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A Simulated Annealing-Based Multiobjective Optimization Algorithm: AMOSA

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Abstract—**This paper describes a simulated annealing based multiobjective optimization algorithm that incorporates the concept of archive in order to provide a set of tradeoff solutions for the problem under consideration. To determine the acceptance probability of a new solution *vis-a-vis* the current solution, an elaborate procedure is followed that takes into account the domination status of the new solution with the current solution, as well as those in the archive. A measure of the amount of domination between two solutions is also used for this purpose. A complexity analysis of the proposed algorithm is provided. An extensive comparative study of the proposed algorithm with two other existing and well-known multiobjective evolutionary algorithms (MOEAs) demonstrate the effectiveness of the former with respect to five existing performance measures, and several test problems of varying degrees of difficulty. In particular, the proposed algorithm is found to be significantly superior for many objective test problems (e.g., 4, 5, 10, and 15 objective problems), while recent studies have indicated that the Pareto ranking-based MOEAs perform poorly for such problems. In a part of the investigation, comparison of the real-coded version of the proposed algorithm is conducted with a very recent multiobjective simulated annealing algorithm, where the performance of the former is found to be generally superior to that of the latter.**

Index Terms—**Amount of domination, archive, clustering, multiobjective optimization (MOO), Pareto-optimal (PO), simulated annealing (SA).**

I. INTRODUCTION

THE MULTIOBJECTIVE OPTIMIZATION (MOO) problem has a rather different perspective compared with one having a single objective. In the single-objective optimization there is only one global optimum, but in multiobjective optimization there is a set of solutions, called the Pareto-optimal (PO) set, which are considered to be equally important; all of them constitute global optimum solutions. Over the past decade, a number of multiobjective evolutionary algorithms (MOEAs) have been suggested (see, [1] and [2] for some reviews). The main reason for the popularity of evolutionary algorithms (EAs) for solving multiobjective optimization is their population-based nature and ability to find multiple optima simultaneously.

Simulated annealing (SA) [3] another popular search algorithm, utilizes the principles of statistical mechanics regarding the behavior of a large number of atoms at low temperature, for finding minimal cost solutions to large optimization problems by minimizing the associated energy. In statistical mechanics, investigating the ground states or low-energy states of matter is of fundamental importance. These states are achieved at very low temperatures. However, it is not sufficient to lower the temperature alone since this results in unstable states. In the annealing process, the temperature is first raised, then decreased gradually to a very low value ($T\min$), while ensuring that one spends sufficient time at each temperature value. This process yields stable low-energy states. Geman and Geman [4] provided proof that SA, if annealed sufficiently slowly, converges to the global optimum. Being based on strong theory, SA has applications in diverse areas [5]–[7] by optimizing a single criterion. However, there have been only a few attempts in extending SA to MOO, primarily because of its search-from-a-point nature. In most of the earlier attempts, a single-objective function is constructed by combining the different objectives into one using a weighted sum approach [8]–[13]. The problem here is how to choose the weights in advance. Some alternative approaches have also been used in this regard. In [11] and [12], different nonlinear and stochastic composite energy functions have been investigated. In [11], six different criteria for energy difference calculation are suggested and evaluated. These are: 1) minimum cost criterion; 2) maximum cost criteria; 3) random cost criteria; 4) self cost criteria; 5) average cost criteria; and 6) fixed cost criteria. Since each run of the SA provides just a single solution, the algorithm attempted to evolve the set of PO solutions by using multiple SA runs. As a result of the independent runs, the diversity of the set of solutions suffered.

Multiobjective SA with a composite energy clearly converges to the true Pareto front if the objectives have ratios given by w_i^{-1}, if such points, in general, exist. Here, w_i is the weight assigned to the ith objective. In [14], it has been proven that part of the front will be inaccessible with fixed weights. In [15], several different schemes were explored for adapting the w_i's during the annealing process to encourage exploration along the front. However, a proper choice of the w_i's remains a challenging task.

In addition to the earlier aggregating approaches of multiobjective SA (MOSA), there have been a few techniques that incorporate the concept of Pareto-dominance. Some such methods are proposed in [16] and [17] which use Pareto-domination-based acceptance criterion in MOSA. A good review of several MOSA algorithms and their comparative performance analysis can be found in [18]. Since the technique in [17] has been used in this paper for the purpose of comparison, it is described in detail later.

In Pareto-domination-based MOSAs developed so far, the acceptance criterion between the current and a new solution

has been formulated in terms of the difference in the number of solutions that they dominate [16], [17]. The amount by which this domination takes place is not taken into consideration. In this paper, a new MOSA is proposed, hereafter referred to as archived multiobjective simulated annealing (AMOSA), which incorporates a novel concept of amount of dominance in order to determine the acceptance of a new solution. The PO solutions are stored in an archive. A complexity analysis of the proposed AMOSA is provided. The performance of the newly proposed AMOSA is compared with two other well-known MOEAs, namely, NSGA-II [19] and PAES [20] for several function optimization problems when binary encoding is used. The comparison is made in terms of several performance measures, namely, *Convergence* [19], *Purity* [21], [22], *Spacing* [23], and *MinimalSpacing* [21]. Another measure called *displacement* [8], [24], that reflects both the proximity to and the coverage of the true PO front is also used here for the purpose of comparison. This measure is especially useful for discontinuous fronts where we can estimate if the solution set is able to approximate all the subfronts. Many existing measures are unable to achieve this.

It may be noted that the MOSA methods developed in [16] and [17] are on lines similar to ours. The concept of archive or a set of potentially PO solutions is also utilized in [16] and [17] for storing the nondominated solutions. Instead of scalarizing the multiple objectives, a domination-based energy function is defined. However, there are notable differences. First, while the number of solutions that dominate the new solution x determines the acceptance probability of x in the earlier attempts, in the present paper this is based on the amount of domination of x with respect to the solutions in the archive and the current solution. In contrast to the works in [16] and [17] where a single form of acceptance probability is considered, the present paper deals with different forms of acceptance probabilities depending on the domination status, the choice of which are explained intuitively later on.

In [17], an unconstrained archive is maintained. Note that theoretically, the number of PO solutions can be infinite. Since the ultimate purpose of an MOO algorithm is to provide the user with a set of solutions to choose from, it is necessary to limit the size of this set for it to be usable by the user. Though maintaining unconstrained archives as in [17] is novel and interesting, it is still necessary to finally reduce it to a manageable set. Limiting the size of the population (as in NSGA-II) or the archive (as in AMOSA) is an approach in this direction. Clustering appears to be a natural choice for reducing the loss of diversity, and this is incorporated in the proposed AMOSA. Clustering has also been used earlier in [25].

For comparing the performance of real-coded AMOSA with that of the MOSA [17], six three objective test problems, namely, DTLZ1–DTLZ6 are used. Results demonstrate that the performance of AMOSA is comparable to, often better than that of MOSA in terms of *Purity*, *Convergence*, and *MinimalSpacing*. Comparison is also made with real-coded NSGA-II for the above mentioned six problems, as well as for some 4, 5, 10, and 15 objective test problems. Results show that the performance of AMOSA is superior to that of NSGA-II specially for the test problems with many objective functions. This is interesting and the most desirable feature of AMOSA

since Pareto ranking-based MOEAs, such as NSGA-II [19] do not work well on many-objective optimization problems as pointed out in some recent studies [26], [27].

II. MULTIOBJECTIVE ALGORITHMS

The MOO can be formally stated as follows [1]. Find the vectors $\overline{x}^* = [x_1^*, x_2^*, \ldots, x_n^*]^T$ of decision variables that simultaneously optimize the M objective values $\{f_1(\overline{x}), f_2(\overline{x}), \ldots, f_M(\overline{x})\}$, while satisfying the constraints, if any.

An important concept of MOO is that of domination. In the context of a maximization problem, a solution $\overline{x_i}$ is said to dominate $\overline{x_j}$ if $\forall k \in 1, 2, \ldots, M, f_k(\overline{x_i}) \geq f_k(\overline{x_j})$ and $\exists k \in 1, 2, \ldots, M$, such that $f_k(\overline{x_i}) > f_k(\overline{x_j})$.

Among a set of solutions P, the nondominated set of solutions P' are those that are not dominated by any member of the set P. The nondominated set of the entire search space S is the globally PO set. In general, a MOO algorithm usually admits a set of solutions that are not dominated by any solution encountered by it.

A. Recent MOEAs

During 1993–2003, a number of different EAs were suggested to solve MOO problems. Among these, two well-known ones, namely, PAES [20] and NSGA-II [19], are used in this paper for the purpose of comparison. These are described in brief.

Knowles and Corne [20] suggested a simple MOEA using a single parent, single child EA, similar to $(1 + 1)$ evolutionary strategy. Instead of using real parameters, binary strings, and bitwise mutation are used in this algorithm to create the offspring. After creating the child and evaluating its objectives, it is compared with respect to the parent. If the child dominates the parent, then the child is accepted as the next parent and the iteration continues. On the other hand, if parent dominates the child, the child is discarded and a new mutated solution (a new solution) is generated from the parent. However, if the parent and the child are nondominating to each other, then the choice between the child and the parent is resolved by comparing them with an archive of best solutions found so far. The child is compared with all members of the archive to check if it dominates any member of the archive. If yes, the child is accepted as the new parent and all the dominated solutions are eliminated from the archive. If the child does not dominate any member of the archive, both the parent and the child are checked for their *nearness* with the solutions of the archive. If the child resides in a less crowded region in the parameter space, it is accepted as a parent and a copy is added to the archive. Generally, this crowding concept is implemented by dividing the whole solution space into d^M subspaces, where d is the depth parameter and M is the number of objective functions. The subspaces are updated dynamically.

The other popular algorithm for MOO is NSGA-II proposed by Deb *et al.* [19]. Here, initially a random parent population P_0 of size N is created. Then, the population is sorted based on the nondomination relation. Each solution of the population is assigned a fitness which is equal to its nondomination level. A child population Q_0 is created from the parent population P_0

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by using binary tournament selection, recombination, and mutation operators. Generally, according to this algorithm, initially a combined population $R_t = P_t + Q_t$ is formed of size R_t, which is $2N$. Now, all the solutions of R_t are sorted based on their nondomination status. If the total number of solutions belonging to the best nondominated set F_1 is smaller than N, F_1 is completely included into $P_{(t+1)}$. The remaining members of the population $P_{(t+1)}$ are chosen from subsequent nondominated fronts in the order of their ranking. To choose exactly N solutions, the solutions of the last included front are sorted using the crowded comparison operator and the best among them (i.e., those with larger values of the crowding distance) are selected to fill in the available slots in $P_{(t+1)}$. The new population $P_{(t+1)}$ is now used for selection, crossover and mutation to create a new population $Q_{(t+1)}$ of size N, and the process continues. The crowding distance operator is also used in the parent selection phase in order to break a tie in the binary tournament selection. This operator is basically responsible for maintaining diversity in the Pareto front.

B. Recent MOSA[17]

One of the recently developed MOSA algorithms is by Smith *et al.* [17]. Here, a dominance-based energy function is used. If the true Pareto front is available, then the energy of a particular solution x is calculated as the total number of solutions that dominates x. However, as the true Pareto front is not available all the time, a proposal has been made to estimate the energy-based on the current estimate of the Pareto front F', which is the set of mutually nondominating solutions found thus far in the process. Then, the energy of the current solution x is the total number of solutions in the estimated front which dominates x. If $\|F'_{x'}\|$ is the energy of the new solution x' and $\|F'_x\|$ is the energy of the current solution x, then energy difference between the current and the proposed solution is calculated as $\delta E(x', x) = (\|F'_{x'}\| - \|F'_x\|)/\|F'\|$. Division by $\|F'\|$ ensures that δE is always less than unity and provides some robustness against fluctuations in the number of solutions in F'. If the size of F' is less than some threshold, then attainment surface sampling method is adopted to increase the number of solutions in the final Pareto front. Authors have perturbed a decision variable with a random number generated from the laplacian distribution. Two different sets of scaling factors, traversal scaling which generates moves to a nondominated proposal within a front, and location scaling which locates a front closer to the original front, are kept. These scaling factors are updated with the iterations.

III. ARCHIVED MULTIOBJECTIVE SIMULATED ANNEALING (AMOSA)

As mentioned earlier, the AMOSA algorithm is based on the principle of SA [3]. In this paper, at a given temperature T, a new state s is selected with a probability

$$p_{qs} = \frac{1}{1 + e^{\frac{-(E(q,T) - E(s,T))}{T}}} \quad (1)$$

where q is the current state and $E(s, T)$ and $E(q, T)$ are the corresponding energy values of s and q, respectively. Note that

the above equation automatically ensures that the probability value lies in between 0 and 1. AMOSA incorporates the concept of an *Archive* where the nondominated solutions seen so far are stored. In [28], the use of unconstrained *Archive* size to reduce the loss of diversity is discussed in detail. In our approach, we have kept the archive size limited since finally only a limited number of well distributed PO solutions are needed. Two limits are kept on the size of the *Archive*: a hard or strict limit denoted by HL, and a soft limit denoted by SL. During the process, the nondominated solutions are stored in the *Archive* as and when they are generated until the size of the *Archive* increases to SL. Thereafter, if more nondominated solutions are generated, these are added to the *Archive*, the size of which is thereafter reduced to HL by applying clustering. The structure of the proposed SA-based AMOSA is shown in Fig. 1. The parameters that need to be set *a priori* are mentioned below.

- HL: The maximum size of the *Archive* on termination. This set is equal to the maximum number of nondominated solutions required by the user.
- SL: The maximum size to which the *Archive* may be filled before clustering is used to reduce its size to HL.
- Tmax: Maximum (initial) temperature.
- Tmin: Minimal (final) temperature.
- iter: Number of iterations at each temperature.
- α: The cooling rate in SA.

The different steps of the algorithm are now explained in detail.

A. Archive Initialization

The algorithm begins with the initialization of a number $\gamma \times \text{SL}(\gamma > 1)$ of solutions. Each of these solutions is refined by using a simple hill-climbing technique, accepting a new solution only if it dominates the previous one. This is continued for a number of iterations. Thereafter, the nondominated solutions (ND) that are obtained are stored in the *Archive*, up to a maximum of HL. In case the number of nondominated solutions exceeds HL, clustering is applied to reduce the size to HL (the clustering procedure is explained below). That means, initially, *Archive* contains a maximum of HL number of solutions.

In the initialization phase, it is possible to get an *Archive* of size one. In MOSA [17], in such cases, other newly generated solutions which are dominated by the archival solution will be indistinguishable. In contrast, the amount of domination as incorporated in AMOSA will distinguish between "more dominated" and "less dominated" solutions. However, in the future, we intend to use a more sophisticated scheme, in line with that adopted in MOSA.

B. Clustering the Archive Solutions

Clustering of the solutions in the *Archive* has been incorporated in AMOSA in order to explicitly enforce the diversity of the nondominated solutions. In general, the size of the *Archive* is allowed to increase up to SL $(> \text{HL})$, after which the solutions are clustered for grouping the solutions into HL clusters. Allowing the *Archive* size to increase up to SL not only reduces excessive calls to clustering, but also enables the formation of more spread out clusters and hence better diversity. Note that in the initialization phase, clustering is executed once even if the number of solutions in the *Archive* is less than SL, as long as it

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Algorithm AMOSA
Set *Tmax, Tmin, HL, SL, iter,* α, temp=*Tmax*.
Initialize the *Archive*.
current-pt = random(*Archive*). /* randomly chosen solution from the *Archive* */
while (temp > *Tmin*)
    for (i=0; i< iter; i++)
        new-pt=perturb(*current-pt*).
        Check the domination status of *new-pt* and *current-pt*.
        /* Code for different cases */
        if (*current-pt* dominates *new-pt*) /* Case 1*/
            $\Delta dom_{avg} = \frac{\left(\sum_{i=1}^{k} \Delta dom_{i,new-pt}\right)+\Delta dom_{current-pt,new-pt}}{(k+1)}$.
            /* *k*=total-no-of points in the *Archive* which dominate *new-pt*, $k \geq 0$. */
            prob= $\frac{1}{1+exp(\Delta dom_{avg}*temp)}$.
            Set *new-pt* as *current-pt* with probability=*prob*.
        if (*current-pt* and *new-pt* are non-dominating to each other) /* Case 2*/
            Check the domination status of *new-pt* and points in the *Archive*.
            if (*new-pt* is dominated by *k* ($k \geq 1$) points in the *Archive*) /* Case 2(a)*/
                prob= $\frac{1}{1+exp(\Delta dom_{avg}*temp)}$.
                $\Delta dom_{avg} = \frac{\left(\sum_{i=1}^{k} \Delta dom_{i,new-pt}\right)}{k}$.

                Set *new-pt* as *current-pt* with probability=*prob*.
            if (*new-pt* is non-dominating w.r.t all the points in the *Archive*) /* Case 2(b)*/
                Set *new-pt* as *current-pt* and add *new-pt* to the *Archive*.
                if *Archive-size* > *SL*
                    Cluster *Archive* to *HL* number of clusters.
            if (*new-pt* dominates *k*, ($k \geq 1$) points of the *Archive*) /* Case 2(c)*/
                Set *new-pt* as *current-pt* and add it to the *Archive*.
                Remove all the *k* dominated points from the *Archive*.
        if (*new-pt* dominates *current-pt*) /* Case 3 */
            Check the domination status of *new-pt* and points in the *Archive*.
            if (*new-pt* is dominated by *k* ($k \geq 1$) points in the *Archive*) /* Case 3(a)*/
                Δdom_{min} = minimum of the difference of domination amounts between the *new-pt*
                        and the *k* points
                prob= $\frac{1}{1+exp(-\Delta dom_{min})}$.
                Set point of the archive which corresponds to Δdom_{min} as *current-pt* with probability=*prob*
                else set *new-pt* as *current-pt*.
            if (*new-pt* is non-dominating with respect to the points in the *Archive*) /* Case 3(b) */
                Set *new-pt* as the *current-pt* and add it to the *Archive*.
                if *current-pt* is in the *Archive*, remove it from the *Archive*.
                else if *Archive-size*> *SL*.
                    Cluster *Archive* to *HL* number of clusters.
            if (*new-pt* dominates *k* other points in the *Archive*) /* Case 3(c)*/
                Set *new-pt* as *current-pt* and add it to the *Archive*.
                Remove all the *k* dominated points from the *Archive*.
    End for
temp= α*temp.
End while
if *Archive-size* > *SL*
    Cluster *Archive* to *HL* number of clusters.

Fig. 1. The AMOSA algorithm.

is greater than HL. This enables it to start with at most HL non-dominated solutions and reduces excessive calls to clustering in the initial stages of the AMOSA process.

For clustering, the well-known single linkage algorithm [29] is used. Here, the distance between any two clusters corresponds to the length of the shortest link between them. This is similar to the clustering algorithm used in SPEA [25], except that they have used average linkage method [29]. After HL clusters are obtained, the member within each cluster whose average distance to the other members is the minimum, is considered as

the representative member of the cluster. A tie is resolved arbitrarily. The representative points of all the HL clusters are thereafter stored in the *Archive*.

C. Amount of Domination

As already mentioned, AMOSA uses the concept of amount of domination in computing the acceptance probability of a new solution. Given two solutions a and b, the amount of domination is defined as $\Delta \mathrm{dom}_{a,b} = \prod_{i=1, f_i(a) \neq f_i(b)}^{M} (|f_i(a) - f_i(b)|/R_i)$, where $M =$ number

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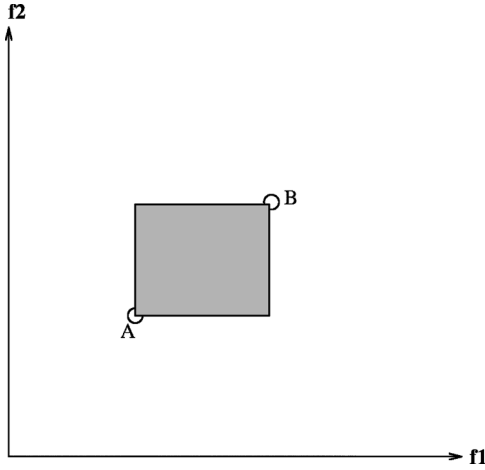
Fig. 2. Total amount of domination between the two solutions A and $B =$ the area of the shaded rectangle.

of objectives and R_i is the range of the ith objective. Note that in several cases, R_i may not be known *a priori*. In these situations, the solutions present in the *Archive* along with the new and the current solutions are used for computing it. The concept of $\Delta \text{dom}_{a,b}$ is illustrated pictorially in Fig. 2 for a two objective case. $\Delta \text{dom}_{a,b}$ is used in AMOSA while computing the probability of acceptance of a newly generated solution.

D. The Main AMOSA Process

One of the points, called *current-pt*, is randomly selected from *Archive* as the initial solution at temperature $\text{temp} = T\max$. The *current-pt* is perturbed to generate a new solution called *new-pt*. The domination status of *new-pt* is checked with respect to the *current-pt* and solutions in *Archive*.

Based on the domination status between *current-pt* and *new-pt*, three different cases may arise. These are enumerated below.

- Case 1: *current-pt* dominates the *new-pt* and k ($k \geq 0$) points from the *Archive* dominate the *new-pt*.
  This situation is shown in Fig. 3. Here, Fig. 3(a) and (b) denote the situations where $k = 0$ and $k \geq 1$, respectively. (Note that all the figures correspond to a two objective maximization problem.) In this case, the *new-pt* is selected as the *current-pt* with

$$\text{probability} = \frac{1}{1 + \exp(\Delta \text{dom}_{\text{avg}} * \text{temp})} \quad (2)$$

where $\Delta \text{dom}_{\text{avg}} = ((\sum_{i=1}^{k} \Delta \text{dom}_{i,new\text{-}pt}) + \Delta \text{dom}_{current\text{-}pt,new\text{-}pt})/(k + 1)$. Note that $\Delta \text{dom}_{\text{avg}}$ denotes the average amount of domination of the *new-pt* by $(k + 1)$ points, namely, the *current-pt* and k points of the *Archive*. Also, as k increases, $\Delta \text{dom}_{\text{avg}}$ will increase since here the dominating points that are farther away from the *new-pt* are contributing to its value.

Lemma: When $k = 0$, the *current-pt* is on the archival front.

Proof: If this is not the case, then some point, say A, in the *Archive* dominates it. Since *current-pt* dominates the *new-pt*, by transitivity, A will also dominate the *new-pt*. However, we

have considered that no other point in the *Archive* dominates the *new-pt* as $k = 0$. Hence proved.

However, if $k \geq 1$, this may or may not be true.

- Case 2: *current-pt* and *new-pt* are nondominating with respect to each other.
  Now, based on the domination status of *new-pt* and members of *Archive*, the following three situations may arise.
  1) *new-pt* is dominated by k points in the *Archive* where $k \geq 1$. This situation is shown in Fig. 4(a). The *new-pt* is selected as the *current-pt* with

$$\text{probability} = \frac{1}{(1 + \exp(\Delta \text{dom}_{\text{avg}} * \text{temp}))} \quad (3)$$

where $\Delta \text{dom}_{\text{avg}} = \sum_{i=1}^{k} (\Delta \text{dom}_{i,new\text{-}pt})/k$. Note that here the *current-pt* may or may not be on the archival front.
  2) *new-pt* is nondominating with respect to the other points in the *Archive* as well. In this case, the *new-pt* is on the same front as the *Archive*, as shown in Fig. 4(b). Therefore, the *new-pt* is selected as the *current-pt* and added to the *Archive*. In case the *Archive* becomes overfull (i.e., the SL is exceeded), clustering is performed to reduce the number of points to HL.
  3) *new-pt* dominates $k(k \geq 1)$ points of the *Archive*. This situation is shown in Fig. 4(c). Again, the *new-pt* is selected as the *current-pt*, and added to the *Archive*. All the k dominated points are removed from the *Archive*. Note that here too the *current-pt* may or may not be on the archival front.
- Case 3: *new-pt* dominates *current-pt*.
  Now, based on the domination status of *new-pt* and members of *Archive*, the following three situations may arise.
  1) *new-pt* dominates the *current-pt* but $k(k \geq 1)$ points in the *Archive* dominate this *new-pt*. Note that this situation [shown in Fig. 5(a)] may arise only if the *current-pt* is not a member of the *Archive*. Here, the minimum of the difference of domination amounts between the *new-pt* and the k points, denoted by $\Delta \text{dom}_{\text{min}}$, of the *Archive* is computed. The point from the *Archive* which corresponds to the minimum difference is selected as the *current-pt* with probability $= 1/(1 + \exp(-\Delta \text{dom}_{\text{min}}))$. Otherwise, the *new-pt* is selected as the *current-pt*. Note that according to the SA paradigm, the *new-pt* should have been selected with probability 1. However, due to the presence of *Archive*, it is evident that solutions still better than *new-pt* exist. Therefore, the *new-pt* and the dominating points in the *Archive* that are closest to the *new-pt* (corresponding to $\Delta \text{dom}_{\text{min}}$) compete for acceptance. This may be considered a form of informed reseeding of the annealer only if the *Archive* point is accepted, but with a solution closest to the one which would otherwise have survived in the normal SA paradigm.
  2) *new-pt* is nondominating with respect to the points in the *Archive* except the *current-pt* if it belongs to the *Archive*. This situation is shown in Fig. 5(b). Thus *new-pt*, which is now accepted as the *current-pt*, can
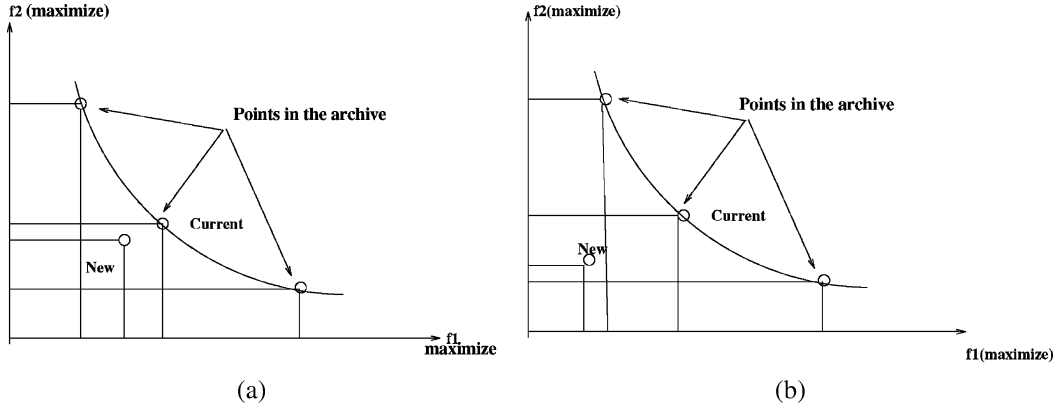
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Fig. 3. Different cases when *New* is dominated by *Current*. (a) *New* is nondominating with respect to the solutions of *Archive* except *Current*. if it is in the *Archive*. (b) Some solutions in the *Archive* dominate *New*.
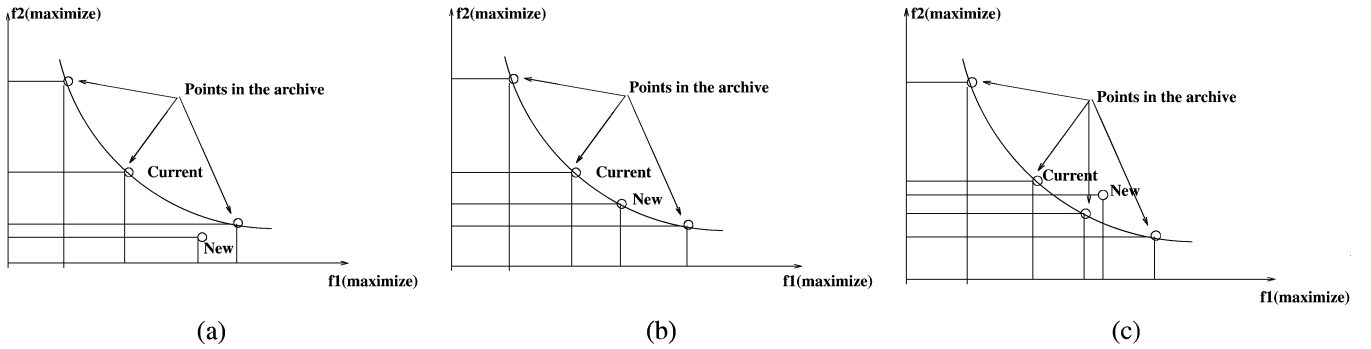

Fig. 4. Different cases when *New* and *Current* are nondominating. (a) Some solutions in *Archive* dominates *New*. (b) *New* is nondominating with respect to all the solutions of *Archive*. (c) *New* dominates $k(k \geq 1)$ solutions in the *Archive*.
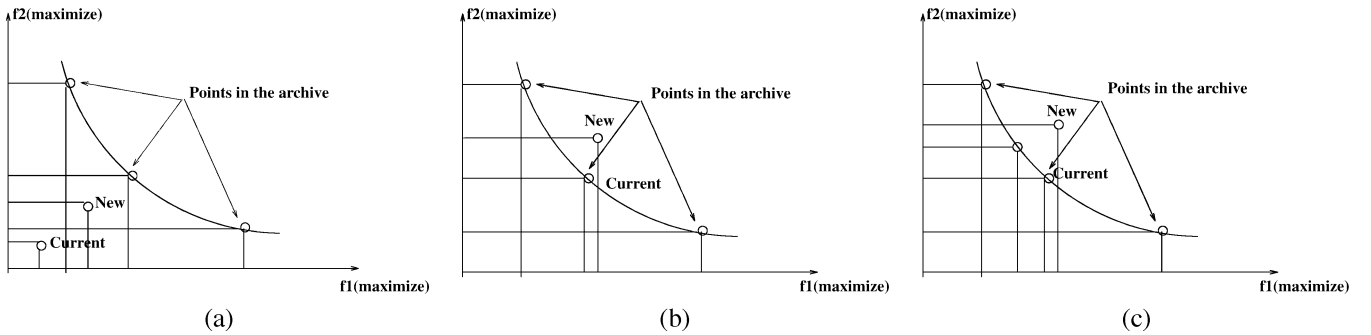

Fig. 5. Different cases when *New* dominates the *Current*. (a) *New* is dominated by some solutions in *Archive*. (b) *New* is nondominating with respect to the solutions in the *Archive* except *Current*, if it is in the *Archive*. (c) *New* dominates some solutions of *Archive* other than *Current*.

be considered as a new nondominated solution that must be stored in *Archive*. Hence, *new-pt* is added to the *Archive*. If the *current-pt* is in the *Archive*, then it is removed. Otherwise, if the number of points in the *Archive* becomes more than the SL, clustering is performed to reduce the number of points to HL. Note that here the *current-pt* may or may not be on the archival front.

3) *new-pt* also dominates $k(k \geq 1)$, other points, in the *Archive* [see Fig. 5(c)]. Hence, the *new-pt* is selected as the *current-pt* and added to the *Archive*, while all the dominated points of the *Archive* are removed. Note that here the *current-pt* may or may not be on the archival front.

The above process is repeated iter times for each temperature (temp). Temperature is reduced to $\alpha \times$ temp, using the cooling rate of α till the minimum temperature Tmin is attained. The process thereafter stops, and the *Archive* contains the final nondominated solutions.

Note that in AMOSA, as in other versions of MOSA algorithms, there is a possibility that a new solution worse than the current solution may be selected. In most other MOEAs, e.g., NSGA-II and PAES, if a choice needs to be made between two solutions $\overline{x}$ and $\overline{y}$, and if $\overline{x}$ dominates $\overline{y}$, then $\overline{x}$ is always selected. It may be noted that in single-objective EAs or SA, usually a worse solution also has a nonzero chance of surviving in subsequent generations; this leads to a reduced possibility of getting stuck at suboptimal regions. However, most of the

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MOEAs have been so designed that this characteristic is lost. The present SA-based algorithm provides a way of incorporating this feature.

E. Complexity Analysis

The complexity analysis of AMOSA is provided in this section. The basic operations and their worst case complexities are as follows:

1) Archive initialization: $O(\text{SL})$.
2) Procedure to check the domination status of any two solutions: $O(M)$, $M = \#$ objectives.
3) Procedure to check the domination status between a particular solution and the *Archive* members: $O(M \times \text{SL})$.
4) Single linkage clustering: $O(\text{SL}^2 \times \log(\text{SL}))$ [30].
5) Clustering procedure is executed:
   - once after initialization if $|\text{ND}| > \text{HL}$;
   - after each $(\text{SL} - \text{HL})$ number of iterations;
   - at the end if final $|Archive| > \text{HL}$.

   Therefore, the maximum number of times the Clustering procedure is called$= (TotalIter/(\text{SL} - \text{HL})) + 2$.

   Therefore, total complexity due to Clustering procedure is $O((TotalIter/(\text{SL} - \text{HL})) \times \text{SL}^2 \times \log(\text{SL}))$.

Total complexity of AMOSA becomes

$$(\text{SL}+M+M\times\text{SL})\times(TotalIter)+\frac{TotalIter}{\text{SL}-\text{HL}}\times\text{SL}^2\times\log(\text{SL}). \tag{4}$$

Let $\text{SL} = \beta \times \text{HL}$, where $\beta \geq 2$ and $\text{HL} = N$ where N is the population size in NSGA-II and archive size in PAES. Therefore, overall complexity of the AMOSA becomes

$$(TotalIter) \times (\beta \times N + M + M \times \beta \times N \\ + (\beta^2/(\beta - 1)) \times N \times \log(\beta N)) \tag{5}$$

or

$$O(TotalIter \times N \times (M + \log(N))). \tag{6}$$

Note that the total complexity of NSGA-II is $O(TotalIter \times M \times N^2)$ and that of PAES is $O(TotalIter \times M \times N)$. NSGA-II complexity depends on the complexity of nondominated procedure. With the best procedure, the complexity is $O(TotalIter \times M \times N \times \log(N))$.

IV. SIMULATION RESULTS

In this section, we first describe comparison metrics used for the experiments. The performance analysis of both the binary-coded AMOSA and the real-coded AMOSA are also provided in this section.

A. Comparison Metrics

In MOO, there are basically two functionalities that an MOO strategy must achieve regarding the obtained solution set [1]. It should converge as close to the true PO front as possible and it should maintain as diverse a solution set as possible.

The first condition clearly ensures that the obtained solutions are near optimal and the second condition ensures that a wide range of tradeoff solutions is obtained. Clearly, these two tasks cannot be measured with one performance measure adequately. A number of performance measures have been suggested in the past. Here, we have mainly used three such performance measures. The first measure is the *Convergence* measure γ [19]. It measures the extent of convergence of the obtained solution set to a known set of PO solutions. The lower the value of γ, the better is the convergence of the obtained solution set to the true PO front. The second measure called *Purity* [21], [22] is used to compare the solutions obtained using different MOO strategies. It calculates the fraction of solutions from a particular method that remains nondominating when the final front solutions obtained from all the algorithms are combined. A value near 1 indicates better performance whereas a value near 0 indicates poorer performance. The third measure named *Spacing* was first proposed by Schott [23]. It reflects the uniformity of the solutions over the nondominated front. It is shown in [21] that this measure will fail to give adequate results in some situations. In order to overcome the above limitations, a modified measure, named *MinimalSpacing* is proposed in [21]. Smaller values of *Spacing* and *MinimalSpacing* indicate better performance.

It may be noted that if an algorithm is able to approximate only a portion of the true PO front and not its full extent, none of the existing measures will be able to reflect this. In case of discontinuous PO front, this problem becomes severe when an algorithm totally misses a subfront. Here, a performance measure which is very similar to the measure used in [8] and [24] named *displacement* is used that is able to overcome this limitation. It measures how far the obtained solution set is from a known set of PO solutions. In order to compute *displacement* measure, a set P^* consisting of uniformly spaced solutions from the true PO front in the objective space is found (as is done while calculating γ). Then, *displacement* is calculated as

$$\text{displacement} = \frac{1}{|P^*|} \times \sum_{i=1}^{|P^*|} \left(\min_{j=1}^{|Q|} d(i,j) \right) \tag{7}$$

where Q is the obtained set of final solutions, and $d(i,j)$ is the Euclidean distance between the ith solution of P^* and jth solution of Q. The lower the value of this measure, the better is the convergence to and extent of coverage of the true PO front.

B. Comparison of Binary Encoded AMOSA With NSGA-II and PAES

First, we have compared the binary encoded AMOSA with the binary-coded NSGA-II and PAES algorithms. For AMOSA, binary mutation is used. Seven test problems have been considered for the comparison purpose. These are SCH1 and SCH2 [1], Deb1 and Deb4 [31], and ZDT1, ZDT2, ZDT6 [1]. All the algorithms are executed ten times per problem and the results reported are the average values obtained for the ten runs. In NSGA-II, the crossover probability (p_c) is kept equal to 0.9. For PAES, the depth value d is set equal to 5. For AMOSA, the cooling rate α is kept equal to 0.8. The number of bits assigned to encode each decision variable depends on the problem. For example, in ZDT1, ZDT2, and ZDT6 which all are 30-variable problems, 10 bits are used to encode each variable, for SCH1

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TABLE I

CONVERGENCE AND *PURITY* MEASURES ON THE TEST FUNCTIONS FOR BINARY ENCODING

Test	*Convergence*			*Purity*		
Problem	AMOSA	PAES	NSGA-II	AMOSA	PAES	NSGA-II
SCH1	0.0016	0.0016	0.0016	0.9950(99.5/100)	0.9850(98.5/100)	1(94/94)
SCH2	0.0031	0.0015	0.0025	0.9950(99.5/100)	0.9670(96.7/100)	0.9974(97/97.3)
ZDT1	0.0019	0.0025	0.0046	0.8350(83.5/100)	0.6535(65.4/100)	0.970(68.64/70.6)
ZDT2	0.0028	0.0048	0.0390	0.8845(88.5/100)	0.4050(38.5/94.9)	0.7421(56.4/76)
ZDT6	0.0026	0.0053	0.0036	1(100/100)	0.9949(98.8/99.3)	0.9880(66.5/67.3)
Deb1	0.0046	0.0539	0.0432	0.91(91/100)	0.718(71.8/100)	0.77(71/92)
Deb4	0.0026	0.0025	0.0022	0.98(98/100)	0.9522(95.2/100)	0.985(88.7/90)

TABLE II

SPACING AND *MINIMALSPACING* MEASURES ON THE TEST FUNCTIONS FOR BINARY ENCODING

Test	*Spacing*			*MinimalSpacing*		
Problem	AMOSA	PAES	NSGA-II	AMOSA	PAES	NSGA-II
*SCH*1	0.0167	0.0519	0.0235	0.0078	0.0530	0.0125
*SCH*2	0.0239	0.5289	0.0495	*N.A.*	*N.A.*	*N.A.*
*ZDT*1	0.0097	0.0264	0.0084	0.0156	0.0265	0.0147
*ZDT*2	0.0083	0.0205	0.0079	0.0151	0.0370	0.0130
*ZDT*6	0.0051	0.0399	0.0089	0.0130	0.0340	0.0162
*Deb*1	0.0166	0.0848	0.0475	0.0159	0.0424	0.0116
*Deb*4	0.0053	0.0253	0.0089	*N.A.*	*N.A.*	*N.A.*

and SCH2 which are single variable problems and for Deb1 and Deb4 which are two variable problems, 20 bits are used to encode each decision variable. In all the approaches, binary mutation applied with a probability of $p_m = 1/l$, where l is the string length, is used as the perturbation operation. We have chosen the values of $T\max$ (maximum value of the temperature), $T\min$ (minimum value of the temperature), and iter (number of iterations at each temperature) so that total number of fitness evaluations of the three algorithms becomes approximately equal. For PAES and NSGA-II, identical parameter settings as suggested in the original studies have been used. Here, the population size in NSGA-II, and archive sizes in AMOSA and PAES are set to 100. Maximum iterations for NSGA-II and PAES are 500 and 50 000, respectively. For AMOSA, $T\max = 200$, $T\min = 10^{-7}$, and iter $= 500$. The parameter values were determined after extensive sensitivity studies, which are omitted here to restrict the size of this paper.

1) Discussions of the Results: The *Convergence* and *Purity* values obtained using the three algorithms are shown in Table I. AMOSA performs the best for ZDT1, ZDT2, ZDT6, and Deb1 in terms of γ. For SCH1, all three are performing equally well. NSGA-II performs well for SCH2 and Dev4. Interestingly, for all the functions, AMOSA is found to provide a number of more overall nondominated solutions than NSGA-II. (This is evident from the quantities in parentheses in Table I, where x/y indicates that on an average the algorithm produced y solutions of which x remained good even when solutions from other MOO strategies are combined). AMOSA took 10 s to provide the first PO solution compared with 32 s for NSGA-II in case of ZDT1.

From Table I, it is again clear that AMOSA and PAES are always giving a number of more distinct solutions than NSGA-II.

Table II shows the *Spacing* and *MinimalSpacing* measurements. AMOSA is giving the best performance of *Spacing* most of the times, while PAES performs the worst. This is also evident from Figs. 6 and 7 which show the final PO fronts of SCH2 and Deb4 obtained by the three methods for the purpose of illustration (due to lack of space final PO fronts given by three methods for some test problems are omitted). With respect to *MinimalSpacing*, the performances of AMOSA and NSGA-II are comparable.

Table III shows the value of *displacement* for five problems, two with discontinuous and three with continuous PO fronts. AMOSA performs the best in almost all the cases. The utility of the new measure is evident, in particular, for Deb4, where PAES performs quite poorly (see Fig. 7). Interestingly, the *Convergence* value for PAES (Table I) is very good here, though the *displacement* correctly reflects that the PO front has been represented very poorly.

Table IV shows the time taken by the algorithms for the different test functions. It is seen that PAES takes less time in six of the seven problems because of its smaller complexity. AMOSA takes less time than NSGA-II in 30 variable problems like ZDT1, ZDT2, 10 variable problem ZDT6. However, for single and two variable problems, SCH1, SCH2, Deb1, and Deb4, AMOSA takes more time than NSGA-II. This may be due to complexity of its clustering procedure. Generally, for single or two variable problems, this procedure dominates the crossover and ranking procedures of NSGA-II. However, for 30

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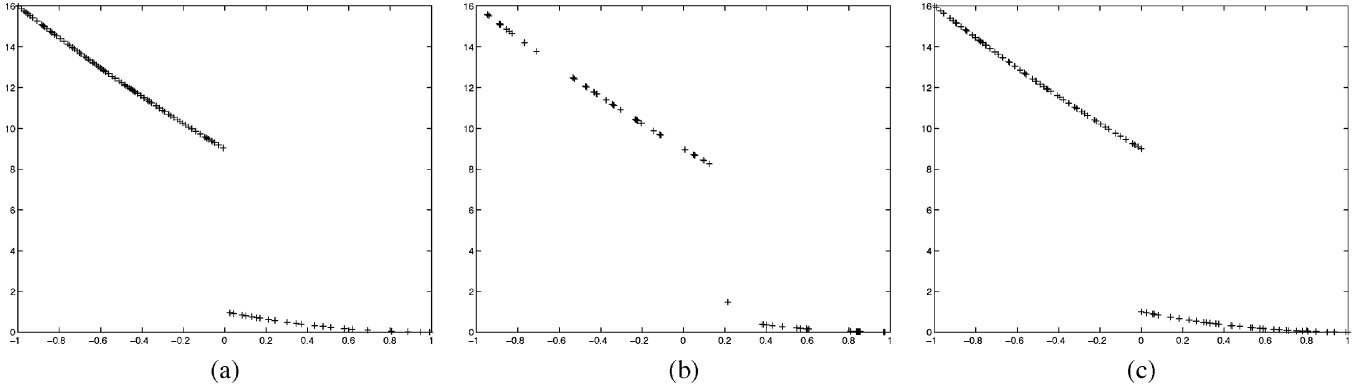
Fig. 6. The final nondominated front for SCH2 obtained by (a) AMOSA, (b) PAES, and (c) NSGA-II.
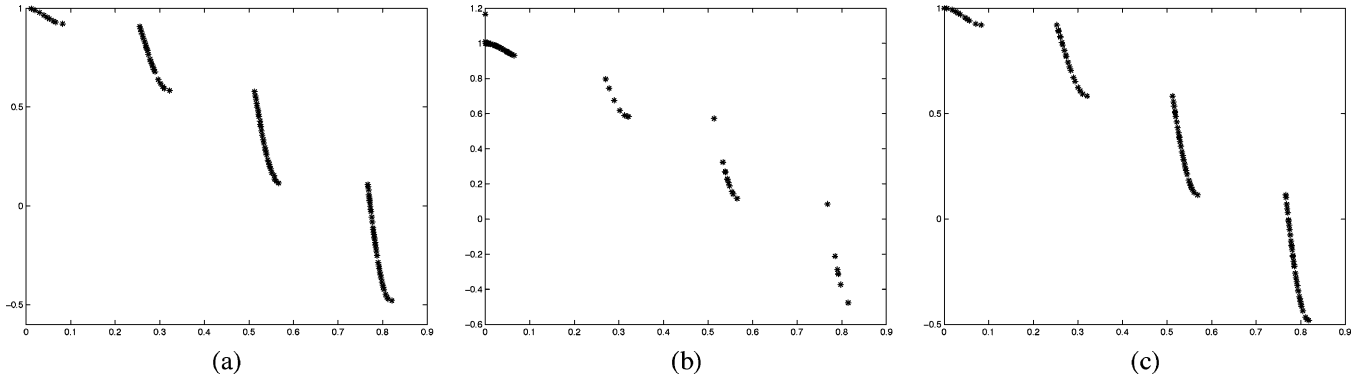

Fig. 7. The final nondominated front for Deb4 obtained by (a) AMOSA, (b) PAES, and (c) NSGA-II.

TABLE III
NEW MEASURE *DISPLACEMENT* ON THE TEST FUNCTIONS
FOR BINARY ENCODING

Algorithm	*SCH*2	*Deb*4	*ZDT*1	*ZDT*2	*ZDT*6
AMOSA	0.0230	0.0047	0.0057	0.0058	0.0029
PAES	0.6660	0.0153	0.0082	0.0176	0.0048
NSGA-II	0.0240	0.0050	0.0157	0.0096	0.0046

TABLE IV
TIME TAKEN BY DIFFERENT PROGRAMS (IN SEC) FOR BINARY ENCODING

Algorithm	*SCH*1	*SCH*2	*Deb*1	*Deb*4	*ZDT*1	*ZDT*2	*ZDT*6
AMOSA	15	14.5	20	20	58	56	12
PAES	6	5	5	15	17	18	16
NSGA-II	11	11	14	14	77	60	21

variable problems, the scenario is reversed. This is because of the increased complexity of ranking and crossover (due to increased string length) in NSGA-II.

C. Comparison of Real-Coded AMOSA With the Algorithm of Smith et al. [17] and Real-Coded NSGA-II

The real-coded version of the proposed AMOSA has also been implemented. The mutation is done, as suggested in [17]. Here, a new string is generated from the old string x by perturbing only one parameter or decision variable of x. The parameter to be perturbed is chosen at random and perturbed with a random variable ϵ drawn from a Laplacian distribution $p(\epsilon) \propto e^{-\|\sigma\epsilon\|}$, where the scaling factor σ sets magnitude of the perturbation. A fixed scaling factor equals to 0.1 is used for mutation. The initial temperature is selected by the procedure mentioned in [17]. That is, the initial temperature T max is calculated by using a short "burn-in" period during which all solutions are accepted and setting the temperature equal to the average positive change of energy divided by

$\ln(2)$. Here, T min is kept equal to 10^{-5} and the temperature is adjusted according to $T_k = \alpha^k T$ max, where α is set equal to 0.8. For NSGA-II, population size is kept equal to 100 and the total number of generations is set such that the total number of function evaluations of AMOSA and NSGA-II are the same. For AMOSA, the archive size is set equal to 100. (However, in part of the investigation, the archive size is kept unlimited as in [17]. The results are compared with those obtained by MOSA [17] and provided in [32].) AMOSA is executed for a total of 5000, 1000, 15 000, 5000, 1000, 5000, and 9000 run lengths, respectively, for DTLZ1, DTLZ2, DTLZ3, DTLZ4, DTLZ5, DTLZ, and DTLZ6. Total number of iterations *iter* per temperature is set accordingly. We have run real-coded NSGA-II (code obtained from KANGAL site: http://www.iitk.ac.in/kangal/codes.html). For NSGA-II, the following parameter setting is used: probability of crossover = 0.99, probability of mutation = $(1/l)$, where l is the string length, distribution index for the crossover operation = 10, and distribution index for the mutation operation = 100.

In MOSA [17], authors have used unconstrained archive size. Note that the archive size of AMOSA and the population size

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TABLE V
CONVERGENCE, PURITY, AND MINIMALSPACING MEASURES ON THE THREE OBJECTIVE TEST FUNCTIONS, WHILE ARCHIVE IS BOUNDED TO 100

Test Problem	Convergence			Purity			MinimalSpacing		
	AMOSA	MOSA	NSGA-II	AMOSA	MOSA	NSGA-II	AMOSA	MOSA	NSGA-II
$DTLZ1$	0.01235	0.159	13.695	0.857 (85.7/100)	0.56 (28.35/75)	0.378 (55.7/100)	0.0107	0.1529	0.2119
$DTLZ2$	0.014	0.01215	0.165	0.937 (93.37/100)	0.9637 (96.37/100)	0.23 (23.25/100)	0.0969	0.1069	0.1236
$DTLZ3$	0.0167	0.71	20.19	0.98 (93/95)	0.84 (84.99/100)	0.232 (23.2/70.6)	0.1015	0.152	0.14084
$DTLZ4$	0.28	0.21	0.45	0.833 (60/72)	0.97 (97/100)	0.7 (70/100)	0.20	0.242	0.318
$DTLZ5$	0.00044	0.0044	0.1036	1 (97/97)	0.638 (53.37/83.6)	0.05 (5/100)	0.0159	0.0579	0.128
$DTLZ6$	0.043	0.3722	0.329	0.9212 (92.12/100)	0.7175 (71.75/100)	0.505 (50.5/100)	0.1148	0.127	0.1266

TABLE VI
CONVERGENCE, PURITY, AND MINIMALSPACING MEASURES ON THE THREE OBJECTIVE TEST FUNCTIONS
BY AMOSA AND MOSA, WHILE ARCHIVE IS UNBOUNDED

Test Problem	Convergence		Purity		MinimalSpacing	
	AMOSA	MOSA	AMOSA	MOSA	AMOSA	MOSA
$DTLZ1$	0.010	0.1275	0.99(1253.87/1262.62)	0.189(54.87/289.62)	0.064	0.083.84
$DTLZ2$	0.0073	0.0089	0.96(1074.8/1116.3)	0.94(225/239.2)	0.07598	0.09595
$DTLZ3$	0.013	0.025	0.858(1212/1412.8)	0.81(1719/2003.9)	0.0399	0.05
$DTLZ4$	0.032	0.024	0.8845(88.5/100)	0.4050(38.5/94.9)	0.1536	0.089
$DTLZ5$	0.0025	0.0047	0.92(298/323.66)	0.684(58.5/85.5)	0.018	0.05826
$DTLZ6$	0.0403	0.208	0.9979(738.25/739.75)	0.287(55.75/194.25)	0.0465	0.0111

of NSGA-II are both 100. For the purpose of comparison with MOSA that has an unlimited archive [17], the clustering procedure (adopted for AMOSA), is used to reduce the number of solutions [32] to 100. Comparison is performed in terms of *Purity*, *Convergence*, and *MinimalSpacing*. Table V shows the *Purity*, *Convergence*, and *MinimalSpacing* measurements for DTLZ1–DTLZ6 problems obtained after the application of AMOSA, MOSA, and NSGA-II. It can be seen from this table that AMOSA performs the best in terms of *Purity* and *Convergence* for DTLZ1, DTLZ3, DTLZ5, and DTLZ6. In DTLZ2 and DTLZ4, the performance of MOSA is marginally better than that of AMOSA. NSGA-II performs the worst among all. Table V shows the *MinimalSpacing* values obtained by the three algorithms for DTLZ1-DTLZ6. AMOSA performs the best in all the cases.

As mentioned earlier, for comparing the performance of MOSA (by considering the results reported in [32]), a version of AMOSA without clustering and with unconstrained archive is executed. The results reported here are the average over ten runs. Table VI shows the corresponding *Purity*, *Convergence*, and *MinimalSpacing* values. Again, AMOSA performs much better than MOSA for all the test problems except DTLZ4. For DTLZ4, the MOSA performs better than that of AMOSA in terms of both *Purity* and *Convergence* values. Fig. 8 shows

the final PO front obtained by AMOSA and MOSA for DTLZ1–DTLZ3, while Fig. 9 shows the same for DTLZ5 and DTLZ6. As can be seen from the figures, AMOSA appears to be able to better approximate the front with more dense solutions as compared with MOSA.

It was mentioned in [33] that for a particular test problem, almost 40% of the solutions provided by an algorithm with truncation of archive got dominated by the solutions provided by an algorithm without archive truncation. However, the experiments we conducted did not adequately justify this finding. Let us denote the set of solutions of AMOSA with and without clustering as S_c and S_{wc}, respectively. We found that for DTLZ1, 12.6% of S_c were dominated by S_{wc}, while 4% of S_{wc} were dominated by S_c. For DTLZ2, 5.1% of S_{wc} were dominated by S_c, while 5.4% of S_c were dominated by S_{wc}. For DTLZ3, 22.38% of S_{wc} were dominated by S_c, while 0.53% of S_c were dominated by S_{wc}. For DTLZ4, all the members of S_{wc} and S_c are nondominating to each other and the solutions are the same, since execution of AMOSA without clustering does not provide more than 100 solutions. For DTLZ5, 10.4% of S_{wc} were dominated by S_c, while 0.5% of S_c were dominated by S_{wc}. For DTLZ6, all the members of S_{wc} and S_c are nondominating to each other.

To have a look at the performance of the AMOSA on a four-objective problem, we apply AMOSA and NSGA-II to

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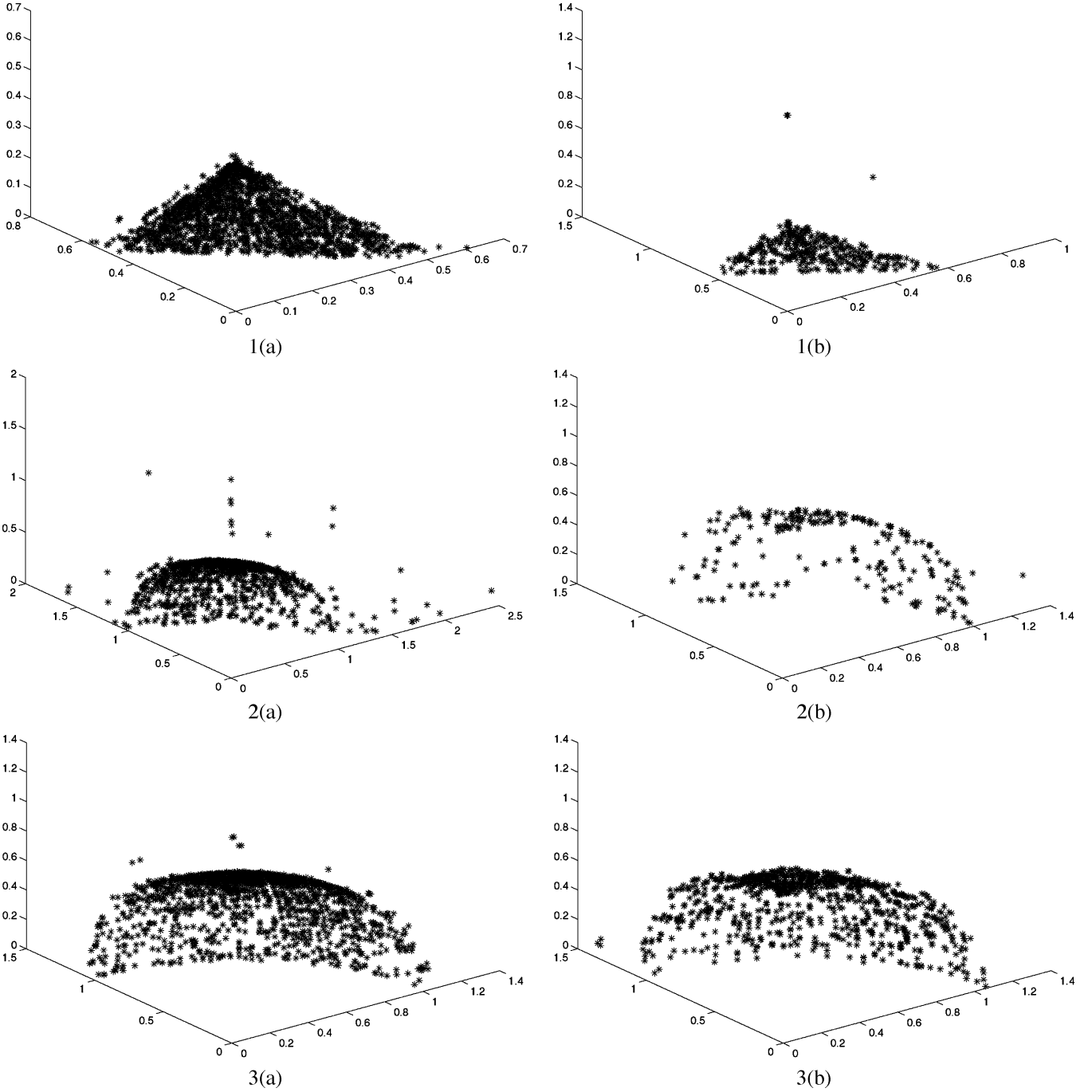

Fig. 8. The final nondominated front obtained by (a) AMOSA and (b) MOSA for the test problems (1) DTLZ1, (2) DTLZ2, and (3) DTLZ3.

the 13-variable DTLZ2 test problem. This is referred to as DTLZ2_4. The problem has a spherical Pareto-front in four dimensions given by the equation: $f_1^2 + f_2^2 + f_3^2 + f_4^2 = 1$ with $f_i \in [0, 1]$ for $i = 1$ to 4. Both the algorithms are applied for a total of 30 000 function evaluations (for NSGA-II popsize $= 100$ and number of generations $= 300$) and the *Purity*, *Convergence*, and *MinimalSpacing* values are shown in Table VII. AMOSA performs much better than NSGA-II in terms of all the three measures.

The proposed AMOSA and NSGA-II are also compared for DTLZ1_5 (9-variable 5 objective version of the test problem DTLZ1), DTLZ1_10 (14-variable 10 objective ver-

sion of DTLZ1) and DTLZ1_15 (19-variable 15 objective version of DTLZ1). The three problems have a spherical Pareto-front in their respective dimensions given by the equation $\sum_{i=1}^{M} f_i = 0.5$, where M is the total number of objective functions. Both the algorithms are executed for a total of 100 000 function evaluations for these three test problems (for NSGA-II, popsize $= 200$, number of generations $= 500$) and the corresponding *Purity*, *Convergence*, and *MinimalSpacing* values are shown in Table VII. The *Convergence* value indicates that NSGA-II does not converge to the true PO front, whereas AMOSA reaches the true PO front for all the three cases. The *Purity* measure also indicates this. The results on the many
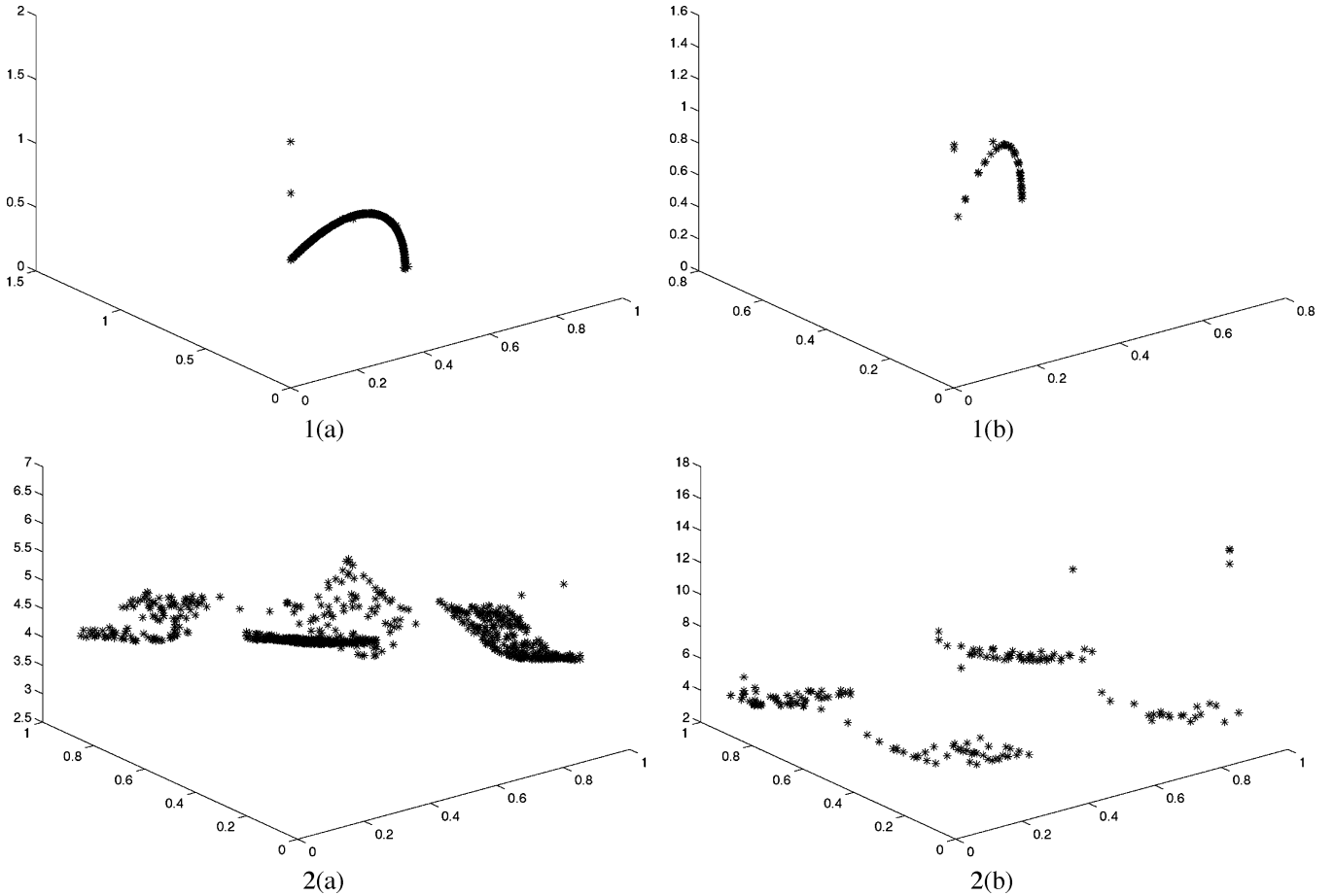
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Fig. 9.   The final nondominated front obtained by (a) AMOSA and (b) MOSA for the test problems (1) DTLZ5 and (2) DTLZ6.

TABLE VII
Convergence, *Purity*, and *Minimal Spacing* Measures on the DTLZ2_4, DTLZ1_5, DTLZ1_10,
and DTLZ1_15 Test Functions by AMOSA and NSGA-II

Test	$Convergence$		$Purity$		$Minimal Spacing$	
Problem	AMOSA	NSGA-II	AMOSA	NSGA-II	AMOSA	NSGA-II
$DTLZ2\_4$	0.2982	0.4563	0.9875(98.75/100)	0.903(90.3/100)	0.1876	0.22
$DTLZ1\_5$	0.0234	306.917	1	0	0.1078	0.165
$DTLZ1\_10$	0.0779	355.957	1	0	0.1056	0.2616
$DTLZ1\_15$	0.193	357.77	1	0	0.1	0.271

objective optimization problems show that AMOSA performs much better than NSGA-II. These results support the fact that Pareto ranking-based MOEAs such as NSGA-II do not work well on many objective optimization problems as pointed out in some recent studies [26], [27].

D. Discussion on Annealing Schedule

The annealing schedule of an SA algorithm consists of: i) initial value of temperature $(T\max)$; ii) cooling schedule; iii) number of iterations to be performed at each temperature; and iv) stopping criterion to terminate the algorithm. The initial value of the temperature should be chosen so that it allows the SA to perform a random walk over the landscape. Some methods to select the initial temperature are given in detail in

[18]. In this paper, as in [17], we have set the initial temperature to achieve an initial acceptance rate of approximately 50% on derogatory proposals. This is described in Section IV-C.

The cooling schedule determines the functional form of the change in temperature required in SA. The most frequently used decrement rule, also used in this paper, is the geometric schedule given by $T_{k+1} = \alpha \times T_k$, where $\alpha \; (0 < \alpha < 1)$ denotes the cooling factor. Typically, the value of α is chosen in the range between 0.5 and 0.99. This cooling schedule has the advantage of being very simple. Some other cooling schedules available in the literature are logarithmic, Cauchy, and exponential. More details about these schedules are available in [18]. The cooling schedule should be so chosen that it is able to strike a good balance between exploration and exploitation of the search space.

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In order to investigate the performance of AMOSA with another cooling schedule, the following is considered (obtained from http://www.members.aol.com/btluke/simanf1.htm)

$$T_i = T_0 \left(\frac{T_N}{T_0} \right)^{i/N}.$$

Here, N is the total number of iterations, T_N is the final temperature, and T_0 is the initial temperature. T_i is the temperature at iteration i. AMOSA with the above cooling schedule is applied on ZDT1. The *Convergence* and *MinimalSpacing* values obtained are 0.008665 and 0.017, respectively. Comparing with the corresponding values in Tables I and II, it is found that the results with this cooling schedule are somewhat poorer. However, an exhaustive sensitivity study needs to be performed for AMOSA.

The third component of an annealing schedule is the number of iterations performed at each temperature. It should be so chosen that the system is sufficiently close to the stationary distribution at that temperature. As suggested in [18], the value of the number of iterations should be chosen depending on the nature of the problem. Several criteria for termination of an SA process have been developed. In some of them, the total number of iterations that the SA procedure must execute is given, where as in some others, the minimum value of the temperature is specified. Detailed discussion on this issue can be found in [18].

V. DISCUSSION AND CONCLUSION

In this paper, a SA-based MOO algorithm has been proposed. The concept of amount of domination is used in solving the MOO problems. In contrast to most other MOO algorithms, AMOSA selects dominated solutions with a probability that is dependent on the amount of domination measured in terms of the hypervolume between the two solutions in the objective space. The results of binary-coded AMOSA are compared with those of two existing well-known MOO algorithms—NSGA-II (binary-coded) [19] and PAES [20] for a suite of seven 2-objective test problems having different complexity levels. In a part of the investigation, a comparison of the real-coded version of the proposed algorithm is conducted with a very recent multiobjective simulated annealing algorithm [17] and real-coded NSGA-II for six 3-objective test problems. Real-coded AMOSA is also compared with real-coded NSGA-II for some 4-, 5-, 10-, and 15-objective test problems. Several different comparison measures like *Convergence*, *Purity*, *MinimalSpacing*, and *Spacing*, and the time taken are used for the purpose of comparison. In this regard, a measure called *displacement* has also been used that is able to reflect whether a front is close to the PO front as well as its extent of coverage. A complexity analysis of AMOSA is performed. It is found that its complexity is more than that of PAES but smaller than that of NSGA-II.

It is seen from the given results that the performance of the proposed AMOSA is better than that of MOSA and NSGA-II in a majority of the cases, while PAES performs poorly in general. AMOSA is found to provide more distinct solutions than NSGA-II in each run for all the problems; this is a desirable feature in MOO. AMOSA is less time consuming than NSGA-II for complex problems like ZDT1, ZDT2, and ZDT6. Moreover, for problems with many objectives, the performance of AMOSA is found to be much better than that of NSGA-II. This is an interesting and appealing feature of AMOSA since Pareto ranking-based MOEAs, such as NSGA-II [19] do not work well on many objective optimization problems as pointed out in some recent studies [26], [27]. An interesting feature of AMOSA, as in other versions of MOSA algorithms, is that it has a nonzero probability of allowing a dominated solution to be chosen as the current solution in favour of a dominating solution. This makes the problem less greedy in nature; thereby leading to better performance for complex and/or deceptive problems. Note that it may be possible to incorporate this feature as well as the concept of amount of domination in other MOO algorithms in order to improve the performance.

There are several ways in which the proposed AMOSA algorithm may be extended in future. The main time consuming procedure in AMOSA is the clustering part. Some other more efficient clustering techniques or even the PAES like grid-based strategy, can be incorporated for improving its performance. Implementation of AMOSA with unconstrained archive is another interesting area to pursue in the future. An algorithm, unless analyzed theoretically, is only useful for the experiments conducted. Thus, a theoretical analysis of AMOSA needs to be performed in the future in order to study its convergence properties. Authors are currently trying to develop a proof for the convergence of AMOSA in the lines of the proof for single-objective SA given by Geman and Geman [4]. As has been mentioned in [18], there are no firm guidelines for choosing the parameters in an SA-based algorithm. Thus, an extensive sensitivity study of AMOSA with respect to its different parameters, notably the annealing schedule, needs to be performed. Finally, application of AMOSA to several real-life domains, e.g., VLSI system design [34], remote sensing imagery [35], data mining, and bioinformatics [36], needs to be demonstrated. The authors are currently working in this direction.

REFERENCES

[1] K. Deb, *Multiobjective Optimization Using Evolutionary Algorithms*. New York: Wiley, 2001.

[2] C. Coello, D. V. Veldhuizen, and G. Lamont, *Evolutionary Algorithms for Solving Multi-Objective Problems*. Norwell, MA: Kluwer, 2002.

[3] S. Kirkpatrick, C. Gelatt, and M. Vecchi, "Optimization by simulated annealing," *Science*, vol. 22, pp. 671–680, 1983.

[4] S. Geman and D. Geman, "Stochastic relaxation, Gibbs distributions and the Bayesian restoration of images," *IEEE Trans. Pattern Anal. Mach. Intell.*, vol. 6, no. 6, pp. 721–741, 1984.

[5] S. Bandyopadhyay, U. Maulik, and M. K. Pakhira, "Clustering using simulated annealing with probabilistic redistribution," *Int. J. Pattern Recogn. Artif. Intell.*, vol. 15, no. 2, pp. 269–285, 2001.

[6] R. Caves, S. Quegan, and R. White, "Quantitative comparison of the performance of SAR segmentation algorithms," *IEEE Trans. Image Process.*, vol. 7, no. 11, pp. 1534–1546, Nov. 1998.

[7] U. Maulik, S. Bandyopadhyay, and J. Trinder, "SAFE: An efficient feature extraction technique," *J. Knowl. Inf. Syst.*, vol. 3, pp. 374–387, 2001.

[8] P. Czyzak and A. Jaszkiewicz, "Pareto simulated annealing—A meta-heuristic technique for multiple-objective combinatorial optimization," *J. Multi-Criteria Decision Anal.*, vol. 7, pp. 34–47, 1998.

[9] M. Hapke, A. Jaszkiewicz, and R. Slowinski, "Pareto simulated annealing for fuzzy multi-objective combinatorial optimization," *J. Heuristics*, vol. 6, no. 3, pp. 329–345, 2000.

[10] A. Suppapitnarm, K. A. Seffen, G. T. Parks, and P. Clarkson, "A simulated annealing algorithm for multiobjective optimization," *Eng. Opt.*, vol. 33, pp. 59–85, 2000.

[11] D. K. Nam and C. Park, "Multiobjective simulated annealing: A comparative study to evolutionary algorithms," *Int. J. Fuzzy Syst.*, vol. 2, no. 2, pp. 87–97, 2000.

[12] E. L. Ulungu, J. Teghaem, P. Fortemps, and D. Tuyttens, "MOSA method: A tool for solving multiobjective combinatorial decision problems," *J. Multi-Criteri Decision Anal.*, vol. 8, pp. 221–236, 1999.

[13] D. Tuyttens, J. Teghem, and N. El-Sherbeny, "A particular multiobjective vehicle routing problem solved by simulated annealing," *Metaheuristics for Multiobjective Optimization*, vol. 535, pp. 133–152, 2003.

[14] I. Das and J. Dennis, "A closer look at drawbacks of minimizing weighted sums of objectives for pareto set generation in multicriteria optimization problems," *Structural Opt.*, vol. 14, no. 1, pp. 163–69, 1997.

[15] A. Jaszkiewicz, "Comparison of local search-based metaheuristics on the multiple objective knapsack problem," *Foundations of Comput. Decision Sci.*, vol. 26, no. 1, pp. 99–120, 2001.

[16] B. Suman, "Study of self-stopping PDMOSA and performance measure in multiobjective optimization," *Comput. Chem. Eng.*, vol. 29, no. 5, pp. 1131–1147, Apr. 15, 2005.

[17] K. Smith, R. Everson, and J. Fieldsend, "Dominance measures for multi-objective simulated annealing," in *Proc. 2004 IEEE Congr. Evol. Comput.*, 2004, pp. 23–30.

[18] B. Suman and P. Kumar, "A survey of simulated annealing as a tool for single and multiobjective optimization," *J. Oper. Res. Soc.*, vol. 57, no. 10, pp. 1143–1160, 2006.

[19] K. Deb, A. Pratap, S. Agarwal, and T. Meyarivan, "A fast and elitist multiobjective genetic algorithm: NSGA-II," *IEEE Trans. Evol. Comput.*, vol. 6, no. 2, pp. 182–197, Apr. 2002.

[20] J. D. Knowles and D. W. Corne, "Approxmating the nondominated front using the Pareto archived evolution strategy," *Evol. Comput.*, vol. 8, no. 2, pp. 149–172, 2000.

[21] S. Bandyopadhyay, S. K. Pal, and B. Aruna, "Multi-objective GAs, quantitative indices and pattern classification," *IEEE Trans. Syst., Man, Cybern.—B*, vol. 34, no. 5, pp. 2088–2099, Oct. 2004.

[22] H. Ishibuchi and T. Murata, "A multi-objective genetic local search algorithm and its application to flowshop scheduling," *IEEE Trans. Systems, Man, Cybern.—Part C: Applications and Reviews*, vol. 28, no. 3, pp. 392–403, Aug. 1998.

[23] J. R. Schott, "Fault tolerant design using single and multi-criteria genetic algorithms," Ph.D. dissertation, Massachusetts Inst. Technol., Cambridge, MA, 1995.

[24] H. Ishibuchi, T. Yoshida, and T. Murata, "Balance between genetic search and local search in memetic algorithms for multiobjective permutation flowshop scheduling," *IEEE Trans. Evol. Comput.*, vol. 6, no. 6, pp. 721–741, 1984.

[25] E. Zitzler and L. Thiele, An evolutionary algorithm for multiobjective optimization: The strength Pareto approach Zurich, Switzerland, Tech. Rep. 43, 1998, Gloriastrasse 35, CH-8092.

[26] E. J. Hughes, "Evolutionary many-objective optimization: Many once or one many?," in *Proc. Congr. Evol. Comput.*, Edinburgh, Scotland, U.K., Sep. 2–5, 2005, pp. 222–227.

[27] H. Ishibuchi, T. Doi, and Y. Nojima, "Incorporation of scalarizing fitness functions into evolutionary multiobjective optimization algorithms," in *Parallel Problem Solving From Nature IX (PPSN-IX)*, Sep. 2006, vol. 4193, pp. 493–502.

[28] J. Fieldsend, R. Everson, and S. Singh, "Using unconstrained elite archives for multi-objective optimization," *IEEE Trans. Evol. Comput.*, vol. 7, no. 3, pp. 305–323, Jun. 2003.

[29] A. K. Jain and R. C. Dubes, *Algorithms for Clustering Data*. Englewood Cliffs, NJ: Prentice-Hall, 1988.

[30] G. Toussaint, "Pattern recognition and geometrical complexity," in *Proc. 5th Int. Conf. Pattern Recogn.*, Miami Beach, FL, Dec. 1980, pp. 1324–1347.

[31] K. Deb, "Multi-objective genetic algorithms: Problem difficulties and construction of test problems," *Evol. Comput.*, vol. 7, no. 3, pp. 205–230, 1999.

[32] [Online]. Available: http://www.dcs.ex.ac.uk/people/kismith/mosa/results/tec/.

[33] E. Zitzler, K. Deb, and L. Thiele, "Comparison of multiobjective evolutionary algorithms: Empirical results," *Evol. Comput.*, vol. 8, no. 2, pp. 173–195, 2000.

[34] S. Saha, S. Sur-Kolay, S. Bandyopadhyay, and P. Dasgupta, "Multiobjective genetic algorithm for k-way equipartitioning of a point set with application to CAD-VLSI," in *Proc. 9th Int. Conf. Inf. Technol.*, Dec. 2006, pp. 281–284.

[35] S. Bandyopadhyay, U. Maulik, and A. Mukhopadhyay, "Multiobjective genetic clustering for pixel classification in remote sensing imagery," *IEEE Trans. Geosci. Remote Sensing*, vol. 45, no. 5, pp. 1506–1511, May 2007.

[36] A. Mukhopadhyay, U. Maulik, and S. Bandyopadhyay, "Efficient two-stage fuzzy clustering of microarray gene expression data," in *Proc. 9th Int. Conf. Inf. Technol.*, Dec. 2006, pp. 11–14.

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