideline

**Guideline 3 (Enhancement of robustness):** To make search more robust, the children generated by a crossover and mutation operations should distribute slightly wider than the distribution of parents.

This guideline may seems inconsistent with the previous guidelines. However, Guidelines 1 and 2 give reference de-
sign and the third guideline gives direction of adjustment. Implementation of this guideline should carried out considering of trade off between robustness and efficiency.

It should be noted that the guidelines proposed above assume that the initial population distributes in the region contains the optimum. Further, while discontinuity and multimodality of the fitness are not taken into consideration in the above discussion well, it doesn’t strongly restrict global search ability of GAs to achieve efficient local search.

Now, we can examine the conventional crossovers including the UNDX along the proposed guidelines,

- In the crossovers such as the one-point, multi-point, uniform and blend crossovers, correlation among variables are gradually lost by applying them to the population due to their component-wise operation. Since the covariances get to zero, they don’t fulfill the Guideline 1. As critically discussed by Salomon, these crossover don’t have sufficient search ability for highly non-separable fitness functions.
- In the crossovers that generate children as the midpoint or interior division points of parents, the children distribute narrower than that of the parents while it preserves the correlation among variables. Hence, these crossovers also don’t fulfill the Guideline 1. Without, e.g., mutation operation, GAs with these crossover will fail in search due to lose of population diversity brought about other than selection operation.
- In the UNDX, the normal component fulfill the Guideline 1.
- However, only with the parallel component, children distributes only on the lines connecting pairs of parents. It may not sufficient from the viewpoint of the Guideline 2.
- In the UNDX, the normal components complement these points, and the work for robustness of the search proposed as Guideline 3. As shown in the analytical and numerical studies in this paper, the contribution of the normal components is not strong and they play the secondary part of the search.
- However, since the normal components use the distance $D$ between the third parent and the primary search line, the distribution of the children is sensitive to the scaling of the coordinate system.

Considering these discussion, we can re-design the UNDX along the design guidelines. The author proposes an extension of the UNDX, and it outperforms the original one.

5. Conclusion

This paper discusses the characteristics of the Unimodal Normal Distribution Crossover (UNDX) proposed by Ono et al. for real-coded genetic algorithms (RCGAs) theoretically, and shows that the UNDX preserves the statistical properties of the parental population well. Based on this finding, the authors propose some design guidelines for crossover operator for RCGAs. The authors are studying improvement of the UNDX based on the proposed design guidelines.

The design guideline of “preservation of the distribution of population” proposed in this paper is realized more concretely as “preservation of the statistics” using continuity of the search space for the RCGAs. To extend this concept to combinatorial optimization in a discrete search space is an interesting subject of future study.

In a discrete space, however, locality of the space is not introduced naturally, and study should be made taking discussion of the fitness landscape into consideration.

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References

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(1) The normal distribution is the distribution having maximum entropy under the constraints on the variance. Hence, if we restrict generation of children on the lines connecting parents, the UNDX is the optimal crossover that maximize the diversity of children under entropy as a criterion, and constraint of the Guideline 1.


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