Rotationally Invariant Crossover Operators in Evolutionary Multi-objective Optimization

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Abstract. Multi-objective problems with parameter interactions can present difficulties to many optimization algorithms. We have investigated the behaviour of Simplex Crossover (SPX), Unimodal Normally Distributed Crossover (UNDX), Parent-centric Crossover (PCX), and Differential Evolution (DE), as possible alternatives to the Simulated Binary Crossover (SBX) operator within the NSGA-II (Non-dominated Sorting Genetic Algorithm II) on four rotated test problems exhibiting parameter interactions. The rotationally invariant crossover operators demonstrated improved performance in optimizing the problems, over a non-rotationally invariant crossover operator.

1 Introduction

Traditional genetic algorithms that use low mutation rates and fixed step sizes have significant trouble with problems with interdependent relationships between decision variables, but are perfectly suited to many of the test functions currently used in the evaluation of genetic algorithms [1]. These test functions are typically linearly separable and can be decomposed into simpler independent problems. Unfortunately, many real-world problems are not linearly separable, although linear approximations may sometimes be possible between decision variables.

Interdependencies between variables can be introduced into a real-coded functional problem by rotating the coordinate system of a test function. A rotated problem cannot be solved efficiently by the directionless step-sizes and low mutation rates that Genetic Algorithms typically use [1]. Although the NSGA-II is a very robust multi-objective optimization algorithm it suffers from similar limitations as traditional Genetic Algorithms on these problems.

Previous work has reported on the poor performance of a number of Multi-objective Evolutionary Algorithms, including the NSGA-II, on a rotated problem [2]. NSGA-II uses a crossover technique called Simulated-Binary Crossover (SBX) [3,4], combined with a uniform crossover operator in which half the time parameters of an offspring solution are replaced with parameters from a parent solution. This crossover technique searches effectively along the principle

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coordinate axes of the decision space. This makes finding more optimal solutions difficult when the decision space is large, and the problem has parameter interactions. Problems which are rotated, and not aligned with the coordinate axes typically require correlated self-adapting mutation step sizes in order to efficiently search for optimal solutions [1].

Differential Evolution (DE) has previously demonstrated rotationally invariant behaviour in the single objective and multiobjective domain [5,6,7]. Simplex Crossover (SPX), Parent Centric Crossover (PCX), and unimodal Normal Distribution Crossover (UNDX-m) have also demonstrated rotationally invariant behaviour on single objective test problems. This provides the motivation to study the worth of these multi-parent crossover techniques on rotated multi-objective optimization problems, where such characteristics are desirable.

Experiments have been conducted on rotated problem from [7]. These problems were rotated arbitrarily and uniformly in the decision space in order to test the rotationally invariant behaviours of the crossover operators.

In Section 2 we will briefly introduce the crossover operators used in this study, followed by Section 3, where the methodology and parameters associated with the experiments are discussed. Section 4 discusses the results of these experiments, followed by the conclusions drawn from this study in Section 5.

2 Background

The NSGA-II uses a simulated binary crossover operator [4] with uniform crossover to generate offspring parameter values. The SBX operator takes two parents and produces two offspring, but does not have the property of rotational invariance because the correlation between the location of parents, and the location of offspring which are generated, is lost under a rotation of the decision space. The discrete crossover of variables also results in non-rotationally invariant behaviour. For example, if an offspring vector has a parameter replaced by a parent parameter, as it might under some uniform crossover scheme, rotational invariance is destroyed [8]. It has been shown that the SBX has a zero probability of generating some points in the space between two parents [9], although in the new version of SBX implemented in the latest revision of NSGA-II, this problem has been addressed by generating offspring in quadrants adjacent to the location of the parents, as well as surrounding the parents.

The UNDX crossover [10] has demonstrated excellent performance in optimizing highly epistatic functions [11]. It generates offspring around a centroid region specified by a number of parents. It has been applied to some difficult real world problems such as design of optical lens systems [12]. A multi-parent variant of the UNDX was proposed, called UNDX-m [13]. The UNDX-m covers the search space more effectively by having a greater diversity of offspring generated, and it is this variant that we will be considering.

The PCX [14,15] is similar to the UNDX-m, but instead of distributing the offspring around the centroid of a number of parents, the offspring distribute around the parents themselves.

The Simplex crossover (SPX) was originally proposed in [16]. It generates a simplex from a number of parents. This simplex is expanded, and offspring are generated inside the expanded region.

The other reproduction technique studied here is Differential Evolution, which differs from other EAs in the mutation and recombination phase. Differential Evolution has also been applied to multi-objective problems [17,18,19,20,6,7]. Unlike stochastic techniques such as Genetic Algorithms and Evolutionary Strategies, where perturbation occurs in accordance with a random quantity, Differential Evolution uses weighted differences between solution vectors to perturb the population. The variant of differential evolution used in this study is known as *DE/current-to-rand/1* [8]. In order to maintain diversity, a Log-normal *dithering* operator was employed as well [21]. This operator maintains rotational invariance, while helping to randomly perturb individuals within the population.

3 Experiments

In order to test each of the crossover techniques, the crossover operator of NSGA-II was replaced with one of the rotationally invariant crossover operators. For the SPX, UNDX-m, and PCX, a single set of parents was randomly selected each generation from the mating pool. These parents were used to generate 100 new offspring individuals. For the DE and SBX variants, parents were randomly selected from the mating pool, and this was repeatedly done in a single generation for each of the 100 offspring generated. A population size of 100 individuals was used for each of the algorithms on each of the test problems. A number of the crossover techniques investigated here have not previously been studied within the NSGA-II framework, and we expect that some of the choices of our parameter settings to be sub-optimal for the problems explored. It is not our intention to perform a comparative study in order to find the best parameter settings of these crossover techniques, but we do expect non-specifically tuned settings to demonstrate improvements in the performance of the NSGA-II with the rotationally invariant behaviour of the DE, SPX, UNDX-m, and PCX operators. A number of appropriate parameter settings have been reported for these operators and we have utilised these reported settings where possible. It should be noted that these settings were reported with respect to single-objective optimization problems. We leave a more detailed comparative study of these operators on rotated multi-objective problems, as an area of future study.

For the DE variant of NSGA-II, F was set to 0.8 and K was set to 0.6. Suggestions from the literature helped guide our choice of parameter values for the NSDE [5]. The factor which controls the spread of the distribution for F in the dithering operator was set to 0.5 [21].

In the SPX operator, the simplex size, ϵ, determines the size of the expanded simplex, and we have used $\sqrt{n+1}$ which was used in previous studies in the single objective domain, where n is the decision space dimension. A mutation rate of 0.1 was also used with the UNDX-m, PCX, SPX, and SBX variants, using the mutation operator in NSGA-II. For the UNDX-m operator, the parameters

$\sigma_\xi = \frac{1}{\sqrt{m}}$ and $\sigma_\eta = \frac{0.35}{\sqrt{n-m}}$ were recommended in [13] and we have used these values in this study. For the PCX, the σ_ξ and σ_η parameters were set to 0.7 and 0.2 respectively. The PCX variant is sensitive to the σ_ξ parameter. If σ_ξ is too small the offspring generated do not spread across the Pareto-optimal front. In the UNDX-m and PCX version of NSGA-II, m was assigned a value of 3. The NSGA-II used a crossover rate of 0.9, but the other variants each used a crossover rate of 1.0.

Experiments were conducted on the unimodal problem R1, R2, R3, and R4, from [7]. Each of these problems incorporates features which are designed to trap points from progressing along the Pareto-optimal front. Problem R1 is unimodal. Problem R2 is discontinuous in the objective space. Problem R3 has a non-uniform mapping between the decision and objective spaces. Problem R4 is deceptive and has a non-local Pareto-optimal front which can trap points from progressing to the global Pareto-optimal front. These problems are described in more detail in [7]. The problems are also 10-dimensional in the decision space. Rotations were performed in the decision space, on each plane, using a random uniform rotation matrix generated using the technique described in [7]. The rotation introduces non-linear dependencies between all parameters. Each algorithm was run 50 times on each test problem, for a total of 800 generations (80,000 problem evaluations) for each run. A new random uniform rotation matrix was generated for each run of each algorithm. For the purposes of evaluating the algorithms, the generational distance metric was employed, as well as its inverse, in order to measure both the convergence to the Pareto-optimal front, and the diversity of solutions across the front [6]. The GD(Q,P*) metric measure the convergence of the non-dominated set Q, towards the Pareto-optimal set P. Similarly, the GD(P*,Q) metric measure the average distance of P to Q, thereby quantifying the degree that Q covers the set P. As both measures approach zero, one can expect good coverage of the Pareto-optimal set, as well as good convergence.

4 Discussion and Results

Previous work has reported on problem R1 [7] and the tendency of the NSGA-II to migrate non-dominated solutions away from the Pareto-optimal region, as well as the difficulty in expanding across the Pareto-optimal front because of these easily favoured non-dominated solutions.

Each of the rotationally invariant crossover operators apparently yields superior performance over the SBX on this relatively simple problem, with respect to both convergence to the Pareto-optimal front and coverage across the front. The boxplots in Figure 1 also demonstrates that the variation in both the GD(Q,P*) which measures convergence, and the GD(P*,Q) which measure spread, is relatively low for the SPX, DE, UNDX, and PCX variants.

Over successive generations, the SBX operator generates non-dominated solutions which skew away from the Pareto-optimal front [7]. In Problem R2, the Pareto-optimal front is discontinuous. This characteristic exacerbates this behaviour further, because the infeasible regions do not allow better non-dominated

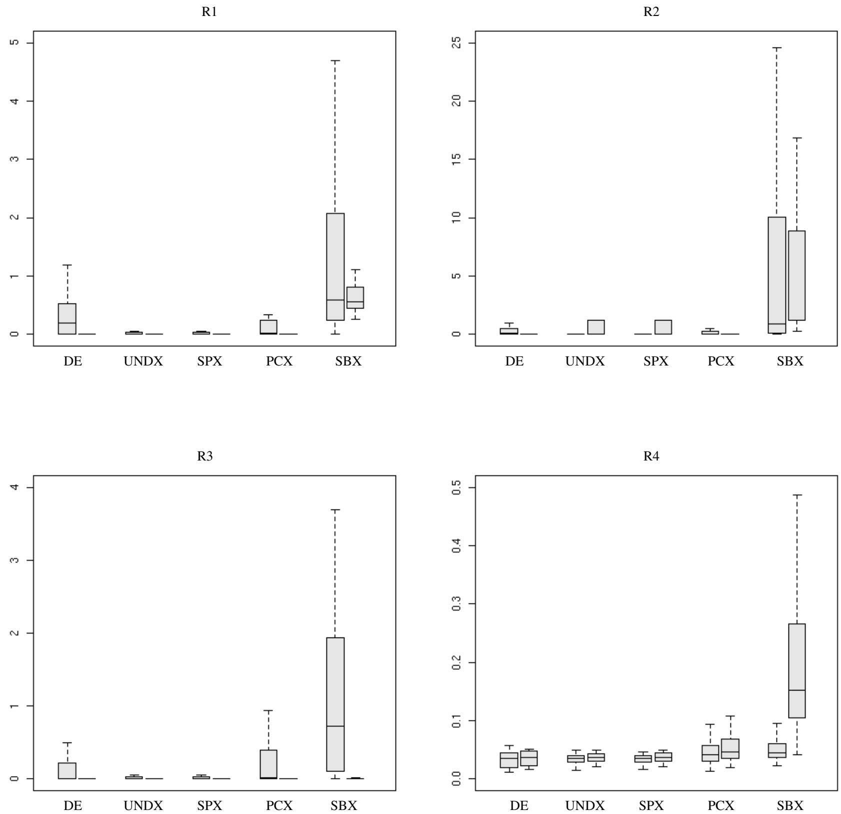

Fig. 1. Boxplots of the $GD(Q, P*)$ and $GD(P*, Q)$ for problem R1, R2, R3, and R4. The $GD(Q, P*)$ boxplot is always to the left of the $GD(P*, Q)$ boxplot.

solutions to be found through independent perturbations of the decision variables when the problem is rotated, as can be seen with the SBX in Figure 2. Contrasting this, from Figure 2, DE does manage to find a variety of solutions close to the Pareto-optimal region. In the boxplots of Figure 1 it is apparent that there is a high variation in the convergence and diversity of the non-dominated solutions found with SBX on R2. The measured convergence and diversity is also worse than the other rotationally invariant operators.

For Problem R3, the NSGA-II wih SBX achieved a rather good spread of non-dominated solutions, but was not able to converge sufficiently to the Pareto-optimal front. Each of the rotationally invariant crossover operators outperformed the SBX on this problem as well.

Problem R4 is highly multimodal, and deceptive. When this problem is rotated, a number of regions can hamper SBX from increasing the spread of solutions across a non-dominated front. This is apparent in the boxplot of Figure 1 as well, where the average of the GD(P*,Q) metric is significantly worse than the rotationally invariant schemes.

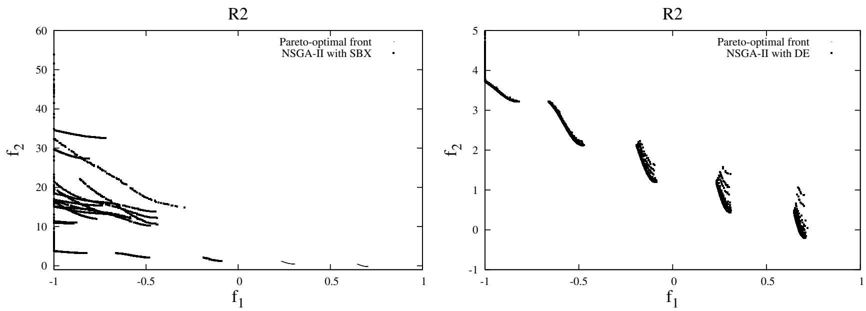

Fig. 2. 50 runs of the NSGA-II with SBX and DE Problem R2

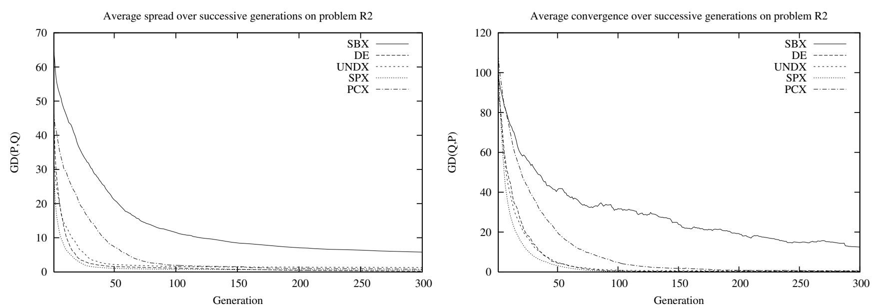

Fig. 3. Average $GD(Q, P*)$ and $GD(P*, Q)$ for problem R2 over 300 generations

From the boxplots in Figure 1 it is apparent that the DE variant demonstrated very competitive performance with respect to the spread of solutions on Problem R1, R2, and R3. It is also of relevance that the number of evaluations required can be significantly reduced through the use of rotationally invariant crossover operator in the presence of parameter interactions. This is demonstrated by the plots in Figure 3. These plots demonstrate the superior performance on Problem R2 of the DE, SPX, UNDX, and PCX variants, in comparison with the baseline NSGA-II with SBX. It is apparent that the rotationally invariant crossover operators have faster convergence to the Pareto-optimal front, while also maintaining a diverse set of solutions across the front. This has important practical relevance to real-world problems which often exhibit parameter interactions and also have computationally expensive evaluations of solutions.

5 Conclusion

This paper has described an empirical study of the effects that rotation of problems has on the NSGA-II. Rotation can trap the search on four problems with the properties of uni-modality, discontinuous Pareto-optimal fronts, a non-uniform mapping between the objective and decision space, and a problem with a deceptive front. We have demonstrated that on these four problems, that the UNDX, SPX, and DE outperformed the SBX, taking into consideration the performance metrics for convergence to the Pareto-optimal front and distribution of solutions across the front.

There are a number of future avenues of work which may be worthwhile considering, such as the effect of rotation on problems with more than two objectives, and when the dimensionality of the decision space increases. One would expect an increase in difficulty with an increase in the decision space dimension, with degraded non-dominated solutions becoming even more likely with non-rotationally invariany algorithms, because there will be far more non-dominated solutions generated which are not Pareto-optimal.

Secondly, it would be useful to conduct further tests on problems which do not have a linearly distributed Pareto-optimal set. This could be achieved using the Okabe framework for constructing multiobjective test problems [22].

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