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K-Bit-Swap: A New Operator For Real-Coded Evolutionary Algorithms

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Abstract

There has been a variety of crossover operators proposed for Real-Coded Genetic Algorithms (RCGAs), which recombine values from the same location in pairs of strings. In this article we present a recombination operator for RC-GAs that selects the locations randomly in both parents, and compare it to mainstream crossover operators in a set of experiments on a range of standard multidimensional optimization problems and a clustering problem. We present two variants of the operator, either selecting both bits uniformly at random in the strings, or sampling the second bit from a normal distribution centered at the selected location in the first string. While the operator is biased towards exploitation of fitness space, the random selection of the second bit for swapping makes it slightly less exploitation-biased. Extensive statistical analysis using a non-parametric test shows the advantage of the new recombination operators on a range of test functions.

1 Introduction

Genetic Algorithms (GAs) are population-based metaheuristic algorithms. They were first introduced in [16], and have demonstrated effectiveness on a wide range of problems, from constrained optimization to design and optimization of neural networks and other classifiers, see e.g. [24, 25]. They are known for their flexibility in terms of the choice of parameters (population and pool sizes, selection function,

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elitism selection, etc) and encodings: binary, integer and real (float).

In the GA framework solutions to a problem are encoded as strings, the fitness of the strings evaluated according to a problem-specific function, and then strings are chosen to enter a 'mating pool' as some function of their fitness. Strings in the mating pool are recombined using genetic operators, and these new offspring strings specify a new population. Over many iterations of the algorithm strings with better fitness (that is, better solutions to the problem) evolve. In general, there are two types of genetic operators that are used: crossover and mutation. Mutation varies the values of entries of a single string, and is effectively a version of local search, exploiting the knowledge encoded in the current string and seeking local improvements in it. In contrast, crossover operators recombine genetic information between parents, which enables a form of global search, exploring the search space more effectively. It has been shown both experimentally and (for some problems) theoretically that GAs with versions of crossover and mutation outperform mutation-only algorithms such as hill-climbers and Randomized Local Search (see e.g. [6, 26]).

While the original GA was based on a binary string, variations based on integer values and floating point numbers are common. Real-Coded Genetic Algorithms (RCGAs) use chromosomes (strings) of floating point numbers and are particularly useful for solving problems where 'real-valued' encoding arises naturally, e.g. training of classifiers, such as neural networks, see [2], signal processing, constrained optimization problems, etc. They are also particularly useful for higher-dimensional optimization problems, where binary encoding is simply infeasible. Readers are referred to [8] for a concise explanation of advantages of RCGAs, and [32] for an extended one.

The development and study of new genetic operators for RCGAs is both a historically rich and active topic of research. Some of the seminal papers include [1,4,8,21,27,32]. Recently, in [14, 15] hybrid crossover operators were thoroughly analyzed, in [34]distance-based crossover operators were studied, in [30] a double Pareto crossover was introduced and successfully tested on a range of multimodal test functions. Also in [30,33] a substantial overview of the history of RCGA crossover operators is given. In many cases parents can generate more (or less) than the standard set of two offspring or an offspring can have more than two parents (see e.g. [7, 13, 19]).

In this paper we follow in these footsteps, and introduce two real-coded versions of the K-Bit Swap (KBS) genetic operator, which is a crossover operator that enables the location of elements of the string to change (transpose) when crossover occurs. We evaluate its use with a RCGA solving multidimensional multimodal realcoded optimization problems, both alone and together with other genetic operators. A version of KBS was introduced in [29] (see also [28] for the extended version of this work) and showed some promise mostly for binary-coded functions.

2 Connection with GA Theory, Exploration vs Exploitation at Population and Gene Levels

Just as with binary GAs, empirical results show a statistically significant advantage of RCGAs with crossover/recombination operators, when compared with mutationonly algorithms. A few probable reasons for this are that crossovers:

- 1. reduce the probability of premature convergence to local optima,
- 2. extend the list of possible offspring that can be generated (especially when probability distributions over offspring are used),
- 3. extend the exploration of fitness space to subsets that are far from the current solution,
- 4. combine exploration and exploitation to some degree, while mutation is primarily an exploitation operator,

The last point is of particular interest when it comes to development of new crossover operators. In the GA community there is little clarity about the definition of the terms 'exploration' and 'exploitation'. Intuitively, exploration deals with sampling from entirely new segments of genotype, while exploitation focuses on sampling in the vicinity of existing solutions. In [3] authors give an overview of approaches to this issue since the early years of GA theory. In short, they can be described as follows:

- 1. Genotype-based, e.g. a distance between individuals of some sort (Manhattan, Hamming, etc),
- 2. Phenotype-based, e.g. a number of different phenotypes (fitness values) in a population that is used to determine diversity.

Hence, the definitions of exploration and exploitation depend on the definition of diversity in the population: finding new individuals outside of the 'basin of similarity' between existing members of the population would be considered exploration. Balancing these two processes, referred to as diversity maintenance (which can be achieved by e.g. niching, crowding, mating restrictions, selection pressure) is crucial to the success of the algorithm. Too much diversity (exploration) can harm by reducing the attention to promising basins around local optima and lack of it (exploitation) reduces the chances of finding good new local optima.

Approaches mentioned above are population-level tools. In this paper we try a genelevel approach (as in, e.g. [7, 13]): given that we have two parents producing two new offspring, there is some distance between the parents and the offspring. Once we have selected the genes/bits for recombination, we use the crossover operator to exchange the information between these genes. Distance from the parents depends on this operator: if it does search strictly in the landscape between the gene values, it is an exploitation operator; if, instead, the operator extends the search space (but doesn't fully exclude the interval between the gene values), it is biased towards exploration.

Arithmetical crossover (AX) is the example of the first type of operator (see [20]):

$$\begin{split} h_i^1 &= \lambda c_i^1 + (1-\lambda) c_i^2 \\ h_i^2 &= \lambda c_i^2 + (1-\lambda) c_i^1 \end{split}$$

where c_i^j are parental gene values, $0 < \lambda < 1$, h_i^j are offspring' gene values. Clearly both h_i^1 and h_i^2 lie strictly between c_i^j , so this operator exploits the interval between the sampled values in each parent. A good example of an exploration-biased operator is BLX- α (see [8]):

$$C_{\max} = \max\{c_i^1, c_i^2\}$$
$$C_{\min} = \min\{c_i^1, c_i^2\}$$
$$I = C_{max} - C_{min}$$
$$h_i^j \in [C_{min} - I\alpha, C_{\max} + I\alpha]$$

The last expression means that new values for the i^{th} gene are sampled from this interval, which stretches beyond the interval by a factor of α . For example, very high values of this parameter ≈ 1 almost triple the interval between gene values. In [8] this operator was introduced as an example of interval schemata.

In Section 3 we introduce two new KBS operators that fit the definition of exploitationbiased operators. Nevertheless, we argue that due to their main property they allow a certain degree of landscape exploration. for i=1: number of pairs in the pool do take the next two strings from the pool for j=1:K do select a bit in the first string uniformly at random select a bit in the second string uniformly at random swap the values of these bits between the two strings end for end for

Figure 1: The K-Bit-Swap Operator for binary coding

3 K-Bit-Swap Genetic Operator for Real-Coded Problems

The original K-Bit-Swap operator was developed for predominantly binary-valued GAs. It was presented in [29], and a pseudo-code description is given in Figure 1. The operator is a form of crossover where, instead of bits being swapped between the strings with their location in the string held fixed, which is standard with most crossovers, the location of the bit in the new string was chosen uniformly at random. The results in [29] demonstrated that the operator improved the results of a GA on numerical optimization problems, but not on an integer-coded variant of the Travelling Salesman Problem.

It is perfectly possible to transfer this version of the KBS to real-valued GAs without substantial changes, just like a standard crossover can be transferred. However, given the success of Arithmetical Crossover (AX) and Blend Crossover (BLX- α) in RCGAs, we use this convention and consider instead variants of KBS that follow the idea behind these two operators, as well as the original KBS, as described next.

3.1 αKBS

The main idea behind KBS is to enable swapping of genetic information between different schemata without binding the choice of the location in the second parent to the location selected in the first parent. Discussion of schemata theory in the context of GAs is beyond the scope of this article, relevant information can be found in [11,22,23]. It is only worth mentioning here that unlike the bulk of crossovers, KBS operators recombine information from unrelated schemata. Simple tweaking of the original KBS idea with an additional feature (parameter α) similar to the one used Set $0 < \alpha \leq 1$ value for i=1:number of pairs in the pool do take the next two strings from the pool for j=1:K do select a value in the first string uniformly at random, v_1 select a value in the second string uniformly at random, v_2 set $v'_1 = \alpha v_1 + (1 - \alpha)v_2$ set $v'_2 = (1 - \alpha)v_1 + \alpha v_2$ replace the values at these locations: $v_1 = v'_1$, $v_2 = v'_2$ end for end for

Figure 2: The αKBS Operator

in AX and BLX- α is presented in Figure 2 (note that the version of KBS described previously is recovered with $\alpha = 0$). This operator resembles both AX and BLX- α in the sense that a value in a parent's gene is multiplied by a coefficient (α or $1 - \alpha$). However, α KBS samples the value to swap with the first parent's value uniformly in the second parent, rather than taking it from the matching location in the string, so that genes from unrelated features (schemata) are swapped. In the current setting, this operator has a greater exploitation, but lesser exploration capacity because the region available for sampling a new value lies strictly between two parental values. This drawback is partly overcome by the main property of randomized bit selection, a feature that AX does not have. Also, unlike BLX- α we do not use an interval around parents' values.

3.2 β KBS

Next, we consider a variant of KBS that samples from a normal (Gaussian) distribution centered on the chosen bit in the first string to select the bit in the second parent. This 'de-randomizes' KBS, making it more of a uniform-type crossover than a mutation operator as, due to lower variance, the selected bit in the second parent is likely to be closer to the original bit. Note that if this normal distribution has 0 variance then this becomes a standard crossover. Empirically, we found the variance of 4 to be a good choice, which is used in the experimental part of the article. One drawback of this algorithm is that the gene location chosen in the second parent can be outside the allowable range (less than 0 or greater than n). In this case we have chosen to replace any outlier values with either 0 or n. This is computationally

for i=1:number of pairs in the pool do

take the next two strings from the pool

```
for j=1:K do
```

select a value in the first string uniformly at random, v_1 , set μ = its position in the string

```
sample u from \mathcal{N}(\mu, \sigma^2)

if u < 0 then

set u = 0

else

if u > n then

set u = n

end if

end if

select the u<sup>th</sup> value in the second parent: v_2

set v'_1 = \alpha v_1 + (1 - \alpha)v_2

set v'_2 = (1 - \alpha)v_1 + \alpha v_2

replace the values of these bits: v_1 = v'_1, v_2 = v'_2

end for

end for
```

Figure 3: The β KBS Operator

simpler than redrawing another random number, but can bias the selection of genes towards these two values. We will address this problem in our future work.

4 Experimental Investigation

4.1 Test Suite

In this paper we only concern ourself with unconstrained multidimensional multimodal (except the Paraboloid function) nonlinear problems. The problem is formulated as:

$$\min f(\mathbf{x}), f: \mathbb{R}^n \to \mathbb{R}$$

We use a range of test functions from the BBOB-2013 (see [9]) list of noiseless functions. Most are well-known examples of minimization problems. Unless otherwise mentioned, the global minimum of the function is at $f(\mathbf{0}) = 0$. All bold values are vectors, i.e. $\mathbf{0} = (0, 0, ..., 0)$, $\|\mathbf{x}\|$ is a square of a vector norm, $\sum_{k=1}^{n} x_k^2$. In the experiments reported in the next section we use values of n in the set $\{2, 5, 10, 20, 50\}$.

Paraboloid This is the only unimodal function we use

$$f_P(\mathbf{x}) = \sum_{k=1}^n x_k^2 = \|\mathbf{x}\|^2, \ -10 \le x_k \le 10$$

Rastrigin This function has $\approx 10^n$ local optima.

$$f_R(\mathbf{x}) = \|\mathbf{x}\|^2 + 10n - 10\sum_{k=1}^n \cos(2\pi k), \ -5.12 \le x_k \le 5.12$$

Rosenbrock

$$f_{Ro}(\mathbf{x}) = \sum_{k=1}^{n-1} (100(x_{k+1}^2 - x_k)^2 - (x_k - 1)^2), \ -5.12 \le x_k \le 5.12$$

with the global minimum at $f(\mathbf{1}) = 0$ (where $\mathbf{1}$ denotes a vector consisting entirely of 1s).

Schwefel

$$f_S(\mathbf{x}) = 418.982n - \sum_{k=1}^n x_k \sin \sqrt{|x_k|}, -500 \le x_k \le 500$$

with the global solution $f(\hat{\mathbf{x}}) = 0$ at $\hat{\mathbf{x}} = (420.9687, 420.9687, \dots, 420.9687)$

Ackley

$$f_A(\mathbf{x}) = 20 + e - 20 \exp\left(-0.2\sqrt{\frac{\|\mathbf{x}\|^2}{n}}\right) - \exp\left(\frac{1}{n}\sum_{k=1}^n \cos(2\pi x_k)\right), \ -32 \le x_k \le 32$$

Griewangk

$$f_G(\mathbf{x}) = 1 + \frac{1}{4000} \|\mathbf{x}\|^2 - \prod_{k=1}^n \cos\left(\frac{x_k}{\sqrt{k}}\right), \ -600 \le x_k \le 600$$

4.2 k-Means Clustering problem

The k-means clustering problem is a very well-known NP-hard problem that arises in many machine learning and signal processing applications. Given a set of n vectors $\mathbf{x}_i \in \mathbb{R}^d (i = 1, ..., n)$, the problem is to find a partition of the data into k clusters (k < n), each represented by the centroid of the data in that partition $(\mu_j \in \mathbb{R}^d, j = 1, ..., k)$, the k^{th} mean, such that the sum of some metric distances, typically the L_2 norm, between all data points $\mathbf{x}_i \forall i$ and the nearest centroid is minimized. In this paper we use Euclidean distance metric:

$$d_{X,Y} = \sum_{j=1}^{k} \sqrt{\sum_{i=1}^{s_j} (x_i - \mu_j)^2}$$
(1)

Here we use Y to denote the set of all centroids (means), x_i and μ_j as defined above and s_j is the number of vectors/observations in the j^{th} subset. There are many local minima in the space, and the standard iterative algorithm (Lloyd's algorithm) typically finds a good one. There has been a lot of interest in heuristic algorithms solving this problem; some well-known implementations include [12, 17, 31]. One of the best-known examples of k-means optimized by a GA is [18].

In our implementation, we consider only the 4-means problem (k = 4), and generate a set of random points \mathbf{x}_i for each dimension and use the same data for all of the algorithms to allow fair comparison. We also report results of using Lloyd's algorithm using the implementation in the Scikit machine learning library for Python.

4.3 Experimental Setup

Each experiment consists of running every algorithm 20 times (from different randomized starting conditions) on a particular function with a pre-chosen dimensionality set η sample $u \sim U(0, 1)$ if u < 0.5 then set $\beta = (2u)^{\frac{1}{\eta+1}}$ else set $\beta = (2(1-u))^{-\frac{1}{\eta+1}}$ end if $x'_k = 0.5(x_k(1-\beta) + y_k(1+\beta))$ $y'_k = 0.5(x_k(1+\beta) + y_k(1-\beta))$

Figure 4: SBX operator

for 5000 generations. For simplicity, all algorithms save a single elite individual at each generation (i.e., the fittest individual is saved at every generation and added to the next generation of individuals, at the same time a randomly chosen offspring is deleted from the pool; thus population size is constant), and we do not vary the size of the population or the recombination pool, which were both fixed at 400 (making this a (400 + 400)EA). Tournament selection was used to select individuals for the recombination pool (see [28] for its description). As well as KBS, we also used two variants of crossover that are well-known in the RCGA literature, BLX- α and SBX. For all recombination operators we use a 100% rate (recombine all pairs in the pool). We also applied two different mutation operators, uniform and Gaussian. In both cases bit mutation probability of $\frac{1}{n}$ was used, so that on the average there was one mutation per string. For the KBS both α and β were set to 0.4, and $K = \lfloor \frac{n}{2} \rfloor$. These values were chosen to make the changes introduced by the KBS operator comparable to those of other crossovers. All values are initiated uniformly at random in the interval specified in Section 4.1. In addition to BLX- α crossover explained in 2, we use Simulated Binary Crossover (SBX, see [1,5]): For our experiments we set $\eta = 2$. We also use the following mutation operators in combination (to reduce bias) with crossovers:

1. Gaussian mutation (GM, see [33]): in our implementation we select a bit x_k with probability $\frac{1}{n}$ and sample from the normal distribution to generate the new value:

$$x'_{k} = \frac{u_{1} + u_{2}}{2} + \sqrt{u_{2} - u_{1}} \cdot Z$$

where $Z \sim N(0, 1)$, u_2 is the maximal value of the bit and u_1 is the minimal value.

2. Simple mutation (SM, each bit is sampled with probability $\frac{1}{n}$):

$$x'_{k} = (u_{2} - u_{1}) \cdot U + u_{1}$$

where $U \sim U[0, 1]$ is a uniform random variable.

We defined success as finding the global minimum to within a tolerance of ε . We set for 2-dimensional problems $\varepsilon = 0.01$, and $\varepsilon = 0.1$ for all of the other problems. If the algorithm was successful, then the generation at which it first happened was recorded. The three measures that we record to establish the efficiency of the algorithm Asolving problem π (where j is j^{th} run out of the total of R runs, x^* is the best solution, and t_j is the number of generations it took the algorithm to find the solution) are:

$$I_j = \begin{cases} 1 & \text{if } f(x^*) < \varepsilon, \\ 0 & \text{otherwise} \end{cases}$$
(2)

$$P(A,\pi) = \frac{\sum_{j=1}^{R} I_j}{R},\tag{3}$$

$$M(A,\pi) = \frac{\sum_{j=1}^{R} t_j I_j}{R} \tag{4}$$

4.4 Experimental Results

The main results of this article are summarized in Tables 1, 2 and 3. In Table 1 in every cell (crossover and mutation types vs function and dimension) the first value is the proportion of successful runs (Equation 3). The second value is mean runtime averaged (applies to successful runs only), computed using Equation 4. A run is considered successful if the ε -tolerance is reached. Tables 2 and 3 simply display the mean fitness value at the end of the run, averaged over 20 runs.

By looking at Tables 1 and 2 we get a good general overview of the performance of algorithms on black-box optimization problems: we know which one does better on which function and can compare rate of convergence, since the faster the algorithm detects the basin of attraction around the global optimum, the better. Further analysis enables us to identify places where the operators tend to lead to convergence to local minima; for example both KBS operators appear to suffer from this (in 10 or more dimensions) for the Rosenbrock and Schwefel function. In contrast, both BLX- α and SBX suffer from slow convergence on these problems: it takes them much longer to explore the landscape segments with promising solutions. It is clear from Tables 1 - 3 that most 2-dimensional problems were very simple, but in most standard optimization problems, KBS algorithms outperform the mainstream crossovers, possibly because they exploit current knowledge more effectively. They do especially well on 20- and 50-dimensional Ackley and Griewangk functions, which we see as a useful contribution to RCGA development if we compare the results, for example, to those in [10].

By looking at the 4-means clustering problem (all dimensions), the results are reversed: KBS does worse compared to both BLX- α and SBX, quickly converging to a local solution and not being able to jump out of it. Although other operators also converge prematurely, this takes rather longer than for KBS, resulting in better solutions. As with the Schwefel function, we attribute this to the lack of exploration capacity of both KBS operators, something that needs to be fixed in the future work.

Nevertheless, all presented algorithms greatly outperform the k-means algorithm in SciKit module for Python, as is shown in Table 3. One surprising result we encountered with Griewangk function (dimensions 2 and 5): Gaussian mutation improved all results by up to a factor of 20, something we did not observe with any other function in our experimentation. Although we attribute it to the structure of the fitness landscape, other factors may be at play that require additional investigation.

| Function | Dims | $\alpha \text{KBS}+$ | | | | | $\beta \text{KBS}+$ | | | | BLX- α + | | | | SBX+ | | | |
|------------|--------|----------------------|--------|------|-------|---------------|---------------------|------|-------|---------------|-----------------|------|--------|---------------|--------|------|-------|--|
| Function | DIIIIS | \mathbf{SM} | | GM | | \mathbf{SM} | | GM | | \mathbf{SM} | | GM | | \mathbf{SM} | | GM | | |
| Paraboloid | 2 | 1 | 7.2 | 1 | 4.75 | 1 | 6.95 | 1 | 4.5 | 1 | 13.7 | 1 | 6.35 | 1 | 13.65 | 1 | 5.75 | |
| | 5 | 1 | 44.8 | 1 | 17.2 | 1 | 45.3 | 1 | 18.5 | 1 | 1643.8 | 1 | 233.15 | 1 | 120.15 | 1 | 60.2 | |
| | 10 | 1 | 134.65 | 1 | 53.7 | 1 | 100.15 | 1 | 46.75 | 0 | - | 0 | - | 0.8 | 2563 | 1 | 1250 | |
| | 20 | 1 | 272.45 | 1 | 94.55 | 1 | 382.55 | 1 | 99.35 | 0 | - | 0 | - | 0 | - | 0 | - | |
| | 50 | 1 | 746 | 1 | 240 | 1 | 866 | 1 | 233 | 0 | - | 0 | - | 0 | - | 0 | - | |
| | 2 | 1 | 20.5 | 1 | 25 | 1 | 32.4 | 1 | 27.45 | 1 | 46.1 | 1 | 38.6 | 1 | 35.45 | 1 | 31.15 | |
| | 5 | 0.05 | 2825 | 0 | - | 0.05 | 4546 | 0.05 | 1424 | 0 | - | 0 | - | 0.05 | 4816 | 0 | - | |
| Rosenbrock | 10 | 0 | - | 0 | - | 0 | - | 0 | - | 0 | - | 0 | - | 0 | - | 0 | - | |
| | 20 | 0 | - | 0 | - | 0 | - | 0 | - | 0 | - | 0 | - | 0 | - | 0 | - | |
| | 50 | 0 | - | 0 | - | 0 | - | 0 | - | 0 | - | 0 | - | 0 | - | 0 | - | |
| | 2 | 0.95 | 2450 | 1 | 1050 | 1 | 1930 | 1 | 1335 | 1 | 3995 | 0.35 | 2155 | 0.15 | 1658 | 0.85 | 2180 | |
| | 5 | 1 | 1431 | 1 | 571 | 1 | 1307 | 1 | 583 | 0 | - | 0 | - | 0 | - | 0.25 | 3422 | |
| Ackley | 10 | 0.6 | 3324 | 1 | 2381 | 1 | 3211 | 0.05 | 1565 | 0 | - | 0 | - | 0 | - | 0 | - | |
| ~~~~ | 20 | 0.25 | 3849 | 0.9 | 2536 | 0.25 | 3981 | 0.75 | 2320 | 0 | - | 0 | - | 0 | - | 0 | - | |
| | 50 | 0.25 | 3652 | 0.95 | 2174 | 1 | 3991 | 0.7 | 2846 | 0 | - | 0 | - | 0 | - | 0 | - | |
| | 2 | 1 | 183 | 1 | 143 | 1 | 176 | 1 | 138 | 1 | 546 | 1 | 424 | 1 | 301 | 1 | 350 | |
| | 5 | 1 | 685 | 1 | 726 | 1 | 594 | 1 | 655 | 0 | - | 0 | - | 0 | - | 0 | - | |
| Rastrigin | 10 | 0.45 | 3303 | 0.7 | 3111 | 0.6 | 2872 | 0.75 | 2538 | 0 | - | 0 | - | 0 | - | 0 | - | |
| | 20 | 0.1 | 4064 | 0.05 | 4196 | 0 | - | 0.1 | 4255 | 0 | - | 0 | - | 0 | - | 0 | - | |
| | 50 | 0 | - | 0 | - | 0 | - | 0 | - | 0 | - | 0 | - | 0 | - | 0 | - | |
| | 2 | 1 | 41 | 1 | 17 | 1 | 23 | 1 | 20 | 1 | 34 | 1 | 30 | 1 | 36 | 1 | 23 | |
| | 5 | 0.05 | 1879 | 0.05 | 1541 | 0.1 | 2144 | 0 | - | 0 | - | 0 | - | 0 | - | 0.05 | 3864 | |
| Schwefel | 10 | 0 | - | 0 | - | 0 | - | 0 | - | 0 | - | 0 | - | 0 | - | 0 | - | |
| | 20 | 0 | - | 0 | - | 0 | - | 0 | - | 0 | - | 0 | - | 0 | - | 0 | - | |
| | 50 | 0 | - | 0 | - | 0 | - | 0 | - | 0 | - | 0 | - | 0 | - | 0 | - | |
| | 2 | 1 | 1388 | 1 | 44.4 | 1 | 1496 | 1 | 38 | 1 | 2362 | 1 | 102 | .8 | 1610 | 1 | 65 | |
| | 5 | 0.9 | 2312 | 1 | 127 | 0.95 | 1970 | 1 | 105 | 0 | - | 0.95 | 1445 | 0 | - | 1 | 1224 | |
| Griewangk | 10 | 0 | - | 0.85 | 1385 | 0 | - | 1 | 1009 | 0 | - | 0 | - | 0 | - | 0 | - | |
| | 20 | 0.05 | 4361 | 0.8 | 1187 | 0 | - | 0.7 | 961 | 0 | - | 0 | - | 0 | - | 0 | - | |
| | 50 | 0.05 | 4830 | 1 | 862 | 0 | - | 1 | 757 | 0 | - | 0 | - | 0 | - | 0 | - | |

Table 1: Success rate (proportion of 20 trials in which the global minimum was reached within tolerance ε) and the mean number of generations required to reach it (mean runtime)

Having established the absolute performance of algorithms, we now rank them based on these results. As our data is not Gaussian-distributed or heteroscedastic, we have chosen to use non-parametric statistical tests, specifically the Mann-Whitney U statistic (also known as the one-sided nonparametric Wilcoxon rank-sum test), which is defined as:

$$U = \min\{U_1, U_2\}$$
$$U_1 = s_1 s_2 + \frac{s_1(s_1 + 1)}{2} - R_1$$
$$U_2 = s_1 s_2 + \frac{s_2(s_2 + 1)}{2} - R_2$$

where s_1, s_2 are sample sizes (equal in our case) and R_1, R_2 are the sums of ranks in each sample. A sample size of 20 (which is our case) is enough to give a reliable estimate of the statistical significance of the difference of the means. The test returns a z-statistic from a normal distribution and *p*-value that is compared to the significance level of $\alpha = 0.05$. The sign of the z-statistic shows which sample's mean is smaller: (-) for the first and (+) for the second.

For reasons of space the particular values are not reported, but the main results we obtain from this analysis can be summarized as follows:

- 1. On the overwhelming majority of the Functional Optimization tasks, KBSbased algorithms outperform both BLX- α and SBX, and this difference is statistically significant (i.e., systematic). Among the exceptions are 2-dimensional Rosenbrock and Schwefel and 5-dimensional Griewangk function, where SBX+GM is equally efficient, because the U-statistic values are not significantly different from 0.
- 2. The 4-means clustering problem is best approximated (the global solution is, of course, unknown) by SBX-based algorithms (up to n = 10) and BLX- α algorithms (for dimensionality n > 10).
- 3. Gaussian mutation improves working on many instances (but never on the 4means problem). This is true for each of the 4 types of crossover. It boosts performance especially well on the Griewangk test functions (all dimensions)
- 4. The two variants of the KBS recombination operator are almost equally good (most differences are not statistically significant). Out of 35 instances (7 functions \times 5 dimensions) α KBS+SM outperforms β KBS+SM in 4 instances, β

| Error et i erro | D: | αK | BS+ | βK | BS+ | BLX | -α + | SBX + | | |
|-----------------|------|---------|---------|---------|---------|---------|---------|---------|---------|--|
| Function | Dims | SM | GM | SM | GM | SM | GM | SM | GM | |
| | 2 | 3.63e-7 | 1.37e-7 | 2.98e-7 | 1.83e-7 | 2.00e-5 | 5.23e-6 | 7.21e-6 | 2.10e-6 | |
| | 5 | 1.13e-5 | 1.91e-6 | 3.26e-6 | 8.49e-7 | 0.045 | 0.018 | 0.003 | 0.0016 | |
| Paraboloid | 10 | 0.0008 | 0.00025 | 0.0004 | 0.00016 | 0.875 | 0.373 | 0.07 | 0.03 | |
| | 20 | 0.0022 | 0.00109 | 0.0049 | 0.001 | 8.102 | 3.616 | 0.67 | 0.31 | |
| | 50 | 0.0078 | 0.003 | 0.012 | 0.006 | 80.76 | 48.16 | 7.78 | 3.87 | |
| | 2 | 2.84e-5 | 1.50e-5 | 4.40e-5 | 3.20e-5 | 7.47e-5 | 5.66e-5 | 2.80e-5 | 2.54e-5 | |
| | 5 | 0.49 | 1.043 | 0.83 | 0.80 | 2.48 | 2.018 | 1.53 | 1.20 | |
| Rosenbrock | 10 | 8.32 | 8.32 | 8.03 | 8.06 | 35.99 | 31.30 | 14.43 | 9.62 | |
| | 20 | 18.86 | 18.78 | 18.97 | 18.74 | 403.57 | 330.97 | 82.83 | 64.14 | |
| | 50 | 48.91 | 48.79 | 48.97 | 48.86 | 7606.79 | 6353.38 | 572.33 | 481.14 | |
| | 2 | 0.003 | 9.66e-4 | 0.003 | 0.002 | 0.05 | 0.01 | 0.02 | 0.006 | |
| | 5 | 0.008 | 0.003 | 0.007 | 0.003 | 2.59 | 0.90 | 0.72 | 0.17 | |
| Ackley | 10 | 0.11 | 0.035 | 0.07 | 0.019 | 5.11 | 2.84 | 2.42 | 0.76 | |
| | 20 | 0.164 | 0.046 | 0.18 | 0.06 | 8.30 | 4.46 | 3.91 | 2.39 | |
| | 50 | 0.165 | 0.044 | 0.25 | 0.08 | 12.62 | 7.76 | 6.41 | 4.03 | |
| | 2 | 1.73e-5 | 2.42e-5 | 7.42e-6 | 1.01e-5 | 1e-3 | 5.19e-4 | 5.15e-4 | 3.71e-4 | |
| | 5 | 2.99e-4 | 1.65e-4 | 1.05e-4 | 1.02e-4 | 2.67 | 2.22 | 1.32 | 0.92 | |
| Rastrigin | 10 | 0.62 | 0.44 | 0.33 | 0.16 | 22.83 | 20.08 | 14.70 | 10.63 | |
| | 20 | 2.72 | 2.32 | 3.38 | 2.56 | 89.97 | 83.62 | 60.24 | 59.30 | |
| | 50 | 9.93 | 3.28 | 10.095 | 4.46 | 376.58 | 366.07 | 315.46 | 301.69 | |
| | 2 | 2.85e-5 | 3.03e-5 | 2.2e-5 | 2.8e-5 | 7.2e-5 | 5.87e-5 | 4.2e-5 | 2.5e-5 | |
| | 5 | 0.67 | 0.73 | 0.75 | 0.81 | 2.39 | 2.103 | 1.27 | 1.21 | |
| Schwefel | 10 | 8.33 | 8.18 | 8.13 | 8.02 | 37.59 | 30.4 | 10.15 | 9.71 | |
| | 20 | 18.84 | 18.84 | 18.85 | 18.80 | 424.11 | 310.51 | 83.05 | 67.81 | |
| | 50 | 49.13 | 48.82 | 49.22 | 48.80 | 7678 | 6104 | 553.90 | 501.33 | |
| | 2 | 0.003 | 1.35e-5 | 0.004 | 3.26e-6 | 0.01 | 2.16e-4 | 0.007 | 1e-4 | |
| | 5 | 0.05 | 0.005 | 0.051 | 0.009 | 0.62 | 0.07 | 0.37 | 0.04 | |
| Griewangk | 10 | 0.49 | 0.03 | 0.42 | 0.02 | 1.76 | 0.47 | 1.04 | 0.35 | |
| | 20 | 0.57 | 0.05 | 0.74 | 0.02 | 8.27 | 1.05 | 1.63 | 0.72 | |
| | 50 | 0.59 | 0.007 | 0.78 | 0.01 | 71.18 | 1.75 | 7.49 | 1.07 | |

Table 2: Mean value of the objective function (after 5000 generations), averaged over 20 trials.

| Function | Dims | αKBS | αKBS | βKBS | βKBS | BLX- α | BLX- α | SBX | SBX | SciKit |
|--------------------|------|---------------------|---------------------|--------------------|--------------------|---------------|---------------|--------|--------|---------|
| FUNCTION | Dims | +SM | +GM | +SM | +GM | +SM | +GM | +SM | +GM | |
| | 2 | 10.54 | 10.44 | 10.35 | 10.51 | 8.63 | 8.63 | 8.62 | 8.62 | 10.31 |
| | 5 | 37.05 | 37.24 | 36.97 | 37.002 | 31.51 | 31.54 | 31.37 | 31.40 | 64.07 |
| 4-Means-Clustering | 10 | 61.44 | 61.61 | 61.33 | 61.23 | 50.20 | 50.17 | 49.78 | 49.94 | 167.52 |
| | 20 | 97.29 | 97.14 | 96.96 | 97.15 | 80.58 | 80.55 | 83.62 | 83.28 | 369.13 |
| | 50 | 159.24 | 159.35 | 159.25 | 159.24 | 143.47 | 142.37 | 150.87 | 148.77 | 1063.29 |

Table 3: Mean value of the objective function (after 5000 generations) for the 4means clustering problem (compared to the 4-means classifier in the SciKit toolbox for Python, averaged over 20 trials.

KBS+SM outperforms α KBS+SM in 5 instances, α KBS+GM outperforms β KBS+GM in 6 instances and β KBS+GM outperforms αKBS +GM in 3 (the rest are not statistically significant). Overall, αKBS has a slight advantage over the other variant.

Overall, we attribute the relative underperformance of BLX- α and SBX operators to our choice of elitism and selection function that prevent successful exploitation of promising fitness basins. We intend to address this problem in our future work.

5 Conclusions and Future Work

In this article we have presented and tested a new recombination operator for RC-GAs, a variant of the K-Bit-Swap that shares certain features with AX and BLX- α crossovers and Gaussian mutation. The principal difference is that in the KBS operator the locations of the bits selected in the two strings do not match, but are chosen randomly. We have considered two versions: chosen the two sites both uniformly at random, and using a normal distribution centered on the selected bit in the first string.

Both KBS operators have been shown to be superior for functional optimization problems to both BLX- α and SBX crossovers, but underperform on the 4-means approximation problem.

We also looked into some theoretical properties of presented operators. KBS samples different genes in both strings, thus slightly compensating for the absence of an exploration bias. If we consider uniform crossover and a simple 1-bit mutation (a standard choice for many applications), it is clear that fairly quickly the bits in the parents, v_1 and v_2 will be close, and even if we construct a certain interval around these values (as in BLX- α crossover), we can easily get stuck in some unpromising fitness region. KBS offers a workaround: although new values are not sampled from outside of the interval between the two parents, the second parent's value may be very different from the value in the same feature, thus it mimics exploration ability. Since the location selection for KBS is not restricted to the current feature, even if other features have already converged to the local optima, KBS has a relatively high probability of selecting a good schema and sampling in the area close to the optimal solution. Compared to the BLX- α operator new values lie strictly between the values selected in the parents. Therefore, both variants of the KBS operator are heavily biased towards exploitation rather than further exploration of the search space (see [8, 11, 22]).

The logical next step would be to enhance the operator with an interval or other features that would enable generation of values outside of this interval. Also, to explore KBS properties further, we intend to study the selection pressure mechanisms that pushes evolution towards areas with high-quality schemata (in this article a simple tournament selection was used) and more sophisticated elitism functions (instead of the single fittest string). We believe that working along these lines will help improve performance of RCGAs on multidimensional and multimodal functions.

References

- [1] R. B. Agrawal, K. Deb, and R. B. Agrawal. Simulated binary crossover for continuous search space. 1994.
- [2] A. Blanco, M. Delgado, and M. Pegalajar. A real-coded genetic algorithm for training recurrent neural networks. *Neural networks*, 14(1):93–105, 2001.
- [3] M. Crepinšek, S.-H. Liu, and M. Mernik. Exploration and exploitation in evolutionary algorithms: a survey. ACM Computing Surveys (CSUR), 45(3):35, 2013.
- [4] K. Deb, A. Anand, and D. Joshi. A computationally efficient evolutionary algorithm for real-parameter optimization. *Evolutionary computation*, 10(4):371– 395, 2002.

- [5] K. Deb and H.-g. Beyer. Self-adaptive genetic algorithms with simulated binary crossover. In *Complex Systems*. Citeseer, 1995.
- [6] B. Doerr, E. Happ, and C. Klein. Crossover can provably be useful in evolutionary computation. In *Proceedings of the 10th annual conference on Genetic* and evolutionary computation, pages 539–546. ACM, 2008.
- [7] S. M. Elsayed, R. Sarker, D. L. Essam, et al. Ga with a new multi-parent crossover for solving ieee-cec2011 competition problems. In *Evolutionary Computation (CEC), 2011 IEEE Congress on*, pages 1034–1040. IEEE, 2011.
- [8] L. J. Eshelman. Real-coded genetic algorithms and interval-schemata. Foundations of genetic algorithms, 2:187–202, 1993.
- [9] S. Finck, N. Hansen, R. Ros, and A. Auger. Real-parameter black-box optimization benchmarking 2010: Presentation of the noisless functions. Technical report, Citeseer, 2010.
- [10] S. García, D. Molina, M. Lozano, and F. Herrera. A study on the use of nonparametric tests for analyzing the evolutionary algorithms behaviour: a case study on the cec2005 special session on real parameter optimization. *Journal of Heuristics*, 15(6):617–644, 2009.
- [11] D. E. Goldberg. Genetic algorithms in search, optimization, and machine learning, 1989. ISBN: 0-201-15767-5, 1989.
- [12] J. A. Hartigan and M. A. Wong. Algorithm as 136: A k-means clustering algorithm. *Applied statistics*, pages 100–108, 1979.
- [13] F. Herrera, M. Lozano, E. Pérez, A. M. Sánchez, and P. Villar. Multiple crossover per couple with selection of the two best offspring: an experimental study with the blx-α crossover operator for real-coded genetic algorithms. In Advances in Artificial Intelligence, pages 392–401. Springer, 2002.
- [14] F. Herrera, M. Lozano, and A. M. Sánchez. A taxonomy for the crossover operator for real-coded genetic algorithms: An experimental study. *International Journal of Intelligent Systems*, 18(3):309–338, 2003.
- [15] F. Herrera, M. Lozano, and A. M. Sánchez. Hybrid crossover operators for realcoded genetic algorithms: an experimental study. *Soft Computing*, 9(4):280–298, 2005.

- [16] J. H. Holland. Adaptation in natural and artificial systems: an introductory analysis with applications to biology, control, and artificial intelligence. U Michigan Press, 1975.
- [17] T. Kanungo, D. M. Mount, N. S. Netanyahu, C. D. Piatko, R. Silverman, and A. Y. Wu. An efficient k-means clustering algorithm: Analysis and implementation. *Pattern Analysis and Machine Intelligence, IEEE Transactions on*, 24(7):881–892, 2002.
- [18] K. Krishna and M. N. Murty. Genetic k-means algorithm. Systems, Man, and Cybernetics, Part B: Cybernetics, IEEE Transactions on, 29(3):433–439, 1999.
- [19] S.-H. Ling and F. F. Leung. An improved genetic algorithm with average-bound crossover and wavelet mutation operations. *Soft Computing*, 11(1):7–31, 2007.
- [20] Z. Michalewicz. Genetic algorithms+ data structures= evolution programs. Springer Science & Business Media, 2013.
- [21] Z. Michalewicz and C. Z. Janikow. Handling constraints in genetic algorithms. In *ICGA*, pages 151–157, 1991.
- [22] M. Mitchell. An introduction to genetic algorithms, 1996. PHI Pvt. Ltd., New Delhi, 1996.
- [23] M. Mitchell, S. Forrest, and J. H. Holland. The royal road for genetic algorithms: Fitness landscapes and ga performance. In *Proceedings of the first european* conference on artificial life, pages 245–254. Cambridge: The MIT Press, 1992.
- [24] T. Pencheva, M. Angelova, K. Atanassov, and P. Vasant. Genetic algorithms quality assessment implementing intuitionistic fuzzy logic. Handbook of Research on Novel Soft Computing Intelligent Algorithms: Theory and Practical Applications, page 327, 2013.
- [25] O. Roeva, T. Slavov, and S. Fidanova. Population-based vs. single point search meta-heuristics for a pid controller tuning. Handbook of Research on Novel Soft Computing Intelligent Algorithms: Theory and Practical Applications, P. Vasant (Ed.), IGI Global, pages 200–233, 2013.
- [26] W. M. Spears et al. Crossover or mutation. Foundations of genetic algorithms, 2:221–237, 1992.

- [27] M. Srinivas and L. M. Patnaik. Adaptive probabilities of crossover and mutation in genetic algorithms. Systems, Man and Cybernetics, IEEE Transactions on, 24(4):656–667, 1994.
- [28] A. Ter-Sarkisov. Computational Complexity of Elitist Population-Based Evolutionary Algorithms. PhD thesis, Massey University, 2012.
- [29] A. Ter-Sarkisov, S. Marsland, and B. Holland. The k-Bit-Swap: A New Genetic Algorithm Operator. In *Genetic and Evolutionary Computing Conference* (GECCO) 2010, pages 815–816, 2010.
- [30] M. Thakur. A new genetic algorithm for global optimization of multimodal continuous functions. *Journal of Computational Science*, 2013.
- [31] K. Wagstaff, C. Cardie, S. Rogers, S. Schrödl, et al. Constrained k-means clustering with background knowledge. In *ICML*, volume 1, pages 577–584, 2001.
- [32] A. H. Wright et al. Genetic algorithms for real parameter qptimization. In FOGA, pages 205–218. Citeseer, 1990.
- [33] Y. Yoon and Y.-H. Kim. The roles of crossover and mutation in real-coded genetic algorithms. *Bio-Inspired Computational Algorithms and Their Applications, InTech*, 2012.
- [34] Y. Yoon and Y.-H. Kim. Geometricity of genetic operators for real-coded representation. Applied Mathematics and Computation, 219(23):10915–10927, 2013.