Diversity Management in Evolutionary Many-Objective Optimization

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***Abstract*—In evolutionary multiobjective optimization, the task of the optimizer is to obtain an accurate and useful approximation of the true Pareto-optimal front. Proximity to the front and diversity of solutions within the approximation set are important requirements. Most established multiobjective evolutionary algorithms (MOEAs) have mechanisms that address these requirements. However, in *many*-objective optimization, where the number of objectives is greater than 2 or 3, it has been found that these two requirements can conflict with one another, introducing problems such as dominance resistance and speciation. In this paper, two diversity management mechanisms are introduced to investigate their impact on overall solution convergence. They are introduced separately, and in combination, and tested on a set of test functions with an increasing number of objectives (6–20). It is found that the inclusion of one of the mechanisms improves the performance of a well-established MOEA in *many*-objective optimization problems, in terms of both convergence and diversity. The relevance of this for *many*-objective MOEAs is discussed.**

***Index Terms*—Diversity requirement, evolutionary multiobjective optimization.**

I. Introduction

In MULTIOBJECTIVE optimization objectives are often in conflict with one another. In such cases, there is no single ideal “optimal” solution, rather a set of solutions for which an improvement in one of the objectives will lead to a degradation in one or more of the remaining objectives. Such solutions are known as *Pareto-optimal* or *non-dominated* solutions to the multiobjective optimization problem (MOP) and multiobjective evolutionary algorithms (MOEAs) strive to obtain an accurate and useful approximation of the true Pareto-optimal front that comprises the set of Pareto-optimal solutions.

Proximity to the true Pareto front and diversity of solutions within the approximation set are important requirements. Most established MOEAs have mechanisms that address these requirements [1], [2].

For many years, most evolutionary multiobjective optimization (EMO) applications focused on problems containing two or three conflicting objectives. *Many*-objective optimization, where the number of objectives is greater than 2 or 3, poses special problems for MOEAs. Recently, *many*-objective optimization has attracted great attention by the EMO research community which has studied the *many*-objective scalability of MOEAs.

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In popular MOEAs, such as NSGA-II [3], the solution’s convergence is usually biased and prioritized over its diversity. As a result, diversity promotion is usually deployed as a secondary consideration to proximity promotion in many MOEAs. Bosman and Thierens [4] justify this approach thus:

... the goal is to preserve diversity along an approximation set that is as close as possible to the Pareto-optimal front, rather than to preserve diversity in general, the exploitation of diversity should not precede the exploitation of proximity.

However, in *many*-objective optimization the proportion of non-dominated objective vectors in a MOEA population becomes very large as the number of objectives increases (see [5], [6]). Early papers by Purshouse and Fleming [7], [8] and Hughes [9] highlight some of the issues.

Recently, these challenges have stimulated a considerable body of continuing research. Wagner *et al.* [10] have undertaken a benchmarking exercise and investigated the behavior of some well-established MOEAs, contributing some valuable insights.

For example, a key issue is the fact that while dominance is used to drive the search toward the true Pareto front, in *many*-objective optimization it is less of a discriminator since there may be insufficient selective pressure to make progress in a given population. In such cases, the diversity criterion can begin to assume a greater (and unwanted) importance. Purshouse and Fleming [11] report that this can have a detrimental impact on the optimization process.

To offset the issue of loss of selective pressure, researchers have sought to reduce the proportion of non-dominated objective vectors by either modifying Pareto dominance [12] or through the introduction of different ranking schemes (e.g., [13]–[16]). Tsuchida *et al.* [17] have proposed a scheme for enhancing the performance of a widely used MOEA, NSGA-II [3] by controlling the degree of expansion or contraction of the dominance area of solutions. Preference information has also been used to identify the decision maker’s region of interest and thereby restrict the search space [6], [18], [19].

These are amongst a number of useful remedial developments that are being researched and have been briefly reviewed in 2008 by Ishibuchi *et al.* [20].

In fact, in a *many*-objective problem, no matter how far a prospective solution is from the Pareto front, if it performs well in terms of one objective it will have a high chance of being preferred in terms of Pareto dominance *and* the diversity criterion (being considered as an extreme solution) for selection for variation and survival. The increasing proportion of non-dominated solutions explored in large objective hyperspaces leads to diversity promotion mechanisms becoming more prominent and assuming greater importance as the selection criterion. Thus, when performing selection for variation, there will be a greater probability that solutions distant from one another will recombine and produce lower performance offspring known as lethals [11]. The superfluous production of lethals, known as dominance resistance, will consequently impair the optimization process and affect convergence toward the Pareto front. Ikeda *et al.* [21] were the first to recognize the problem of dominance resistance followed by Deb *et al.* [22].

Another impact of the increasing number of outlying non-dominated solutions in the approximation set, the emphasis of diversity over convergence, and the dominance resistance problem, is the combined effect of the aforementioned observations on the selection for survival process. When attempting to downscale the size of the active archive to its pre-determined size by such means as the truncation procedure in SPEA2 [23], *good* locally non-dominated solutions in terms of proximity toward the Pareto front might be filtered out at the expense of keeping good solutions in terms of diversity, but which may be distant from the true Pareto front.

This latter observation introduces an oscillatory behavior [24] in the evolutionary search by repeatedly discovering and filtering out good solutions that might have been previously explored. This oscillatory behavior impairs convergence toward the optimal tradeoff surface. As a result, as the number of competing objectives increases, the occurrence of the problem of *speciation* increases due to the combined effect of Pareto dominance-based selection and the active diversity promotion mechanisms. At the end of the optimization process, the probability of exclusively producing an approximation set with solutions excelling in a certain particular objective will increase. This problem was originally present in Schaffer's VEGA [25], and is widely considered to be the first approach for using EAs to solve multiobjective optimization.

The objective of this paper is to investigate new approaches and strategies for promoting diversity in evolutionary *many*-objective optimization. This is initially motivated by the outcome of the studies by Purshouse and Fleming [8], [11] which show that settings for a representative set of recombination and mutation operators that are suitable for optimization problems with a small number of objectives are inappropriate for optimization frameworks with a large number of conflicting objectives. The experimental results of their study highlight the conflict between the primary MOP requirement for convergence toward the Pareto front, and the secondary requirement for maintaining diversity in the approximation set. This conflict between convergence and diversity requirements in multiobjective optimization has a detrimental impact on the optimization process and is particularly aggravated in *many*-objective optimization frameworks.

Two new approaches for diversity promotion in *many*-objective optimization frameworks are proposed in the next section. Previously introduced in a preliminary form in [26], here we both extend the critical discussion and introduce the following new features:

1) an extension of the testing of *many*-objective problems to include MOPs containing 20 objectives;
2) the study of a second diversity management mechanism, an adaptive mutation operator, which takes into consideration solution diversity and local crowding;
3) a more rigorous evaluation of the introduced diversity mechanisms involving the "optimized" genetic operator parameters proposed by Purshouse and Fleming [11];
4) the inclusion of random search as a basis for the comparison of algorithm performance.

Diversity quality can be expressed in two forms: 1) uniformity, i.e., the evenness of distribution of solutions across the Pareto front, and 2) extent, which describes the spread of the Pareto front. Here, the effect of diversity extent, rather than uniformity, is addressed. We investigate the impact of this approach by also examining the resulting quality of diversity uniformity.

In Section II, two new mechanisms for managing diversity are introduced and the functionality of both mechanisms is described. The experimental setup is described in Section III. This covers the test functions used, optimizer configurations, and the metrics which are to be used to assess the performance of the optimizers. Performance evaluation is based on an analytical comparison of the results produced by a well-established and representative MOEA, NSGA-II, a version incorporating the new diversity management mechanisms, individually and in combination, and, as a baseline, the application of a random search approach. Experimental results are presented and discussed in Section IV. In Section V, a further set of experiments is conducted on more challenging test functions. Research outcomes are summarized in Section VI.

II. *Many*-Objective Optimization and Diversity Management

A. Proposed Diversity Management Mechanisms

In this paper, the requirement for promoting diversity in MOEAs is envisaged as a local, adaptive and varying requirement rather than a global necessity. In this paper, two mechanisms for managing diversity in a *many*-objective (more than three objectives) optimization framework are introduced and hybridized with NSGA-II [3]. NSGA-II is a multiobjective evolutionary algorithm which can be broadly regarded as representative of the larger family of MOEAs and, probably, the most widely used. The two diversity management mechanisms are:

1) DM1, which involves the activation and deactivation of diversity promotion according to the spread of solutions in a population;

2) DM2, which adapts the mutation range for each decision variable according to local conditions of spread and crowding.

The first diversity management mechanism, DM1, is an adaptive strategy that promotes the integration of very effective performance and diversity indicators, such as the *hypervolume* metric [27] and the *maximum spread* metric [27] to efficiently guide the search process of an MOEA toward the tradeoff surface of a MOP while controlling the diversity requirement.

Despite the recognized utility of the hypervolume metric [28] and its potential as a selection for survival strategy [29], [30] and as a solution ranking strategy replacing the Pareto dominance concept (whose practicality is debatable in *many*-objective frameworks), the metric suffers from some limitations [28], [31]. These limitations include the requirement for a judicious choice of non-trivial reference parameters, the multiplication of potentially non-commensurable objectives and, importantly, the computational complexity of calculating the hypervolume metric, which is exponential in the number of objectives [32].

In this paper, a particular, computationally efficient diversity metric which is based on the *maximum spread indicator* introduced by Zitzler [27] and is defined in (1), has been incorporated in the first diversity management mechanism, DM1. Purshouse and Fleming [11] previously used this indicator in an exploratory study aimed at investigating the suitability of some classical settings of MOEA parameters for optimization problems with more than three objectives.

In (1), D represents the measure of the diagonal of the hypercube formed by the extreme objective values attained in a certain approximation set Z_A. M denotes the number of objectives, and Z_A is a candidate objective vector solution which belongs to the approximation set Z_A

$$D = \left[\sum_{m=1}^{M} \left(\max_{z_A \in Z_A} \{z_{A_m}\} - \min_{z_A \in Z_A} \{z_{A_m}\} \right)^2 \right]^{1/2}. \quad (1)$$

In order to track the diversity quality of the manipulated set of solutions, the value of the spread indicator, D, presented in (1) is normalized with respect to the targeted spread corresponding to the set of solutions representing the expected Pareto front. It is only by knowing the normal and the desired condition that the abnormal and the undesired conditions, such as the dispersal of solutions in suboptimal regions of the objective space or, alternatively, the convergence to Pareto-optimal solutions outside the region of interest, can be defined and avoided. In other words, an application-dependent scale defining the approximate notion of a *low*, *ideal*, and *high* diversity is required to overcome the conflicting requirements of convergence and diversity, which is especially evident in high-dimensional problems.

In the context of the proposed mechanism, DM1, the decision maker, usually, and preferably, a domain expert, is only required to suggest an approximate estimate of the defining extremities of the *desired* tradeoff surface. These extremities will then serve as the vertices of the hypercube containing the ideally sought Pareto front.

Equation (1) will then be normalized with respect to the length of the diagonal of such a hypercube and the normalized diversity indicator is defined as

$$I_S = D \Bigg/ \left[\sum_{m=1}^{M} \left(\max_{z_* \in Z_*} \{z_{*_m}\} - \min_{z_* \in Z_*} \{z_{*_m}\} \right)^2 \right]^{1/2} \quad (2)$$

where z_t is a member of Z_t, which represents the targeted set of Pareto-optimal solutions.[1] The spread indicator (I_S) can take any positive real value. Ideally, an indicator value close to unity ($I_S = 1$) is sought (*ideal* diversity). Indicator values smaller than one ($I_S < 1$) signify *low* diversity among the solutions manipulated compared with the desired spread of solutions. On the other hand, indicator values larger than one ($I_S > 1$) highlight an excessive dispersal of the solutions in the objective space (*high* diversity). This kind of excessive dispersal in the hyperspace most likely causes the divergence of the solutions from the Pareto-optimal front and hampers the optimization process by introducing a cyclic behavior forcing the MOEA to repeatedly explore previously visited regions of the space.

The second diversity management mechanism, DM2, anticipates the possible wide dispersion of potential solution points by the polynomial mutation operator used in NSGA-II. DM2 seeks to control this dispersion in a managed way through the introduction of an adaptive mutation operator. This new mutation operator seeks to define the mutation range for the *set of decision variables* at each generation on the basis of the diversity *extent* of the locally non-dominated set of solutions and, for each *individual decision variable* within that set, on the local diversity as measured by NSGA-II's crowding measure.

A schematic presentation of how both diversity management mechanisms, DM1 and DM2, are incorporated in NSGA-II is illustrated in Fig. 1. A pseudo-code description is presented in Appendix A.

B. DM1 Functionality

Diversity management mechanism, DM1, is implemented as follows.

```
Calculate the spread indicator I_s for the current approximation set at generation i.
    If I_s < 1
Activate the diversity promotion mechanism in the selection for variation and the selection for survival process.
    Else If I_s ≥ 1
Deactivate the diversity promotion mechanism in the selection for variation and the selection for survival process.
```

This consists of calculating the spread indicator defined in (2) for the local front of non-dominated solutions achieved. The calculation of the spread indicator takes place at every generation of the optimization process prior to the execution

[1] If objectives are of different order of magnitude, it may be appropriate to normalize their values when calculating I_s.

of the genetic operators (selection for variation and selection for survival).

DM1 then adjusts and controls the global search processes of the MOEA in an informed way based on the local level of spread optimality. In other words, if the spread indicator reports an excessive dispersal of the local front of solutions in the objective space (i.e., $I_s \geq 1$), DM1 switches off the diversification mechanisms within the subsequent selection for variation and selection for survival procedures. The goal is to maintain the optimal tradeoff between convergence and diversity requirements. In the context of NSGA-II, therefore, at the selection for variation stage, deploying the binary tournament selection procedure, two candidate solutions are picked randomly and compared in terms of their Pareto dominance rank. The solution with the highest Pareto dominance rank is inserted in the mating pool. In the case where the two solutions share the same Pareto dominance rank, one of the two solutions is chosen randomly and included in the mating pool, disregarding the NSGA-II crowding measure which usually constitutes the secondary criterion for selection for variation. The selection for variation process continues until the mating pool is filled.

At the selection for survival stage, the diversity measure is again eliminated as a discriminatory criterion for selection. In the situation where the number of locally non-dominated solutions exceeds the prefixed size of the active archive, the solutions are selected randomly for survival and propagation to the succeeding generation of the optimization process.

On the other hand, when required (i.e., $I_s < 1$), the diversity promotion mechanisms are automatically activated in the selection for variation and the selection for survival procedures based on the diversity indicator monitoring the diversity of the locally non-dominated solutions.

C. DM2 Functionality

Diversity management mechanism, DM2, consists of an adaptive mutation operator designed to ensure the usual explorative and diversity-preserving benefits of the mutation process in evolutionary algorithms. Moreover, DM2's mutation operator is designed to avoid the problem of the mutation process causing deterioration by uncovering, *in a high-dimensional search space*, a locally non-dominated approximate solution which is remote from the true Pareto front and which can hinder the search process.

DM2's adaptive mutation operator is modeled on Deb and Goyal's polynomial mutation operator [33], where the magnitude of the variation of a certain decision variable is inversely proportional to a mutation distribution parameter. In the DM2, the magnitude of the normalized variation of each decision variable is governed by:

1) the value of the spread indicator (I_s) measuring the diversity extent of the locally non-dominated set of solutions;
2) the NSGA-II "crowding" measure which highlights the "*local*" diversity around each single solution.

Specific details are provided in Appendix B.

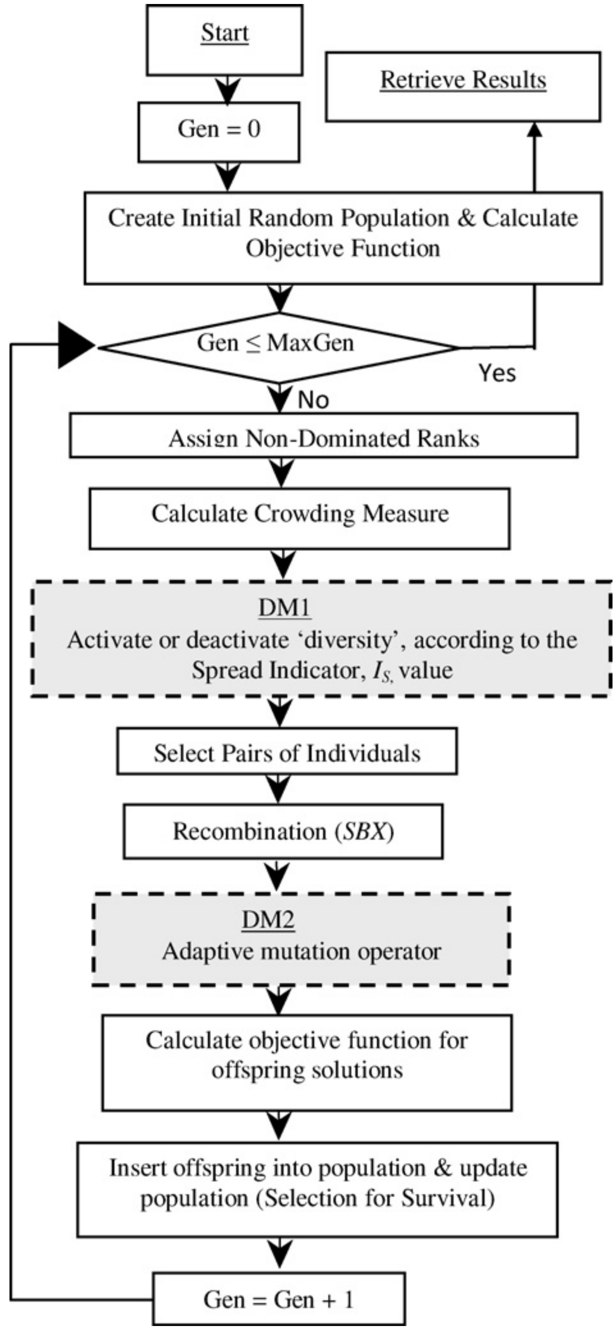

Fig. 1. NSGA-II with the addition of the DM mechanisms.

In the next section, the experimental framework used to test the performance of DM1, DM2, and their combined effect (DM) is presented. This includes a summary of the different optimization problems used, the configuration of the optimizers and the different performance metrics utilized for assessing the utility of the DMO.

III. Test Functions, Configurations, and Performance Metrics

A. Test Functions and Optimizer Configurations

Here, we adopt a similar approach to that of Purshouse and Fleming [11]. Our investigative study experiments with different versions of the scalable DTLZ2 test function introduced by Deb *et al*. [22]. DTLZ2 possesses a continuous and non-convex global Pareto front and comprises two types of decision variables responsible for controlling convergence of solutions toward the global Pareto front and the distribution of solutions in the objective space, respectively. DTLZ2, with its well-defined Pareto fronts, small computational cost, and effortless scalability is a suitable problem for the theoretical analysis and examination of new MOEA performances especially in the *many*-objective optimization contexts. Four different versions of the DTLZ2 test function, featuring 6, 8, 12, and 20-objective optimization problems, are used to assess the impact of the new diversity management mechanisms on NSGA-II. These four instances of DTLZ2 will be referred to as DTLZ2 (6), DTLZ2 (8), DTLZ2 (12), and DTLZ (20), respectively.

In order to assess the performance of the mechanisms, nine algorithms were executed on each of the DTLZ2 functions and their performances in terms of convergence and diversity were simultaneously visualized. The nine algorithms are summarized in Table I where Algorithms 3–8 present different variations of how DM1 and DM2 can be integrated with NSGA-II. Algorithms 3–6 were designed to assess the usefulness of each of the diversity management mechanisms, and Algorithms 7 and 8 assess their combined impact. Finally, for each of the DTLZ2 functions investigated, a random search (Algorithm 9) was also performed in order to baseline and put into context the performance of Algorithms 1–8.

The simulated binary crossover (SBX) [34], a two-parent crossover operator that produces two new solutions, is used in this paper.[2] Similar to the study by Purshouse and Fleming [11], each decision variable is independently considered for undertaking the variation operator. The probability of uniformly applying the variation operator on a certain decision variable, p_{ic}, is commonly set to a value of 0.5 alongside a distribution parameter value, $\eta_c = 15$ [11], [35]. In Purshouse and Fleming [11], these settings were shown to be suitable for optimizing DTLZ2 (3) but inappropriate for DTLZ2 (6) and DTLZ2 (12) problems, in terms of the resulting convergence of the produced results toward the Pareto fronts of these test functions, as well as in terms of solution diversity.

In this paper, two scenarios deploying two different settings for the SBX operator are investigated to assess the performance of the DMO when operating in the NSGA-II framework and optimizing each version of the DTLZ2 test function. The first scenario (involving Algorithms 1, 3, 5, and 7) consisted of the SBX operator configured with parameters normally used in the EMO community ($\eta_c = 15$ and $p_{\text{ic}} = 0.5$) [11], [35]. Based on the findings of Purshouse and Fleming [8], [11], the second scenario (involving Algorithms 2, 4, 6, and 8) consisted of well-chosen parameters for the SBX operator and which were expected to be more suitable for each of the DTLZ2 functions investigated. These two scenarios were intended to investigate the impact of the diversity management mechanisms and to quantify the level of improvement or deterioration that they might introduce when operating in the standard or the optimized configurations.

[2]It is a feature of the DTLZ test suite that the number of decision variables, n, is a function of the number of objectives. The use of SBX diminishes the impact of this aspect as SBX is not affected by n.

TABLE I

LIST OF ALGORITHMS INVESTIGATED

	Algorithm Name	Description
1	NSGA-II STD	NSGA-II with STandarD SBX parameters
2	NSGA-II OPT	NSGA-II with OPTimized SBX parameters
3	NSGA-II/DM1 STD	NSGA-II with standard SBX parameters and using DM1 mechanism only
4	NSGA-II/DM1 OPT	NSGA-II with optimized SBX parameters and using DM1 mechanism only
5	NSGA-II/DM2 STD	NSGA-II with standard SBX parameters and using DM2 mechanism only
6	NSGA-II/DM2 OPT	NSGA-II with optimized SBX parameters and using DM2 mechanism only
7	NSGA-II/DM STD	NSGA-II with standard SBX parameters and using both DM1 and DM2 mechanisms
8	NSGA-II/DM OPT	NSGA-II with optimized SBX parameters and using both DM1 and DM2 mechanisms
9	RS	Random search

TABLE II

OPTIMIZER CONFIGURATIONS

Size of population	100				
Number of generations/run	200				
Number of runs	10				
Crossover operator		Standard Configuration		Optimized Configuration	
		η_c	p_{ic}	η_c	p_{ic}
	DTLZ2(6)	15	0.5	15	0.1
	DTLZ2(8)	15	0.5	10	0.1
	DTLZ2(12)	15	0.5	10	0.05
	DTLZ2(20)	15	0.5	5	0.01
Mutation operator	NSGA-II and NSGA-II/DM1: Polynomial Mutation Probability: $1/n$				
		η_m		p_m	
	DTLZ2 (6)	20		≈0.06	
	DTLZ2 (8)	20		≈0.05	
	DTLZ2 (12)	20		≈0.04	
	DTLZ2 (20)	20		≈0.03	
	NSGA-II/DM and NSGA-II/DM2: DM2 adaptive mutation Probability: $1/n$				

In this paper, the polynomial mutation operator [33] was also used in NSGA-II (Algorithms 1 and 2) and NSGA-II/DM1 (Algorithms 3 and 4) when the utility of DM1 is assessed. The polynomial mutation was configured with the standard parameters for each of the DTLZ2 functions. The configuration of NSGA-II and its diversity management variations is presented in Table II.

All nine algorithms had identical numbers of objective function evaluations, population sizes, and number of runs. The performances of all nine algorithms are compared for each of the four instances of DTLZ2 deployed. In order to make a rigorous comparison of the optimizers and an accurate assessment of their performances, all nine algorithms were executed ten times and their results were compared at every execution.

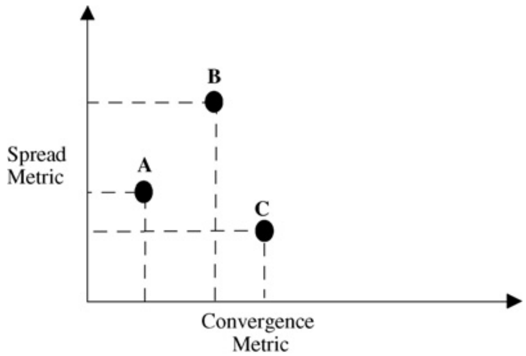

Fig. 2. Non-dominated evaluation metric.

B. Performance Metrics

In order to illustrate the performance of the two optimizers in terms of the desired requirements—convergence and diversity—the *non-dominated evaluation* metric [1] was used to simultaneously visualize the performance of the optimizers in terms of proximity to the Pareto front and in terms of diversity. The spread metric and the generational distance metric were used to evaluate the two competing objectives: Objective 1 is convergence and Objective 2 is diversity. The problem can then be formulated as a two-objective optimization scenario optimizing (minimizing) these two objectives. As a result, the performance of an optimizer **A** would be deemed superior to the performance of another optimizer **B** if its approximation set for the posed bi-objective optimization problem dominates the approximation set achieved by **B**. The non-dominated evaluation metric is illustrated in Fig. 2, where it can be inferred that optimizer **A** outperforms optimizer **B** in terms of convergence and diversity but it cannot be concluded that **A** outperforms **C**.

The normalized *maximum spread metric* (2) was used to measure the performance of the two optimizers in terms of the diversity quality of their produced results.

The convergence quality of the achieved approximation sets is assessed in terms of their proximity to the well-defined Pareto fronts of the DTLZ2 test function. The *convergence metric* used (Fig. 3) is the generational distance (GD) metric [36] for the case of a continuous Pareto-optimal reference set Z_* is used to measure the median proximity of the achieved approximation sets (Z_A) to the Pareto fronts of each of the DTLZ2 versions investigated. The proximity metric is presented in (3), where the value of $\left[\sum_{m=1}^{M}(z_m)^2\right]^{1/2}$ denotes the Euclidean distance from a certain objective vector z to the origin of the Cartesian coordinate system. This Euclidean distance is larger or equal to one with the equality only holding when the objective vector z is a Pareto-optimal solution

$$GD = median_{z_A \in Z_A}\left\{\left[\sum_{m=1}^{M}(z_{A_m})^2\right]^{1/2} - 1\right\}. \tag{3}$$

In order to better illustrate the results of the non-dominated evaluation metric produced by the different investigated algorithms, confidence ellipses [37] are also drawn around each algorithm's results. The confidence ellipses are used in this paper to establish the 95% confidence interval that might be used to predict new observations about a specific algorithm's performance. Confidence ellipses are drawn assuming that the two variables (convergence metric and diversity metric results) follow a bivariate normal distribution, and the longer axis of the ellipse is overlaid on the regression line formed by the data.

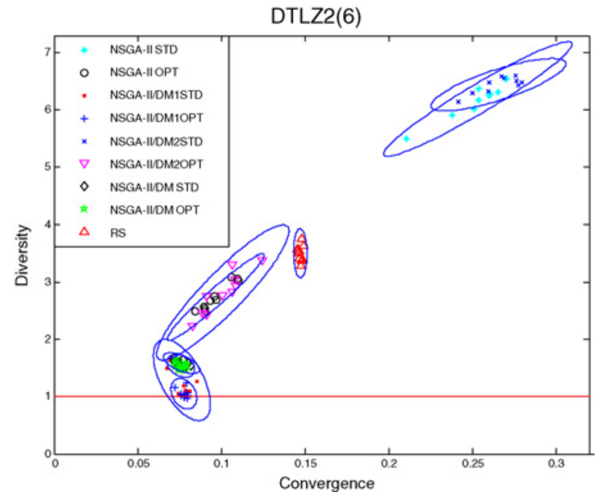

Fig. 3. Non-dominated evaluation metric results for Algorithms 1–9 on DTLZ2 (6).

Although management of diversity extent is the target of this paper, its impact on the quality of diversity uniformity is also investigated. An entropy-based metric [38] is used to measure the quality of the results produced by a certain optimizer in terms of the diversity uniformity. Mehr and Azarm's entropy metric has its roots in Shannon's entropy metric [39] which measures the flatness of a probability distribution function. For a full explanation of the metric, see [38].

IV. Results

In this section, the results achieved by the algorithms presented in Table I are illustrated for the test functions investigated. In Figs. 3 and 4, the values of the non-dominated evaluation metric achieved by all nine algorithms for DTLZ2 (6) and DTLZ2 (20) are presented. In Figs. 3 and 4 and subsequent figures showing the non-dominated evaluation metric results, 95% confidence ellipses are illustrated for the performance of each of the algorithms.

In Figs. 5–8, the values of the non-dominated evaluation metric achieved by Algorithms 5, 6, 7, and 8 (incorporating the DM2 adaptive mutation mechanism) are omitted. Instead, only the values of the non-dominated evaluation metric achieved by Algorithms 1, 2, 3, 4, and 9 for DTLZ2 (6), (8), (12), and (20), respectively, are illustrated. The solid reference line (corresponding to diversity = 1) in all figures represents the ideal diversity extent for the DTLZ2 functions.

From Figs. 3–8, the following general observations can be made.

Three distinct clusters of algorithms' performances are observed.

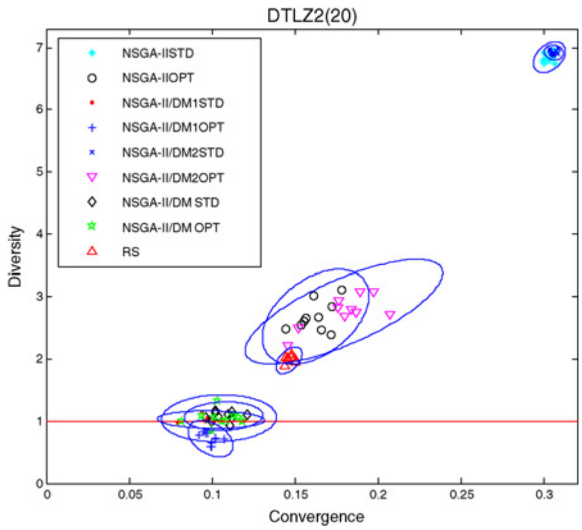

Fig. 4. Non-dominated evaluation metric results for Algorithms 1–9 on DTLZ2 (20).

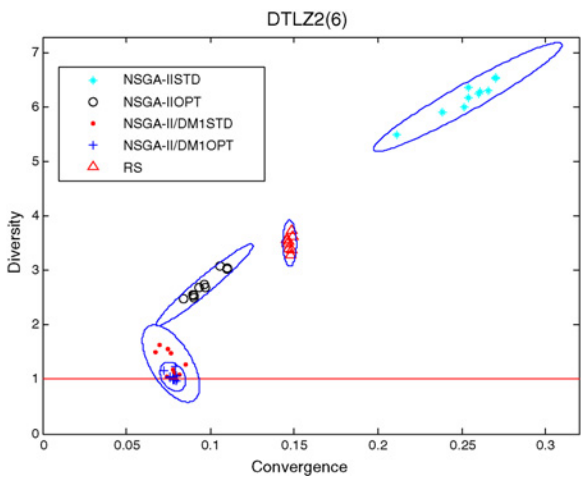

Fig. 5. Non-dominated evaluation metric results for Algorithms 1–4 and 9 on DTLZ2 (6).

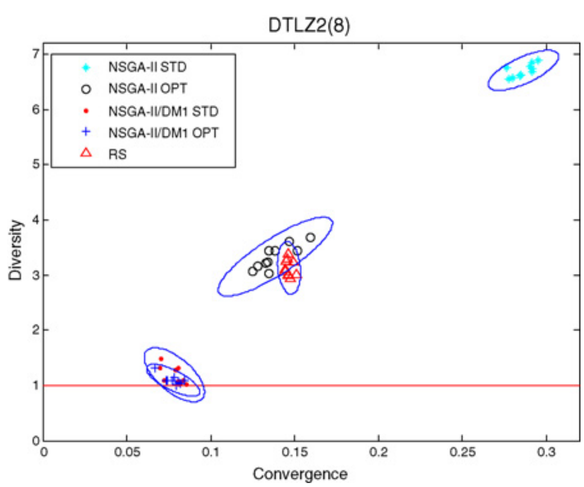

Fig. 6. Non-dominated evaluation metric results for Algorithms 1–4 and 9 on DTLZ2 (8).

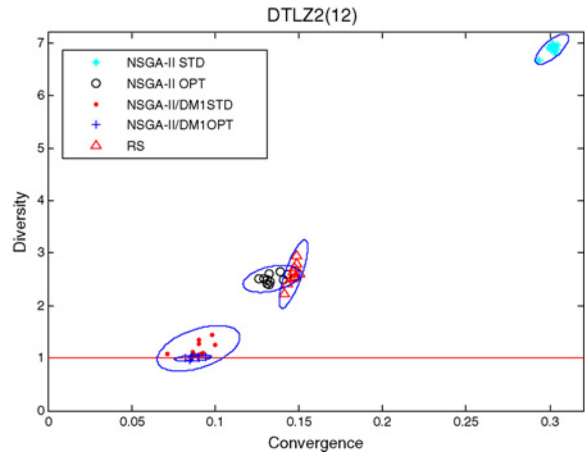

Fig. 7. Non-dominated evaluation metric results for Algorithms 1–4 and 9 on DTLZ2 (12).

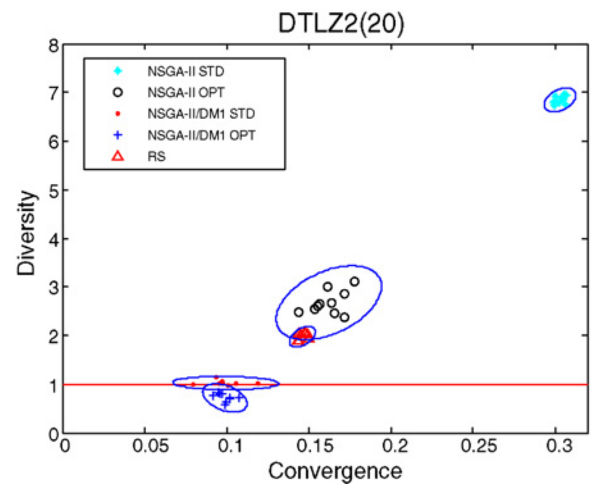

Fig. 8. Non-dominated evaluation metric results for Algorithms 1–4 and 9 on DTLZ2 (20).

TABLE III
PERFORMANCE CLASSIFICATION

Cluster Number	Performance	Algorithms
1	Best	3, 4, 7, and 8
2	Intermediate	2, 6, and 9[3]
3	Worst	1 and 5

[3]Especially when the number of objectives is = 8.

1) The performance of random search (Algorithm 9) seems to progressively improve, relative to the other algorithms, as the number of objectives increased.
2) The diversity extent of the handled approximation sets are excessive most of the time ($I_s > 1$).

The general classification of the algorithm performances is summarized in Table III.

After running the nine algorithms on all DTLZ2 test functions, it is observed that the DM2 mutation operator is not making a notable contribution and consequently the results of all nine algorithms are only shown in Figs. 3 and 4, which provide results for the extreme cases of DTLZ2 (6) and (20).

This decision is made in order to improve the clarity of results illustrated in Figs. 5–8.

In Figs. 3 and 4, the observed results for Algorithms 3, 4, 7, and 8 highlight good convergence (most GD values ≤ 0.12) to the Pareto front alongside a simultaneous near-optimal diversity.[4] The performance of the algorithms within Cluster 1 is insensitive to the choice of SBX parameters or the type of mutation operator. It can therefore be concluded that DM1 is the key mechanism contributing to improved results.

Closer inspection of Cluster 1 results in Figs. 3 and 4 reveals that the DM2 mutation operator might introduce some minor degradation in terms of the convergence criterion compared with the standard polynomial mutation. In hindsight, such a detrimental effect introduced by the DM2 mutation can be attributed to the way it encapsulates the diversity requirement as a goal and tries to control it by reducing the mutation range to handle excessive diversity. The "diversity awareness" design that the DM2 mutation is built upon seems to be limiting the explorative capabilities of the MOEA and slightly impairing the convergence of the solutions in the context of the DTLZ2 function.

Inspection of the results of Clusters 2 and 3 reinforces the findings of Purshouse and Fleming [11] that the use of an optimized configuration for the SBX operator improves performance. Further, the results demonstrate that random search is competitive with NSGA-II OPT when there are many objectives. This outcome is in no way suggesting that NSGA-II is a poor optimizer; instead it highlights the challenges and complexities involved in optimizing problems with increasing number of objectives. It must be stressed, however, that more recent MOEAs which use a modification of the Pareto dominance selection mechanism, such as ε-MOEA (see [40], [41]), are expected to perform better than NSGA-II OPT on *many*-objective problems.

As the number of objectives increases from 6 to 8, 12, and 20, two further observations can be made from Figs. 3–8 and Tables IV–VII. In Figs. 3–8, we observe that the clusters of algorithms become more distinct. This emphasizes the growing influence of the impact of DM1 (Cluster 1) and the effect of the optimized parameters on NSGA-II (Cluster 2), as the number of objectives increases. In Tables IV–VII, we observe that the number of occasions when I_s is less than or equal to 1 only increases for Cluster 1 algorithms.

Thus, Cluster 2 and Cluster 3 algorithms do not need diversification even for the 20-objective case, despite using the same population size. (In a side experiment it was found that population size plays a role for Cluster 1: when the population size was increased there were fewer occasions when I_s was less than or equal to 1.)

Further analysis of Cluster 1 algorithms (see Figs. 9 and 10) reveals that the I_s metric tends to decrease monotonically with the number of generations, and thus the diversity management mechanism is only activated later in an optimization sequence.

The corresponding diversity uniformity for the five algorithms of interest (namely random search and NSGA-II, with

[4]Optimal in terms of diversity extent. Future research will look at optimizing the uniformity of distribution, while controlling diversity extent.

TABLE IV
TOTAL NUMBER OF GENERATIONS (OUT OF A TOTAL OF 2000–200 PER ALGORITHM EXECUTION) WHERE $I_s \leq 1$ ON DTLZ2 (6)

Algorithm No.	Algorithm Name	No. of Generations Where $I_s \leq 1$
1	NSGA-II STD	0
2	NSGA-II OPT	0
3	NSGA-II/DM1 STD	13
4	NSGA-II/DM1 OPT	81
5	NSGA-II/DM2 STD	0
6	NSGA-II/DM2 OPT	0
7	NSGA-II/DM STD	0
8	NSGA-II/DM OPT	0
9	RS	0

TABLE V
TOTAL NUMBER OF GENERATIONS (OUT OF A TOTAL OF 2000–200 PER ALGORITHM EXECUTION) WHERE $I_s \leq 1$ ON DTLZ2 (8)

Algorithm No.	Algorithm Name	No. of Generations Where $I_s \leq 1$
1	NSGA-II STD	0
2	NSGA-II OPT	0
3	NSGA-II/DM1 STD	17
4	NSGA-II/DM1 OPT	109
5	NSGA-II/DM2 STD	0
6	NSGA-II/DM2 OPT	0
7	NSGA-II/DM STD	0
8	NSGA-II/DM OPT	0
9	RS	0

TABLE VI
TOTAL NUMBER OF GENERATIONS (OUT OF A TOTAL OF 2000–200 PER ALGORITHM EXECUTION) WHERE $I_s \leq 1$ ON DTLZ2 (12)

Algorithm No.	Algorithm Name	No. of Generations Where $I_s \leq 1$
1	NSGA-II STD	0
2	NSGA-II OPT	0
3	NSGA-II/DM1 STD	40
4	NSGA-II/DM1 OPT	453
5	NSGA-II/DM2 STD	0
6	NSGA-II/DM2 OPT	0
7	NSGA-II/DM STD	1
8	NSGA-II/DM OPT	54
9	RS	0

TABLE VII
TOTAL NUMBER OF GENERATIONS (OUT OF A TOTAL OF 2000–200 PER ALGORITHM EXECUTION) WHERE $I_s \leq 1$ ON DTLZ2 (20)

Algorithm No.	Algorithm Name	No. of Generations Where $I_s \leq 1$
1	NSGA-II STD	0
2	NSGA-II OPT	0
3	NSGA-II/DM1 STD	72
4	NSGA-II/DM1 OPT	1074
5	NSGA-II/DM2 STD	0
6	NSGA-II/DM2 OPT	0
7	NSGA-II/DM STD	21
8	NSGA-II/DM OPT	361
9	RS	0

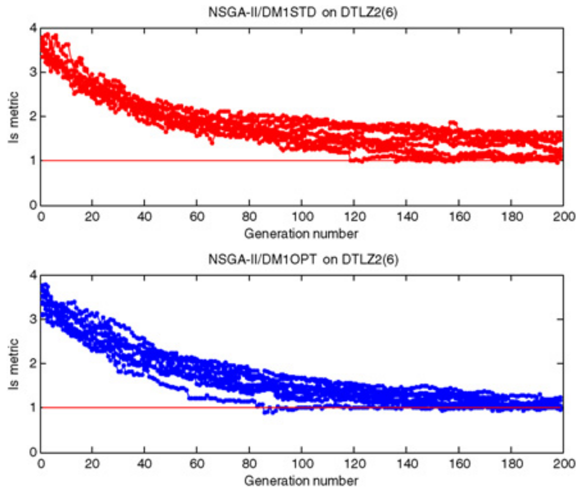

Fig. 9. I_s metric values on DTLZ2 (6).

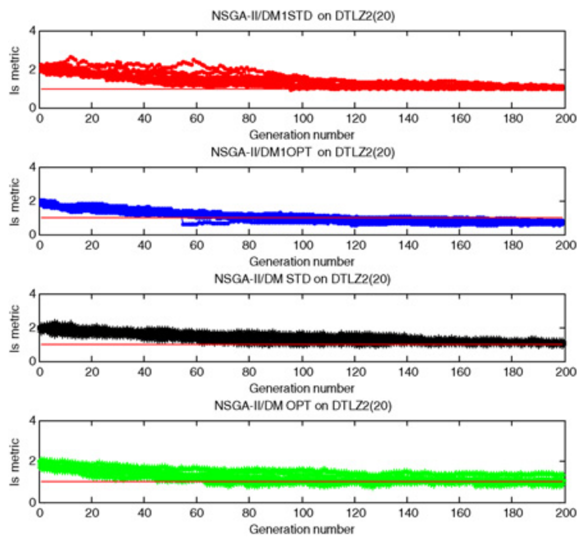

Fig. 10. I_s metric values on DTLZ2 (20).

and without DM1) is illustrated in Figs. 11 and 12 for the extreme cases of 6 and 20 objectives. (For brevity, results from the 8-objective and 12-objective cases and Algorithms 5–8 are omitted.)

The ideal level of diversity uniformity as measured by the normalized entropy metric is unity. The lowest value for diversity uniformity is 0.825 was achieved in one run of NSGA-II/DM1 OPT. Even for this case, such value of diversity uniformity is deemed acceptable. Nonetheless, it is apparent from both Figs. 11 and 12 that NSGA-II/DM1 tends to trade off diversity quality for diversity extent performance. Comparing the performance of the NSGA-II/DM1-OPT for the two cases (see Figs. 11 and 12), this tradeoff effect is lessened for the 20-objective case.

In this paper, our aim was to highlight the effect of excessive diversity on convergence and how the diversity management mechanisms might be good and simple remedial measures to address this. We have not attempted to improve the explorative powers of NSGA-II, as this was outside the scope of this paper.

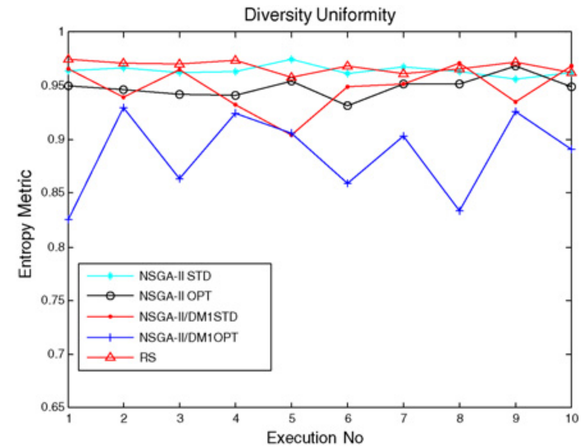

Fig. 11. Diversity uniformity results for Algorithms 1–4 and 9 on DTLZ2 (6).

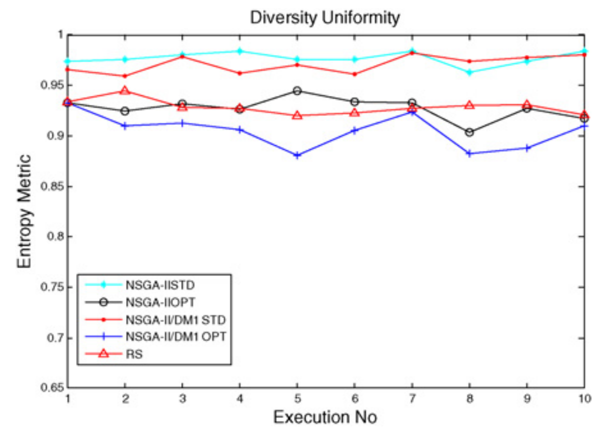

Fig. 12. Diversity uniformity results for Algorithms 1–4 and 9 on DTLZ2 (20).

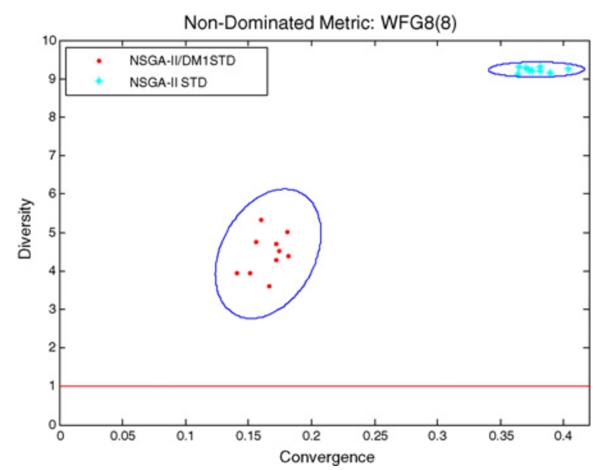

Fig. 13. Non-dominated evaluation metric results for Algorithms 1 and 3 on WFG8 (8).

V. Further Investigations

Shortcomings of the DTLZ2 (and the DTLZ test function suite, in general) are reported in Huband *et al.* [42]. For example, none of the problems are deceptive and none are "(practically) non-separable." As a result, the performance of DM1 is now investigated on two challenging test functions with nonseparable decision variables.

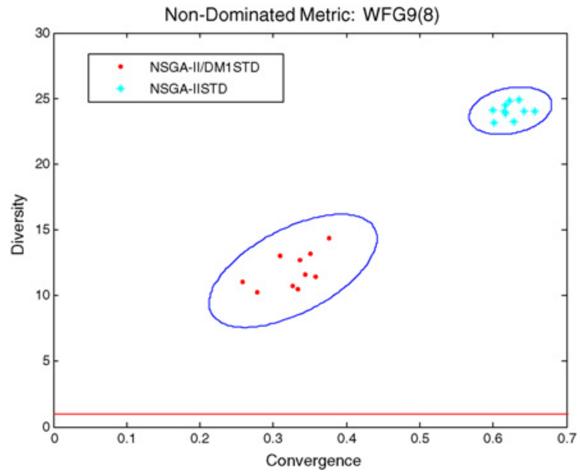

Fig. 14. Non-dominated evaluation metric results for Algorithms 1 and 3 on WFG9 (8).

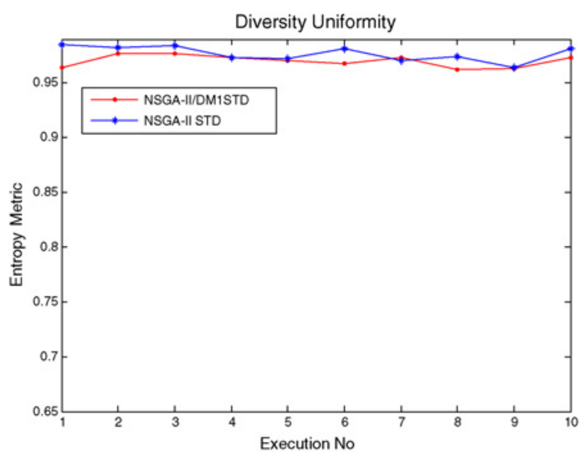

Fig. 15. Diversity uniformity results for Algorithms 1 and 3 WFG8 (8).

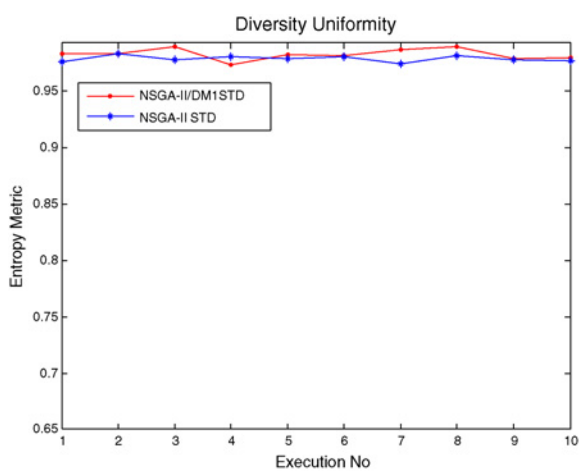

Fig. 16. Diversity uniformity results for Algorithms 1 and 3 WFG9 (8).

A nonseparable MOP is a problem with variable dependencies. Nonseparability is a feature that is common in real-world applications. In [42], Huband *et al.* proposed a test suite of nine scalable multiobjective problems featuring important characteristics such as nonseparability. Experiments involving the use of DM1 have been conducted on the full WFG test suite. In this paper, experiments on 8-objective instances of the test functions WFG8 and WFG9 [WFG8(8) and WFG9(8)], two complex and nonseparable test functions suggested in [42] are reported. These are both challenging and representative cases. WFG9, in particular, presents a deceptive decision space and represents a formidable challenge for most MOEAs.

The focus here is on the comparison of the performance of Algorithms 1 and 3, i.e., NSGA-II with and without DM1 (STD versions are used since the OPT versions are only applicable to the DTLZ2 function). Similar to the configuration described in Table II, the size of population is 100, number of generations is 200 and number of runs is 10.

It is clear from Figs. 13 and 14 that NSGA-II/DM1 is superior to NSGA-II in terms of both convergence and diversity extent. This is consistent with the previous findings reported above for DTLZ2 and with the findings obtained by experiments on the full WFG test suite (WFG1-WFG9). Furthermore, Figs. 15 and 16 reveal that there is now no clear discernible difference in terms of diversity uniformity for the two algorithms over ten runs. This may be attributed to the fact that now the standard value of SBX is used and this is consistent with the performance of NSGA-II/DM1 STD observed in Figs. 11 and 12. It is felt that the optimized value of SBX in conjunction with DM1 further limits the diversification capability of the optimizer.

VI. Conclusion

Many-objective optimization presents fresh challenges for MOEA designers. The increased proportion of non-dominated solutions in each population suggests the need for a new policy to be adopted in respect of diversity promotion.

It is important that convergence retains its status as the primary requirement of an optimizer.

Two new mechanisms for managing diversity have been proposed, which address the conflict between the MOEA requirement for proximity to the Pareto front and the requirement for maintaining a diverse set of solutions.

The two new mechanisms are as follows.

1) *DM1:* activation/deactivation of diversity promotion according to the spread of solutions in a population. Use of DM1 requires that the decision maker select an approximate estimate of the defining extremities of the *targeted* tradeoff surface. *Note*: It is not necessary, of course, that the true Pareto front be known at this stage.
2) *DM2:* adapting the mutation range for each decision variable according to local conditions of spread and crowding.

A rigorous testing program was undertaken to compare the performance of nine algorithms based on NSGA-II and NSGA-II/DMO (i.e., NSGA-II adapted to incorporate DMO). Contrary to expectations, it was found that the second diversity management mechanism, DM2, failed to generate any significant improvement in algorithm performance. This negative outcome is, nonetheless, a useful research finding. The first diversity management mechanism, DM1, on the other hand, did perform a valuable role and its adoption is strongly recommended.

NSGA-II/DM1 repeatedly outperformed NSGA-II by producing solutions closer to the Pareto front and maintaining a near-optimal and desired diversity among the solutions, for a set of *many*-objective optimization problems (6–20 objectives). It is recognized that obtaining good solutions to *many*-objective optimization problems is itself a MOP involving the twin objectives of good proximity and good diversity. For this reason, algorithm performance was assessed against these twin objectives and NSGA-II/DM1 was found to consistently dominate NSGA-II.

Purshouse [24] and Purshouse and Fleming [11] found that, when there are many objectives, a successful configuration for recombination and the mutation operators for one MOP might prove unsuitable for another. As a result, they proposed that the parameters of the recombination and mutation operators might need to be customized for individual MOPs when there are many objectives. However, using a similar experimental framework to that used in Purshouse and Fleming [11] and Purshouse [24], it was shown that NSGA-II/DM1 (and NSGA-II/DM) was less susceptible to changes in the parameter settings of the genetic operators. This, in itself, is another beneficial contribution of DM1.

While the focus of this research was on the management of diversity extent and its impact on convergence, the quality of diversity uniformity was also investigated. DM1 was found to have a limited impact on diversity quality on the DTLZ2 test functions: improvements in diversity extent were offset by a small, but acceptable, reduction in diversity uniformity. When experiments were conducted on more challenging test functions, this discrepancy was not evident and the superior performance of DM1 was maintained.

Thus, one of the proposed diversity management mechanisms, DM1, has proved to be an effective mechanism for managing diversity promotion and requires only very modest additional computing effort. The decision maker is simply required to provide an approximate, targeted or desired, value for the extreme solutions (in terms of each objective) in the objective space. These solutions serve to define an approximation to the vertices of the hypercube which contains the desired region of interest, and therefore define the notion of "good" diversity.

With regard to *many*-objective optimization, in addition to the important optimizer requirements of convergence and diversity, Fleming *et al.* [6] add a third requirement, *pertinency*, i.e., that the approximation set should only contain solutions in the decision maker's region of interest. The MOEA described in Fonseca and Fleming [43] is one algorithm that supports this requirement through provision of decision maker interaction and progressive preference articulation (PPA). (The method of Branke and Deb [43] also supports PPA.) This PPA approach may be extended to accommodate the progressive refinement of the definition of what is meant by "good" diversity by inviting the decision maker to update this definition as solutions converge to the true Pareto front in the region of interest. Future work should also be undertaken to investigate DM1 performance on real-world problems and test functions with more complicated features.

From the set of experiments presented in this paper, the success of exercising control over the activation or deactivation of diversity promotion according to the spread of solutions in a population was established on the set of *many*-objective optimization problems investigated in this paper. It is strongly recommended that existing MOEAs, which use separate Pareto-dominance selection and diversification mechanisms, are adapted to include this mechanism when addressing a MOP which has *many* objectives. This is not the case when algorithms, in which convergence and diversity operations are not separable, such as ε-MOEA, are used.

Initialize random population **P**[5]
-Evaluate the objective values of **P** and store them in **A**[6]
For gen = 1 **to Max_Gen**
  -Assign ranks to the solutions in **P** using non-dominated sorting technique
  -Determine the crowding distance Crd_{Z_A} for each solution z_A in **P**
  -Generate offspring population **Q** from **P** (size **Nind)**
  -DM1:
  -Calculate $\mathbf{I_S}$ (2) for the local Pareto front presented in **A**
  -If $\mathbf{I_S} < 1$
    -Binary tournament selection (Standard Tie Breaking—diversity promotion active)
  -Else
    -Binary tournament selection (Random Tie Breaking—diversity promotion inactive)
  -Selection for recombination and recombination processes
  -DM2:
  Adaptive Mutation Operator
  -Evaluate objective values for the offspring population **Q**
  -Combine parent population **P** and offspring Population **Q** (size: **2xNind)**
  -Assign ranks to the combined population using non-dominated sorting technique
  -Determine the crowding distance for each solution in the combined population
  -DM1 continued:
  -If $\mathbf{I_S} < 1$
    Select **Nind** solutions to propagate to the next generation (Selection Criteria: 1st: elitist—biased toward lower ranks—2nd: crowding distance—bias less crowded solutions—diversity promotion active)
  -Else
    Select **Nind** solutions to propagate to the next generation (Selection Criteria: 1st: elitist—biased toward lower ranks—2nd: random—diversity promotion inactive)
End loop

---

[5] 'P' is a 2-D array of decision variables and its dimension is Nind x n, where Nind is the size of the population of candidate solutions and n is the number of decision variables.

[6] 'A' is a 2-D array of objective values and its dimension is Nind x m, where m is the number of objectives being optimized.

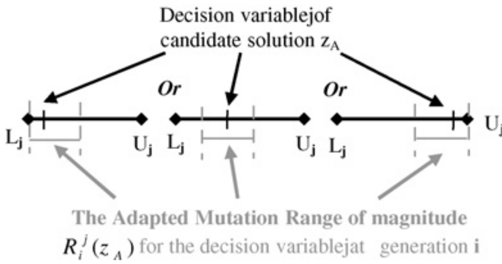

Fig. A.1. DM2: the adaptive mutation.

Appendix A
Pseudo-code Description of NSGA-II Incorporating the Proposed Diversity Management Mechanisms

A pseudo-code description of the proposed DM mechanisms within the context of NSGA-II is presented above. This algorithm is described as NSGA-II/DM.

Appendix B
DM2: Adaptive Mutation Operator

The DM2 mutation operator and Deb and Goyal's polynomial mutation operator [33] are similar in that they both include a control process for the mutation magnitude of a certain candidate solution. However, while the polynomial mutation operator requires a fixed mutation distribution parameter to control the magnitude of the expected mutation of a certain decision variable, the DM2 mutation operator adapts the magnitude of the expected mutation for a certain decision variable based on two complementary criteria:

1) the value of the spread indicator (I_s) measuring the diversity extent of the locally non-dominated set of solutions;
2) the NSGA-II "crowding" measure which highlights the "*local*" diversity around each single solution.

The DM2 mutation operator is a three-step process, which operates on the set of decision variable vectors representing the whole population of solutions at a certain generation "i." These decision variables vectors are produced by the selection for variation process from the active archive, containing the set of locally non-dominated solutions, following the recombination process.

The three steps of the DM2 mutation operator are as follows.

Step 1) Determine a maximum mutation magnitude R_i^j for all decision variables "j" ($j = 1, \ldots n$, where n is the total number of decision variables) of any candidate solution in the population at generation "i" using (A.1) ("n" such maximum mutation magnitudes will be calculated in total). For every decision variable "j" of each candidate solution z_A, R_i^j represents a certain proportion of the magnitude $|\mathbf{U_j} - \mathbf{L_j}|$, where U_j and L_j are the upper and lower bounds for the jth decision variable

$$R_i^j = k_1 \times \left|U_j - L_j\right| \tag{A.1}$$

and k_1 is determined by normalizing the value of I_s in the range [ε, 1]. I_s is a positive real number whose minimum value is zero and ideal value is 1. A value of I_s tending to zero represents a very poor diversity quality, and will correspond to the value k_1 being set to 1 in the normalization range [ε, 1]. This represents a request for the highest level of mutation possible. On the other hand, for $I_s > 1$, the value of k_1 will tend to ε, where ε is an application-dependent, positive non-zero tolerance value defined by the decision maker, to reduce the amplitude of the mutation process.

Step 2) For each decision variable j of each candidate solution z_A in the population, separately customize a maximum mutation magnitude $R_i^j(z_A)$ (A.2). $R_i^j(z_A)$ represents a certain proportion of the global magnitude R_i^j previously calculated

$$R_i^j(z_A) = k_2 \times R_i^j \tag{A.2}$$

where k_2 is determined for each candidate solution, z_A, by normalizing the value of z_A's crowding measure crd(z_A) at generation "i" in the range [ε, 1]. At generation "i," the minimum crowding measure crd_{max} which corresponds to the most crowded solution is mapped to the value $k_2 = 1$, while the maximum crowding measure crd_{max} is mapped to $k_2 = 1 = \varepsilon$.

This represents a request for higher mutation magnitudes for the crowded solutions and vice versa. The normalized values of the crowding measures separately define the amplitude of the mutation range for each decision variable, j, of each candidate solution z_A. These calculated local mutation ranges are then centered over the values of each decision variable chosen to undertake mutation (Fig. A.1).

Step 3) After defining the local mutation range for each decision variable of each candidate solution, the value of a certain decision variable j chosen to undertake mutation is perturbed randomly within its determined local mutation range (Fig. A.1).

The DM2 mutation operator is applied uniformly to every decision variable j with a probability $p_m = 1/n$, where n is the total number of decision variables. This is a standard probability for uniform mutation operators and is used in studies deploying the polynomial mutation for solving real-coded multiobjective optimization problems (see [11], [35]).

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