On Set-Based Multiobjective Optimization

Eckart Zitzler, Lothar Thiele, and Johannes Bader

***Abstract*— Assuming that evolutionary multiobjective optimization (EMO) mainly deals with set problems, one can identify three core questions in this area of research: 1) how to formalize what type of Pareto set approximation is sought; 2) how to use this information within an algorithm to efficiently search for a good Pareto set approximation; and 3) how to compare the Pareto set approximations generated by different optimizers with respect to the formalized optimization goal. There is a vast amount of studies addressing these issues from different angles, but so far only a few studies can be found that consider all questions under one roof. This paper is an attempt to summarize recent developments in the EMO field within a unifying theory of set-based multiobjective search. It discusses how preference relations on sets can be formally defined, gives examples for selected user preferences, and proposes a general preference-independent hill climber for multiobjective optimization with theoretical convergence properties. Furthermore, it shows how to use set preference relations for statistical performance assessment and provides corresponding experimental results. The proposed methodology brings together preference articulation, algorithm design, and performance assessment under one framework and thereby opens up a new perspective on EMO.**

***Index Terms*— Convergence, evolutionary algorithms, multiobjective optimization, Pareto set approximation, preference articulation.**

I. Introduction

BY FAR, MOST PUBLICATIONS within the field of evolutionary multiobjective optimization (EMO) focus on the issue of generating a suitable approximation of the Pareto-optimal set, or Pareto set approximation for short. For instance, the first book on EMO by Kalyanmoy Deb [7] is mainly devoted to techniques of finding multiple tradeoff solutions using evolutionary algorithms.

Taking this view, one can state that EMO in general deals with set problems: the search space Ψ consists of all potential Pareto set approximations rather than single solutions, i.e., Ψ is a set of sets. Furthermore, an appropriate order on Ψ is required to fully specifiy the set problem—this order will here be denoted as set preference relation. A set preference relation provides the information on the basis of which the search is carried out; for any two Pareto set approximations, it says whether one set is better or not. Set preference relations can be defined, e.g., via set quality measures, which can be regarded as objective functions for sets, or directly using a binary relation, e.g., extended Pareto dominance on sets. Transforming the original problem into such a set problem offers many advantages for decision making, but also poses new challenges in terms of search space complexity.

In the light of this dicussion, three core research issues can be identified in the EMO field: 1) how to formalize the optimization goal in the sense of specifying what type of set is sought; 2) how to effectively search for a suitable set to achieve the formalized optimization goal; and 3) how to evaluate the outcomes of multiobjective optimizers with respect to the underlying set problem.

The question of what a good set of compromise solutions is depends on the preferences of the decision maker. Suppose, for instance, that a few representative solutions are to be selected from a large Pareto-optimal set; the actual choice can be quite different for different users. Many multiobjective evolutionary algorithms (MOEAs) aim at generating a subset that is uniformly distributed in the objective space [8], [16], [37]; others consider the subset maximizing the hypervolume of the dominated objective space as the best one [14], [22]. There are many more possibilites depending on the user and the situation: one may be interested in the extreme regions of the Pareto-optimal set [9], in convex portions of the tradeoff surface (knee points) [3], or in regions close to a predefined ideal point [11], to name only a few. These preferences are usually hard-coded in the algorithm, although there have been attemtps to design methods with more flexibility with respect to user preferences [13], [36].

Overall, one can conclude that EMO in general relies on *set preferences*, i.e., preference information that specifies whether one Pareto set approximation is better than another, and that MOEAs usually implement different types of set preferences. There are various studies that focus on the issue of preference articulation in EMO, in particular integrating additional preferences such as priorities, goals, and reference points [2], [4], [6], [11], [17], [23], [28]. However, these studies mainly cover preferences on solutions and not preferences on sets. Furthermore, there is a large amount of publications that deal with the definition and the application of quantitative quality measures for Pareto set approximations [20], [24], [31], [38], [40]. These quality measures or quality indicators reflect set preferences and have been widely employed to compare the outcomes generated by different MOEAs. Moreover, in recent years a trend can be observed to directly use specific measures such as the hypervolume indicator and the epsilon indicator in the search process [1], [10], [14], [15], [21], [22], [25], [27], [36]. Nevertheless, a *general* methodology to formalize set preferences and to use them for optimization is missing.

This paper represents one step toward such an overarching methodology. It:

1) proposes a theory of set preference relations that clarifies how user preferences on Pareto set approximations can

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The authors are with the Computer Engineering and Networks Laboratory (TIK), Eidgenössische Technische Hochschule Zürich, Switzerland (e-mail: zitzler@tik.ee.ethz.ch; thiele@tik.ee.ethz.ch; jbader@tik.ee.ethz.ch).

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TABLE I
OVERVIEW OF IMPORTANT SYMBOLS USED THROUGHOUT THE PAPER

Symbol	Meaning
$\mathcal{X}$	set of feasible solutions resp. decision vectors
$\mathcal{Z}$	objective space with $\mathcal{Z} \subseteq \mathbb{R}^n$
$f = (f_1, \ldots, f_n)$	vector-valued function $f : \mathcal{X} \longrightarrow \mathbb{R}^n$
$a \preceq_{\text{par}} b$	weak Pareto dominance relation on solutions
$a \preceq b$	any preference relation on solutions
$a \prec b$	$a \preceq b \wedge b \not\preceq a$ (strict preference)
$a \parallel b$	$a \not\preceq b \wedge b \not\preceq a$ (incomparability)
$a \equiv b$	$a \preceq b \wedge b \preceq a$ (indifference)
$\text{Min}(\mathcal{X}, \preceq)$	optimal solutions with respect to $\preceq$
Ψ	set of all admissible solutions sets $A \subseteq \mathcal{X}$
Ψ_m	set of all solutions sets $A \subseteq \mathcal{X}$ with $\lvert A \rvert \leq m$
$A \preccurlyeq_{\text{par}} B$	weak Pareto dominance relation on solution sets
$A \preccurlyeq B$	any preference relation on solution sets
$A \preccurlyeq^{\text{minpart}} B$	constructed set preference relation that combines $\preccurlyeq$ with minimum elements partitioning
$A \prec B$	$A \preccurlyeq B \wedge B \not\preccurlyeq A$ (strict preference)
$A \parallel B$	$A \not\preccurlyeq B \wedge B \not\preccurlyeq A$ (incomparability)
$A \equiv B$	$A \preccurlyeq B \wedge B \preccurlyeq A$ (indifference)
$\text{Min}(\Psi, \preccurlyeq)$	optimal solution sets with respect to $\preccurlyeq$

be formalized on the basis of quality indicators and what criteria such formalizations must fulfill;

2) introduces a general set-preference based search algorithm that can be flexibly adapted to arbitrary types of set preference relations and that can be shown to converge under certain mild assumptions; and
3) discusses an approach to statistically compare the outcomes of multiple search algorithms with respect to a specific set preference relation.

The novelty of this approach is that it brings all aspects of preference articulation, multiobjective search, and performance assessment under one roof, while achieving a clear separation of concerns. This offers several benefits: 1) it provides flexibility to the decision maker as he can change his preferences without the need to modify the search algorithm; 2) the search can be better guided which is particularly important in the context of high-dimensional objective spaces; 3) algorithms designed to meet specific preferences can be compared on a fair basis since the optimization goal can be explicitly formulated in terms of the underlying set preference relation. The practicability of this approach has already been demonstrated in a preliminary study which contains selected proof-of-principle results [39]. This paper is the full version of this paper; in particular, it introduces the underlying theoretical framework and contains an extensive investigation of the proposed search methodology.

In the following, we will first provide the formal basis of set preference relations and introduce fundamental concepts. Afterward, we will discuss how set preference relations can be designed using quality indicators and present some example relations. A general, set preference based multiobjective search algorithm will be proposed in Section IV, including a discussion of convergence properties. Finally, Section V presents a methodology to compare algorithms with respect to a given set preference relation and provides experimental results for selected preferences.

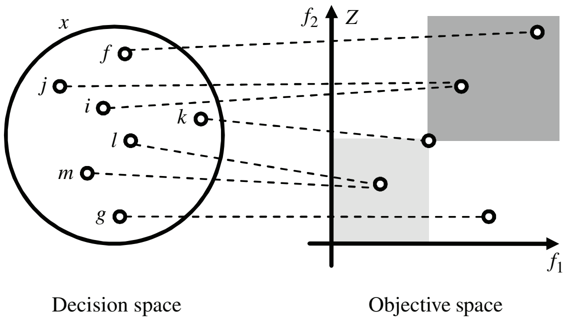


Fig. 1. Optimization scenario with $\mathcal{X} = \{f, g, i, j, k, l, m\}$ and $n = 2$. In the case that the preference relation is the weak Pareto-dominance relation $\preceq_{\text{par}}$, the shaded areas represent locations of solutions that are dominated by k (dark) and that dominate k (light).

II. NEW PERSPECTIVE: SET PREFERENCE RELATIONS

As has been described in the introduction, multiobjective optimization will be viewed as a preference-based optimization on sets. The purpose of this section is to formally define the notation of optimization and optimality in this context and to provide the necessary foundations for the practical algorithms described in the forthcoming sections. Table I serves as a reference for the nomenclature introduced in the following.

A. Basic Terms

We are considering the optimization of vector-valued objective functions $f = (f_1, \ldots, f_n) : \mathcal{X} \longrightarrow \mathbb{R}^n$ where all components f_i are—without loss of generality—to be minimized. Here, $\mathcal{X}$ denotes the feasible set of solutions in the decision space, i.e., the set of alternatives of the decision problem. A single alternative $x \in \mathcal{X}$ will be denoted as a decision vector or solution. The image of $\mathcal{X}$ under f is denoted as the feasible set in the objective space $\mathcal{Z} = f(\mathcal{X}) = \{y \in \mathbb{R}^n \mid \exists x \in \mathcal{X} : y = f(x)\}$ where $\mathcal{Z} \subseteq \mathbb{R}^n$. The objective values of a single alternative x will be denoted as objective vector $y = f(x)$.

For reasons of simplicity, we suppose that the decision space is finite. Nevertheless, almost all results described in the paper hold for infinite sets also or can be generalized. Fig. 1 illustrates a possible scenario with seven solutions in the feasible set and a 2-D objective space ($n = 2$).

In order to allow for optimization in such a situation, we need a preference relation $a \preceq b$ on the feasible set in the decision space which denotes that a solution a is at least as good as a solution b. In the context of this paper, we will suppose that all preference relations are preorders.[1]

[1] A preorder $\leqq$ on a given set S is reflexive and transitive: $a \leqq a$ and $(a \leqq b \wedge b \leqq c) \Rightarrow (a \leqq c)$ holds for all a, b, and c in S.

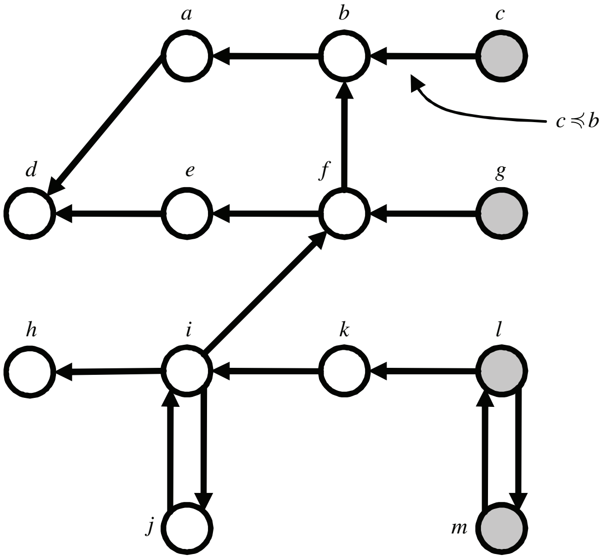


Fig. 2. Representation of a preordered set $(\mathcal{X}, \preceq)$ where $\mathcal{X}$ consists of the solutions $\{a, \dots, m\}$. The optimal solutions are $\text{Min}(\mathcal{X}, \preceq) = \{c, g, l, m\}$. $\{i, j\}$ and $\{l, m\}$ form two equivalence classes, i.e. $i \equiv j$ and $l \equiv m$. As $b \npreceq c$ and $c \preceq b$, we find $c \prec b$.

A well-known preference relation in the context of multiobjective optimization is the (weak) Pareto dominance.

Definition 2.1: A solution $a \in \mathcal{X}$ weakly Pareto-dominates a solution $b \in \mathcal{X}$, denoted as $a \preceq_{\text{par}} b$, if it is at least as good in all objectives, i.e. $f_i(a) \leq f_i(b)$ for all $1 \leq i \leq n$.

Note that $\preceq_{\text{par}}$ is only one example of a useful preference relation. The results described in this paper are not restricted to the concept of Pareto dominance but hold for any preference relation defined on the set of solutions.

The situation that a solution a is at least as good as a solution b will also be denoted as a being weakly preferable to b in this paper. Moreover, we will use the following terms: A solution a is strictly better than or preferable to a solution b (denoted as $a \prec b$) if $a \preceq b \wedge b \npreceq a$. A solution a is incomparable to a solution b ($a \parallel b$) if $a \npreceq b \wedge b \npreceq a$. A solution a is equivalent or indifferent to a solution b (denoted as $a \equiv b$) if $a \preceq b \wedge b \preceq a$. We say that a set of solutions form an equivalence class, if they are mutually equivalent. We denote the set of minimal elements[2] in the ordered set $(S, \leqq)$ as

$$\text{Min}(S, \leqq) = \{x \in S \mid \nexists a \in S : a \leqq x \wedge x \nleqq a\}.$$

We will call the set

$$\mathcal{X}^* = \text{Min}(\mathcal{X}, \preceq)$$

the optimal set of $\mathcal{X}$ with respect to $\preceq$ and an element $x^* \in \mathcal{X}^*$ is an optimal solution. Optimization may now be termed as finding a minimal element in the ordered feasible set $(\mathcal{X}, \preceq)$.

Preference relations can also be depicted graphically. Fig. 2 shows a possible preordered set of solutions $\mathcal{X} = \{a, \dots, m\}$. In particular, the preferences among $\{f, g, i, k, l, m\}$ correspond directly to the scenario shown in Fig. 1.

B. Approximation of the Pareto-Optimal Set

As a preference relation $\preceq$ defined above is usually not a total order on the feasible set,[3] we will often have many optimal solutions, i.e., many minimal elements that reflect the different tradeoffs among the objective functions.

In particular, this holds for the Pareto preference relation $\preceq_{\text{par}}$. As a result, we may not only be interested in one of these minimal elements but also in a carefully selected subset that reflects additional preference information of some decision maker. Traditional evolutionary multiobjective optimization methods attempt to solve this problem by maintaining and improving sets of decision vectors, denoted as populations. The corresponding optimization algorithms are tuned to anticipated preferences of a decision maker.

Thus, the underlying goal of set-based multiobjective optimization can be described as determining a (small-sized) set of alternative solutions:

1) that contains as many different decision vectors as possible that are minimal with respect to a preference relation *on the feasible set in the decision space* (for example the weak Pareto-dominance according to Definition 2.1); and
2) whose selection of minimal and non-minimal decision vectors reflects the preferences of the decision maker.

As pointed out in Section I, the purpose of the paper is to define set-based multiobjective optimization on the basis of these two aspects. In contrast to previous results, the second item as defined above is made formal and treated as a first class citizen in optimization theory and algorithms. This not only leads to a better understanding of classical population-based multiobjective optimization but also allows for defining set-based methods with corresponding convergence results as well as statistical tests to compare different algorithms. Finally, a new set of optimization algorithms can be obtained which can directly take preference information into account.

Therefore, we need to formalize the preferences of a decision maker on the subset of decision vectors in an optimal set of solutions. This will be done by defining a preorder $\preccurlyeq$ on the set of all possible sets of solutions. A set of solutions P is defined as a set of decision vectors, i.e., $x \in P \Rightarrow x \in \mathcal{X}$. A set of all admissible sets, e.g., sets of finite size, is denoted as Ψ, i.e., $P \in \Psi$.

> We define set-based multiobjective optimization as finding a minimal element of the ordered set $(\Psi, \preccurlyeq)$ where Ψ is a set of admissible sets of solutions.

We can summarize the elements of a set-based multiobjective optimization problem as follows:

1) a set of feasible solutions $\mathcal{X}$;
2) a vector-valued objective function $f : \mathcal{X} \longrightarrow \mathbb{R}^n$;
3) a set Ψ of all admissible sets P of decision vectors with $x \in P \Rightarrow x \in \mathcal{X}$;
4) a preference relation $\preccurlyeq$ on Ψ.

In the light of the above discussion, the preference relation $\preccurlyeq$ needs to satisfy the aforementioned two conditions;

[2] A minimal element u of an ordered set $(S, \leqq)$ set with a preorder $\leqq$ satisfies: If $a \leqq u$ for some a in the set, then $u \leqq a$.

[3] A binary relation $\leqq$ on a set S is called total, if $(a \leqq b) \vee (b \leqq a)$ holds for all $a, b \in S$.

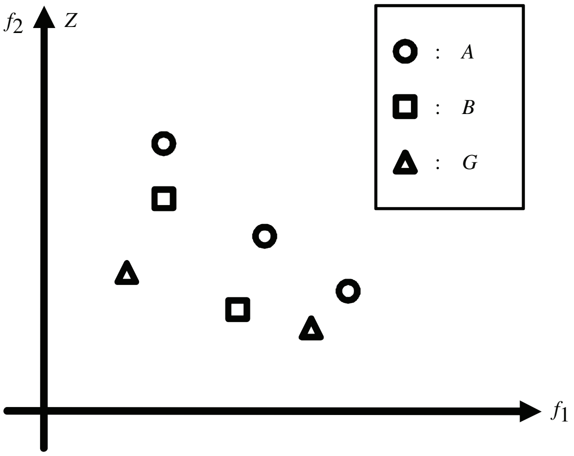


Fig. 3. Representation of a preordered set of sets of solutions $\{A, B, G\} \in \Psi$ where $\preceq_{\text{par}}$ is assumed to be the underlying solution-based preference relation. We find $B \preccurlyeq A$, $G \preccurlyeq A$ and $B \parallel G$, i.e., B and G are incomparable.

the first one guarantees that we actually optimize the objective functions and the second one allows the addition of preferences of the decision maker. In the next section, we will discuss the necessary properties of suitable preference relations and the concept of refinement.

C. Preference Relations

We will construct $\preccurlyeq$ in two successive steps. At first, a general set-based preference relation (a set preference relation) $\preccurlyeq \subseteq \Psi \times \Psi$ will be defined that is *conforming* to a solution-based preference relation $\preceq \subseteq \mathcal{X} \times \mathcal{X}$. This set preference relation will then be *refined* by adding preferences of a decision maker in order to possibly obtain a total order. For a *conforming* set preference relation we require that no solution is excluded that could be interesting to a decision maker. In addition, if for each solution $b \in B$ there is some solution $a \in A$ which is at least as good, then we can safely say that A is at least as good as or weakly preferable to B.

From the above considerations, the definition of a conforming set-based preference relation follows directly; it is in accordance to the formulations used in [20], [40].

Definition 2.2: Let be given a set $\mathcal{X}$ and a set Ψ whose elements are subsets of $\mathcal{X}$, i.e., sets of solutions. Then the preference relation $\preccurlyeq$ on Ψ conforms to $\preceq$ on $\mathcal{X}$ if for all $A, B \in \Psi$

$$A \preccurlyeq B \;\Leftrightarrow (\forall b \in B : (\exists a \in A : a \preceq b)).$$

As an example, Fig. 3 shows three sets of solutions A, B, and G. According to the above definition, we find that $B \preccurlyeq A$ and $G \preccurlyeq A$. As sets B and G are incomparable, we have $B \parallel G$.

Now, it will be shown that the above preference relation is indeed suitable for optimization.

Theorem 2.3: The set preference relation $\preccurlyeq$ as defined in Definition 2.2 is a preorder.

Proof: $A \preccurlyeq A$ is true as $\forall a' \in A : (\exists a \in A : a \preceq a')$ holds with $a' = a$. Now we need to show that $A \preccurlyeq B \wedge B \preccurlyeq C \Rightarrow A \preccurlyeq C$. Given an arbitrary $c^* \in C$. From $B \preccurlyeq C$ we know that $\exists b^* \in B$ such that $b^* \preceq c^*$. From $A \preccurlyeq B$ we know that $\exists a^* \in A$ such that $a^* \preceq b^*$. From the transitivity of $\preceq$ we can conclude that $a^* \preceq c^*$ holds. As a result, $\forall c^* \in C : (\exists a^* \in A : a^* \preceq c^*)$. ■

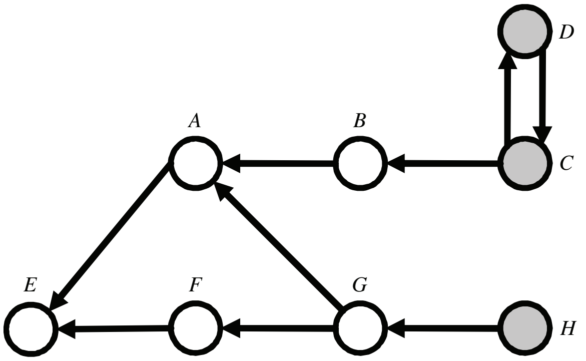


Fig. 4. Representation of a preordered set of sets of solutions $\Psi = \{A, B, C, D, E, F, G, H\}$. The minimal sets are $\text{Min}(\Psi, \preccurlyeq) = \{C, D, H\}$.

Therefore, we can also represent the relations between the sets of solutions in form of an acyclic graph whose nodes correspond to sets of solutions and edges correspond to the set preference relation $\preccurlyeq$. As an example, Fig. 4 represents such a diagram. Note that the relation between the sets A, B, and G corresponds exactly to the scenario shown in Fig. 3. The minimal sets are $\text{Min}(\Psi, \preccurlyeq) = \{C, D, H\}$.

The above definition of a conforming set-based preference relation ensures that each set in $\text{Min}(\Psi, \preccurlyeq)$ contains at least one representative of each equivalence class of $\mathcal{X}^*$. Therefore, no preferences other than that contained in $\preceq$ is included so far.

For practical reasons, one may deal with sets of solutions that have an upper bound m on their size, i.e., if $P \in \Psi_m$, then $|P| \leq m$. In this case, the properties of minimal elements of $(\Psi_m, \preccurlyeq)$ are somewhat more complex.

Let s denotes the number of equivalence classes of $\mathcal{X}^* = \text{Min}(\mathcal{X}, \preceq)$, i.e., the maximal number of solutions that are not equivalent. In the important case $m < s$ (a small set size), a set P is an element of $\text{Min}(\Psi_m, \preccurlyeq)$ (i.e., it is a minimal set of solutions) iff it contains m minimal solutions that are not equivalent, i.e., a minimal set of solutions may contain one representative of each equivalence class only.

If we are interested in the solutions themselves, then we may want to have the possibility to determine all solutions that lead to the same value in objective space. They may well be different in the decision space and, therefore, be interesting to a decision maker, see Fig. 2. This can be achieved by replacing a given solution-based preference relation $\preceq$ that considers objective values only. Equivalent solutions that lead to the same objective values should become incomparable. As a result, solutions will be equivalent only if they are identical in the decision space. We denote such a preference relation as $\dot{\preceq}$ with

$$a \,\dot{\preceq}\, b \Leftrightarrow (a = b) \vee (a \prec b).$$

This new preference relation is a preorder as it is reflexive ($a \,\dot{\preceq}\, a$ clearly holds) and transitive. The latter property can be shown as follows: $a \,\dot{\preceq}\, b \wedge b \,\dot{\preceq}\, c \Rightarrow ((a = b) \vee (a \prec b)) \wedge ((b = c) \vee (b \prec c)) \Rightarrow ((a = c) \vee (a \prec c)) \Rightarrow a \,\dot{\preceq}\, c$. Fig. 5 shows the order graph if $\preceq_{\text{par}}$ is replaced by $\dot{\preceq}_{\text{par}}$ in Fig. 2. As can

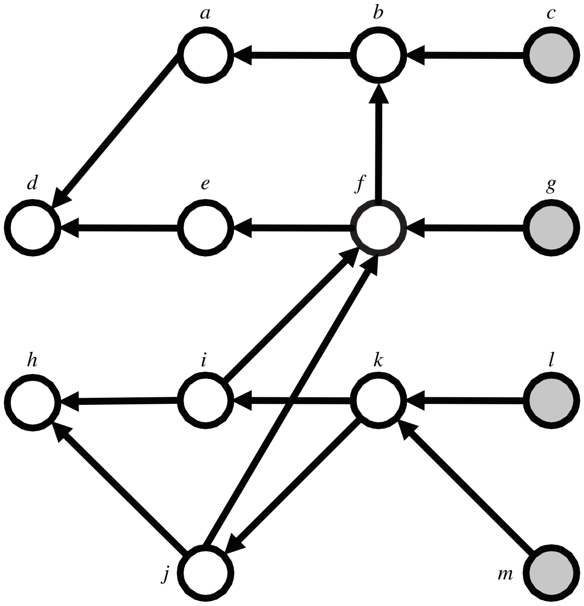


Fig. 5. Representation of the preordered set of solutions from Fig. 2 if $\preceq_{\text{par}}$ is replaced by $\dot{\preceq}_{\text{par}}$.

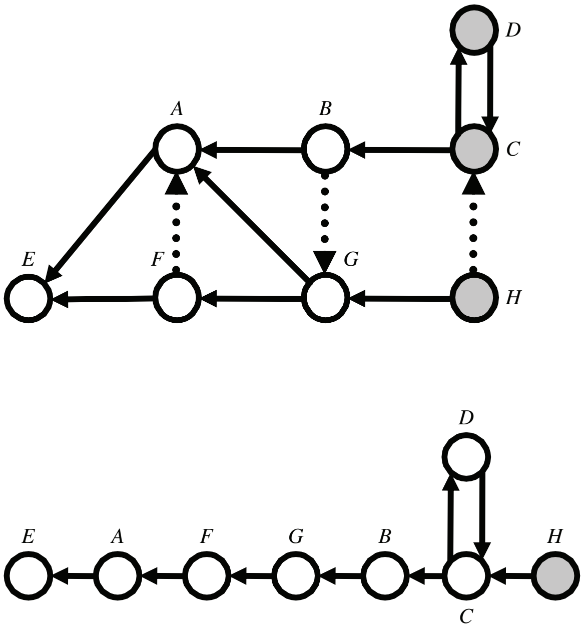


Fig. 6. Including preference information may create a total preorder that can be used for optimization. Here, three preferences $F \preccurlyeq A$, $B \preccurlyeq G$ and $H \preccurlyeq C$ have been added to the preorder shown in Fig. 4. The resulting total preorder is shown at the bottom.

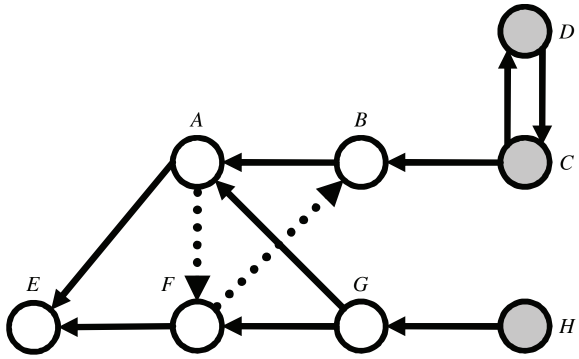


Fig. 7. Including preference information arbitrarily may create cycles in the optimization. Here, two preferences $A \preccurlyeq F$ and $F \preccurlyeq B$ have been added to the preorder shown in Fig. 4.

be seen, the equivalence classes are not present anymore and i, j as well as l, m are now considered as incomparable.

The above definition of a preference relation $\dot{\preceq}$ derived from $\preceq$ ensures that the minimal set of sets $\text{Min}(\Psi, \dot{\preccurlyeq})$ contains sets with all possible combinations of minimal elements $\text{Min}(\mathcal{X}, \preceq)$. More precisely, we can state that each minimal set $P^* \in \text{Min}(\Psi_m, \dot{\preccurlyeq})$ now contains m minimal solutions provided that $m < |\mathcal{X}^*|$.

D. Refinements

What remains to be done is to define the notion of refinement, as we need to have a possibility to include preference information into a conforming preference relation. This way, we can include preference information of a decision maker and optimize toward a set which contains a preferred subset of all minimal solutions, i.e., nondominated solutions in the case of Pareto dominance. The goal of such a refinement is twofold: At first, the given preorder should become "more total." This way, there are less incomparable sets of solutions which are hard to deal with by any optimization method. Second, the refinement will allow us to explicitly take into account preference information of a decision maker.

An example is shown in Fig. 6, where three edges (preference relations) have been added and the resulting ordering is a total preorder with the optimal set of solutions H. Just adding an ordering among incomparable solutions potentially leads to cycles in the ordering, as the resulting structure is no longer a preorder. Using such an approach in optimization will prevent convergence in general, see also Fig. 7.

For the refinement, we require the following properties.

1) The refinement should again be a preorder.
2) If a set is minimal in the refined order for some subset of Ψ, it should also be minimal in the original order in the same subset. This way, we guarantee that we actually optimize the objective functions with respect to some preference relation, e.g., Pareto dominance.

As a result of this discussion, we obtain the following definition:

Definition 2.4: Given a set Ψ. Then the preference relation $\preccurlyeq_{\text{ref}}$ refines $\preccurlyeq$ if for all $A, B \in \Psi$ we have

$$(A \preccurlyeq B) \wedge (B \not\preccurlyeq A) \Rightarrow (A \preccurlyeq_{\text{ref}} B) \wedge (B \not\preccurlyeq_{\text{ref}} A).$$

Examples of legal refinements are depicted in Fig. 8. Note, that the refinement still needs to be a preorder.

If we use the notion of strictly better, we can also derive the condition $A \prec B \Rightarrow A \prec_{\text{ref}} B$. In other words, if in the given preference relation a set A is strictly better than a set B $(A \prec B)$, then it must be strictly better in the refined relation, too $(A \prec_{\text{ref}} B)$. As can be seen, refining a preference relation maintains existing strict preference relationships. If two sets are incomparable, i.e., $A \parallel B \Leftrightarrow (A \not\preccurlyeq B) \wedge (B \not\preccurlyeq A)$, then

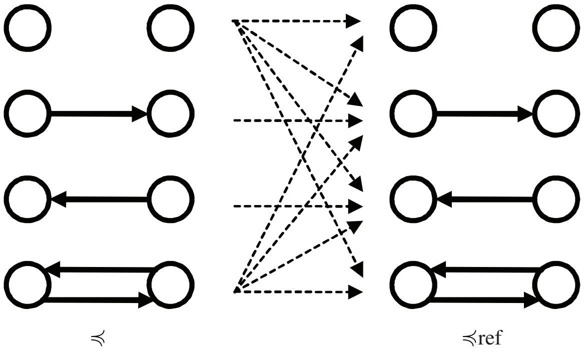


Fig. 8. Left-hand side shows the four different possibilities between two nodes of the given preference relation: no edge (incomparable), single edge (one is better than the other) and double edge (equivalent). The right-hand side shows the possibility in case of the refined relation. The dotted edges represent all possible changes of edges if $\preccurlyeq$ is refined to $\preccurlyeq_{\text{ref}}$.

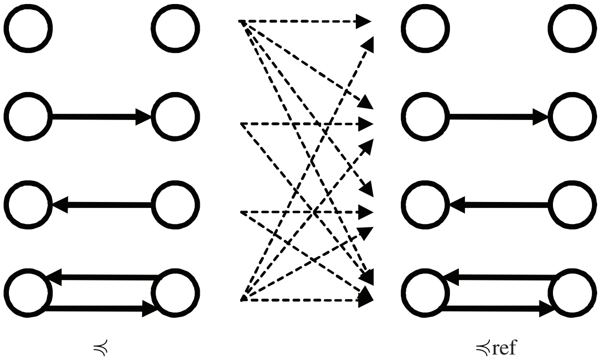


Fig. 9. Left-hand side shows the four different possibilities between two nodes of the given preference relation: no edge (incomparable), single edge (one is better than the other) and double edge (equivalent). The right-hand side shows the possibility in case of the weakly refined relation. The dotted edges represent all possible changes of edges if $\preccurlyeq$ is weakly refined to $\preccurlyeq_{\text{ref}}$.

additional edges can be inserted by the refinement. In case of equivalence, i.e., $A \equiv B \Leftrightarrow (A \preccurlyeq B) \wedge (B \preccurlyeq A)$, edges can be removed.

As will be seen in the next section, some of the widely used preference relations are not refinements in the sense of Definition 2.4, but satisfy a weaker condition.

Definition 2.5: Given a set Ψ. Then the set preference relation $\preccurlyeq_{\text{ref}}$ weakly refines $\preccurlyeq$ if for all $A, B \in \Psi$ we have

$$(A \preccurlyeq B) \wedge (B \not\preccurlyeq A) \Rightarrow (A \preccurlyeq_{\text{ref}} B).$$

In other words, if set A is strictly better than B ($A \prec B$), then A weakly dominates B in the refined preference relation, i.e., $A \preccurlyeq_{\text{ref}} B$. Therefore, A could be incomparable to B in the refined preference relation, i.e., $A \parallel_{\text{ref}} B$. In addition, if a preference relation refines another one, it also weakly refines it. Fig. 9 depicts all possibilities of a weak refinement. The weak refinement still needs to be a preorder.

The following hierarchical construction of refinement relations will be used in later sections for several purposes. At first, it allows the conversion of a given weak refinement into a refinement. This way, a larger class of available indicators and preference relations can be used. In addition, it provides a simple method to add decision maker preference information to a given relation by adding an order to equivalent sets. This way, a preorder can be made "more total." Finally, it enables refining a given preorder in a way that helps to speed up the convergence of an optimization algorithm, e.g., by taking into account also solutions that are worse than others in a set. This way, the successful technique of nondominated sorting can be used in the context of set-based optimization.

The following construction resembles the concept of hierarchy used in [17]; however, here (a) we are dealing with preference relations on sets and (b) the hierarchical construction is different.

Definition 2.6: Given a set Ψ and a sequence S of k preference relations over Ψ with $S = (\preccurlyeq^1, \preccurlyeq^2, \ldots, \preccurlyeq^k)$, the preference relation $\preccurlyeq_S$ associated with S is defined as follows. Let $A, B \in \Psi$; then $A \preccurlyeq_S B$ if and only if $\exists 1 \leq i \leq k$ such that the following two conditions are satisfied:

(i) $(i < k \wedge (A \prec^i B)) \vee (i = k \wedge (A \preccurlyeq^k B))$

(ii) $\forall 1 \leq j < i : (A \preccurlyeq^j B \wedge B \preccurlyeq^j A)$.

With this definition, we can derive the following procedure to determine $A \preccurlyeq_S B$ for two sets A and B.

1) Start from the first preference relation, i.e., $j = 1$. Repeat the following step: If $A \equiv^j B$ holds (A and B are equivalent), then increase j to point to the next relation in the sequence if it exists.
2) If the final j points to the last preference relation ($j = k$), then set $A \preccurlyeq_S B \Leftrightarrow A \preccurlyeq^k B$. Otherwise, set $A \preccurlyeq_S B \Leftrightarrow A \prec^k B$.

As described above, one of the main reasons to define a sequence of preference relations is to upgrade a given weak refinement to a refinement. In addition, it would be desirable to add arbitrary preorders to the sequence S. As they need not to be refinements of the given order $\preccurlyeq$, a decision maker can freely add his preferences this way. The following theorem states the corresponding results. The proof is provided in the Appendix.

Theorem 2.7: Given a sequence of preference relations according to Definition 2.6. Suppose there is a $k' \leq k$ such that $\preccurlyeq^{k'}$ is a refinement of a given preference relation $\preccurlyeq$ and all relations $\preccurlyeq^j$, $1 \leq j < k'$ are weak refinements of $\preccurlyeq$. Then $\preccurlyeq_S$ is a refinement of $\preccurlyeq$. Furthermore, if all relations $\preccurlyeq^j$, $1 \leq j < k$ are preorders, so is $\preccurlyeq_S$; if all relations $\preccurlyeq^j$, $1 \leq j < k$ are total preorders, then $\preccurlyeq_S$ is a total preorder.

All set preference relations $\preccurlyeq^j$, $k' < j \leq k$ can be arbitrary preorders that may reflect additional preferences, see also Fig. 10. Nevertheless, the resulting preference relation $\preccurlyeq_S$ still refines $\preccurlyeq$. The previously described hierarchical construction of refinements will be applied in later sections of the paper to construct preference relations that are useful for set-based multiobjective optimization.

III. Design of Preference Relations Using Quality Indicators

A. Unary Indicators

Unary quality indicators are a possible means to construct set preference relations that on the one hand are total orders and on the other hand satisfy the refinement property, cf. Definition 2.4. They represent set quality measures that

$$S = (\underbrace{\preccurlyeq^{1}, \ldots, \preccurlyeq^{k'-1}}_{\text{Weak refinement}}, \overset{\text{Refinement}}{\preccurlyeq^{k'}}, \underbrace{\preccurlyeq^{k'+1}, \ldots, \preccurlyeq^{k}}_{\text{Preorder}})$$

Fig. 10. Representation of the hierarchical construction of refinements according to Theorem 2.

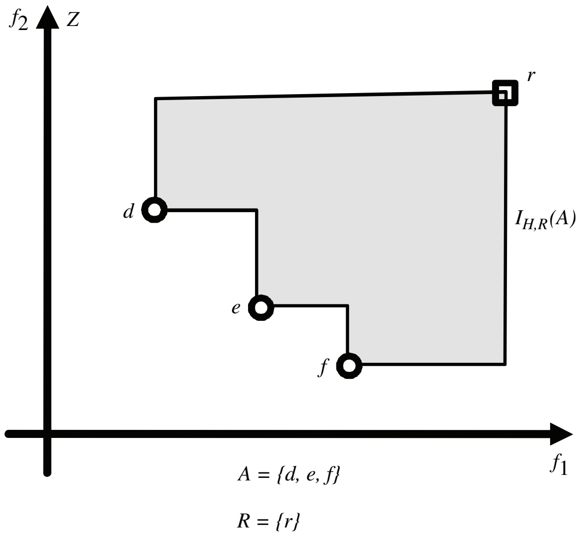


Fig. 11. Graphical representation of the unary hypervolume indicator.

map each set $A \in \Psi$ to a real number $I(A) \in \mathbb{R}$. Given an indicator I, one can define the corresponding preference relation as

$$A \preccurlyeq_{\mathrm{I}} B := (I(A) \leq I(B)) \tag{1}$$

where we assume that smaller indicator values stand for higher quality; in other words, A is as least as good as B if the indicator value of A is not larger than the one of B. By construction, the preference relation $\preccurlyeq_{\mathrm{I}}$ defined above is a preorder as it is reflexive as $I(A) \leq I(A)$ and transitive as $(I(A) \leq I(B)) \wedge (I(B) \leq I(C)) \Rightarrow I(A) \leq I(C)$. Moreover, it is a total preorder because $(I(A) \leq I(B)) \vee (I(B) \leq I(A))$ holds. Note that depending on the choice of the indicator function, there may be still sets that have equal indicator values, i.e., they are indifferent with respect to the corresponding set preference relation $\preccurlyeq_{\mathrm{I}}$. In this case, we may have equivalence classes of sets, each one containing sets with the same indicator value. For multiobjective optimization algorithms that use indicators as their means of defining progress, sets with identical indicator values pose additional difficulties in terms of cyclic behavior and premature convergence. We will later see how these problems can be circumvented by considering hierarchies of indicators.

Clearly, not all possible indicator functions realize a refinement of the orginal preference relation, e.g., weak Pareto dominance. The following theorem provides sufficient conditions for weak refinements and refinements.

Theorem 3.1: If a unary indicator I satisfies

$$(A \preccurlyeq B) \wedge (B \not\preccurlyeq A) \Rightarrow (I(A) \leq I(B))$$

for all $A, B \in \Psi$, then the corresponding preference relation $\preccurlyeq_{\mathrm{I}}$ according to (1) weakly refines the preference relation $\preccurlyeq$ according to Definition 2.5. If

$$(A \preccurlyeq B) \wedge (B \not\preccurlyeq A) \Rightarrow (I(A) < I(B))$$

holds, then $\preccurlyeq_{\mathrm{I}}$ refines $\preccurlyeq$ according to Definition 2.4.

Proof: Consider $A, B \in \Omega$ with $(A \preccurlyeq B) \wedge (B \not\preccurlyeq A)$. If $I(A) \leq I(B)$, then also $A \preccurlyeq_{\mathrm{I}} B$ according to (1). If $I(A) < I(B)$, then $I(A) \leq I(B)$, but $I(B) \not\leq I(A)$, which implies that $A \preccurlyeq_{\mathrm{I}} B$ and $B \not\preccurlyeq_{\mathrm{I}} A$. ■

In other words, if A is strictly better than B, i.e., $A \prec B$, then the indicator value of A must be not worse or must be smaller than the one of B in order to achieve a weak refinement or a refinement, respectively. In practice, this global property may be difficult to prove for a specific indicator since one has to argue over all possible sets. Therefore, the following theorem provides sufficient and necessary conditions that are only based on the local behavior, i.e., when adding a single element. The proof of the theorem is given in the Appendix.

Theorem 3.2: Let I be a unary indicator and $\preccurlyeq$ a preference relation on populations that itself conforms to a preference relation $\preceq$ on its elements (see Definition 2.2). The relation $\preccurlyeq_{\mathrm{I}}$ according to (1) refines $\preccurlyeq$ if the following two conditions hold for all sets $A \in \Psi$ and solutions b with $\{b\} \in \Psi$:

1) if $A \preccurlyeq \{b\}$ then $I(A \cup \{b\}) = I(A)$;
2) if $A \not\preccurlyeq \{b\}$ then $I(A \cup \{b\}) < I(A)$.

For weak refinement one needs to replace the relation $<$ by $\leq$ in the second condition. The second condition is necessary for $\preccurlyeq_{\mathrm{I}}$ being a refinement (in case of $<$) or weak refinement (in case of $\leq$) of $\preccurlyeq$.

Using these two conditions, it is straightforward to prove that an indicator induces a refinement of the weak Pareto dominance relation. The hypervolume indicator [35], [38], for instance, gives the volume of the objective space weakly dominated by a set of solutions with respect to a given set of reference points $R \subset \mathcal{Z}$. We define the corresponding indicator function as the negative volume $I_H(A) = -\lambda(H(A, R))$ where λ denotes the Lebesgue measure with $\lambda(H(A, R)) = \int_{\mathbb{R}^n} \mathbf{1}_{H(A,R)}(z)dz$ and

$$H(A, R) = \{h \mid \exists a \in A \; \exists r \in R \; : \; f(a) \leq h \leq r\}.$$

Now, it is easy to see that the volume is not affected whenever a weakly Pareto dominated solution is added to a set A. Furthermore, any solution b not weakly Pareto dominated by A covers a part of the objective space not covered by A and therefore the indicator value for $A \cup \{b\}$ is better (smaller) than the one for A. These properties can easily be verified by looking at the example shown in Fig. 11; therefore, the hypervolume indicator induces a refinement, see also [15]. Furthermore, there are various other unary indicators which induce weak refinements, e.g., the unary R_2 and R_3 indicators [20] and the epsilon indicator [40]—the above conditions can be used to show this, see also [24], [40] for a more detailed discussion.

Furthermore, the necessary condition can be used to prove that a particular indicator—when used alone—does not lead to a weak refinement or a refinement of the weak Pareto dominance relation. That applies, for instance, to most of the diversity indicators proposed in the literature as they do not fulfill the second condition in Theorem 3.2. Nevertheless, these indicators can be useful in combination with indicators inducing (weak) refinements as we will show in Section III-D.

B. Binary Indicators

In contrast to unary indicators, binary quality indicators assign a real value to ordered pairs of sets (A, B) with $A, B \in \Psi$. Assuming that smaller indicator values stand for higher quality, we can define for each binary indicator I a corresponding set preference relation as follows:

$$A \preccurlyeq_{\mathrm{I}} B := (I(A, B) \leq I(B, A)) \tag{2}$$

Similarly to unary undicators, one can derive sufficient conditions for $\preccurlyeq_{\mathrm{I}}$ being a refinement respectively a weak refinement as the following theorem shows.

Theorem 3.3: Let I be a binary indicator that induces a binary relation $\preccurlyeq_{\mathrm{I}}$ on Ψ according to (2). If I satisfies

$$(A \preccurlyeq B) \wedge (B \not\preccurlyeq A) \Rightarrow (I(A, B) < I(B, A))$$

for all $A, B \in \Psi$, then the corresponding preference relation $\preccurlyeq_{\mathrm{I}}$ refines $\preccurlyeq$ according to Definition 2.4. If $<$ is replaced by $\leq$, then $\preccurlyeq_{\mathrm{I}}$ weakly refines $\preccurlyeq$ according to Definition 2.5.

Proof: Consider $A, B \in \Psi$ with $(A \preccurlyeq B) \wedge (B \not\preccurlyeq A)$. If $I(A, B) \leq I(B, A)$, then also $A \preccurlyeq_{\mathrm{I}} B$ according to (2). If $I(A, B) < I(B, A)$, then $I(A, B) \leq I(B, A)$, but $I(B, A) \not\leq I(A, B)$, which implies that $A \preccurlyeq_{\mathrm{I}} B$ and $B \not\preccurlyeq_{\mathrm{I}} A$. ■

Note that the relation $\preccurlyeq_{\mathrm{I}}$ is not necessarily a preorder, and this property needs to be shown for each specific indicator separately. Obviously, if transitivity and reflexitivity are fulfilled, then $\preccurlyeq_{\mathrm{I}}$ is even a total preorder because either $(I(A, B) \leq I(B, A))$ or $(I(B, A) \leq I(A, B))$ (or both). However, some binary indicators violate transitivity, although $\preccurlyeq_{\mathrm{I}}$ (weakly) refines $\preccurlyeq$ according to Definition 2.5.

Consider, for instance, the coverage indicator [38] which gives the portion of solutions in B to which a weakly preferable solution in A exists. This indicator represents a refinement of $\preccurlyeq_{\mathrm{par}}$, but does not induce a preorder as transitivity cannot be ensured [24].

Another example is the binary epsilon indicator [40]. Its corresponding set preference relation $\preccurlyeq_{I_\epsilon}$ according to (2) is a refinement of $\preccurlyeq_{\mathrm{par}}$. It is defined as follows:

$$I_\epsilon(A, B) = \max_{b \in B} \min_{a \in A} F_\epsilon(a, b)$$

where we use the distance function

$$F_\epsilon(a, b) = \max_{1 \leq i \leq n} (f_i(a) - f_i(b))$$

between two solutions a and b. Informally speaking, $I_\epsilon(A, B)$ denotes the minimum amount one needs to improve every objective value $f_i(a)$ of every solution $a \in A$ such that the resulting set is weakly preferable to B. We will not discuss further properties here and instead refer to [20], [24], [40] for detailed reviews of binary indicators. The following counterexample shows that the binary epsilon indicator does not lead to a preorder. We consider four solutions a, b, c, d with the objective values $f(a) = (0, 8)$, $f(b) = (1.5, 5)$, $f(c) = (2.5, 3)$, and $f(d) = (4, 0)$ in $\mathbb{R}^2$. Using the solution sets $A = \{a, d\}$, $B = \{b, d\}$, and $C = \{c, d\}$, we find $(I_\epsilon(C, B) = 1 \leq I_\epsilon(B, C) = 2) \Rightarrow (C \preccurlyeq_{I_\epsilon} B)$ and $(I_\epsilon(B, A) = 1.5 \leq I_\epsilon(A, B) = 3) \Rightarrow (B \preccurlyeq_{I_\epsilon} A)$ as well as $(I_\epsilon(A, C) = 1.5 \leq I_\epsilon(C, A) = 2.5) \Rightarrow (A \preccurlyeq_{I_\epsilon} C)$. However, since $I_\epsilon(C, A) = 2.5 \not\leq I_\epsilon(A, C) = 1.5$, it holds $C \not\preccurlyeq_{I_\epsilon} A$ which contradicts transitivity.

In contrast to the negative results concerning the binary coverage and epsilon indicators, one can derive valid binary indicators from unary indicators. For example, for every unary indicator I_1 a corresponding binary indicator I_2 can be defined as $I_2(A, B) := I_1(B) - I_1(A)$; it is easy to show that the property of (weak) refinement transfers from the unary indicator to the binary version. In a similar way, one could also use $I_2(A, B) := I_1(B) - I_1(A \cup B)$ as in the case of the binary hypervolume indicator, see, e.g., [34].

On the other hand, every binary indicator I_2 can be transformed into a unary indicator I_1 by using a reference set R: $I_1(A) := I_2(A, R)$.[4] Here, the refinement property is not necessarily preserved, e.g., the unary versions of the binary epsilon indicators induce only weak refinements, while the original binary indicators induce refinements of the weak Pareto dominance relation.

C. Refinement Through Set Partitioning

The Pareto dominance relation $\preccurlyeq_{\mathrm{par}}$ on sets is by definition insensitive to dominated solutions in a set, i.e., whether $A \in \Psi$ weakly dominates $B \in \Psi$ only depends on the corresponding minimal sets: $A \preccurlyeq_{\mathrm{par}} B \Leftrightarrow \mathrm{Min}(A, \preceq_{\mathrm{par}}) \preccurlyeq_{\mathrm{par}} \mathrm{Min}(B, \preceq_{\mathrm{par}})$. The same holds for set preference relations induced by the hypervolume indicator and other popular quality indicators. Nevertheless, preferred solutions may be of importance.

1) When a Pareto set approximation is evaluated according to additional knowledge and preferences—which may be hard to formalize and therefore may not be included in the search process—then preferred solutions can become interesting alternatives for a decision maker.
2) When a set preference relation is used within a (evolutionary) multiobjective optimizer to guide the search, it is crucial that preferred solutions are taken into account—for reasons of search efficiency.

Accordingly, the question is how to refine a given set preference relation that only depends on its minimal elements such that also non-minimal solutions are considered.

This issue is strongly related to fitness assignment in MOEAs. Pareto-dominance-based MOEAs divide the population into dominance classes which are usually hierarchically

[4] Usually, instead of a reference set of solutions a reference set of objective vectors is given. This requires a slight modication of the indicator.

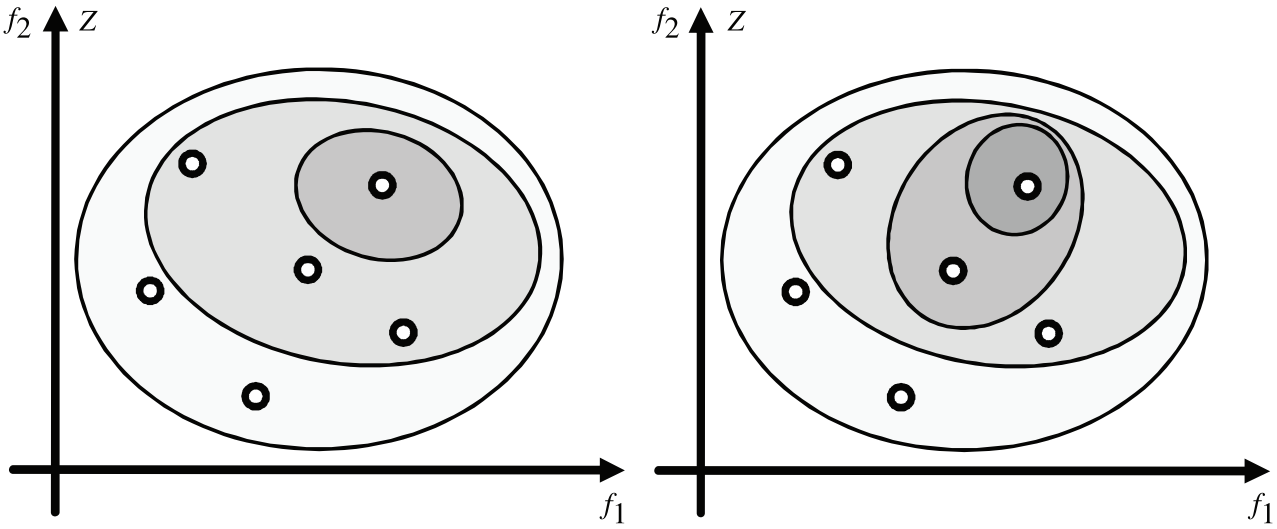


Fig. 12. Illustration of two set partitioning functions, here based on weak Pareto dominance: (left)minpart and (right) rankpart. The light-shaded areas stand for the first subsets (A_1) and the darkest areas represent the lth subsets (A_3 left and A_4 right). As to the resulting partitions, on the left holds $P_1 \prec_{\text{par}} P_2 \prec_{\text{par}} P_3$, while on the right $P_1 \prec_{\text{par}} P_i$ for $2 \leq i \leq 4$, $P_3 \prec_{\text{par}} P_4$, and $P_2 \,||_{\text{par}}\, P_3$ as well as $P_2 \,||_{\text{par}}\, P_4$.

organized. For instance, with dominance ranking [16], individuals that are dominated by the same number of population members are grouped into one dominance class; with nondominated sorting [18], [30], the minimal elements are grouped into the first dominance class, and the other classes are determined by recursively applying this classification scheme to the remaining population members. The underlying idea can be generalized to arbitrary set preference relations. To this end, we introduce the notion of a set partitioning function.

Definition 3.4: A set partitioning function part is a function part: $\Psi \times \mathbb{N} \to \Psi$ such for all $A \in \Psi$ a sequence $(A_1, A_2, \ldots, A_l, \ldots)$ of subsets is determined with $A_i := \text{part}(A, i)$ and it holds:

1) $\forall 1 \leq i \leq l : A_i \subseteq A$;
2) $\forall i > l : A_i = \emptyset$;
3) $\forall 1 \leq i < j \leq l+1 : A_i \supset A_j$.

A set partitioning function indirectly creates l non-empty partitions: the ith partition P_i is defined by the set difference between the ith and the $(i+1)$th subset: $P_i = \text{part}(A, i) \setminus \text{part}(A, i+1)$. By construction, the induced partitions are disjoint. For instance, the following two set partitioning functions resemble the concepts of dominance rank and nondominated sorting:

$$\text{rankpart}(A, i) := \{a \in A : |\{b \in A : b \prec a\}| \geq i - 1\}$$

$$\text{minpart}(A, i) := \begin{cases} A & \text{if } i = 1 \\ \text{minpart}(A, i-1) \setminus & \\ \text{Min}(\text{minpart}(A, i-1), \preceq) & \text{else} \end{cases}$$

where $\preceq$ is the solution-based preference relation under consideration. The second function, i.e., minpart, yields a partitioning such that $P_1 \prec P_2 \prec \cdots \prec P_l$ holds; this is demonstrated in Fig. 12.

Now, given a set partitioning function, part one can construct set preference relations that only refer to specific partitions of two sets $A, B \in \Psi$. By concatenating these relations, one then obtains a sequence of relations that induces a set preference relation according to Definition 2.6.

Definition 3.5: Let $\preccurlyeq$ be a set preference relation and part a set partitioning function. For a fixed l, the partition-based extension of $\preccurlyeq$ is defined as the relation $\preccurlyeq^{\text{part}[l]} := \preccurlyeq_S$ where S is the sequence $(\preccurlyeq^1_{\text{part}}, \preccurlyeq^2_{\text{part}}, \ldots, \preccurlyeq^l_{\text{part}})$ of preference relations with

$$\begin{aligned} A \preccurlyeq^i_{\text{part}} B \quad :\Leftrightarrow \quad & (\text{part}(A, i) \setminus \text{part}(A, i+1)) \\ \preccurlyeq \quad & (\text{part}(B, i) \setminus \text{part}(B, i+1)). \end{aligned}$$

A partition-based extension of a set preference relation $\preccurlyeq$ basically means that $\preccurlyeq$ is successively applied to the hierarchy of partitions defined by the corresponding set partition function. Given $A, B \in \Psi$, first the two first partitions of A and B are compared based on $\preccurlyeq$; if the comparison yields equivalence, then the two second partitions are compared and so forth. This principle reflects the general fitness assignment strategy used in most MOEAs.

One important requirement for such a partition-based extension is that $\preccurlyeq^{\text{part}[l]}$ refines $\preccurlyeq$. Provided that $\preccurlyeq$ depends only on the minimal elements in the sets, both rankpart and minpart induce refinements. The argument is simply that $\preccurlyeq^1_{\text{part}}$ is the same as $\preccurlyeq$ because the first partition corresponds for both functions to the set of minimal elements; that means $\preccurlyeq^1_{\text{part}}$ is a refinement of $\preccurlyeq$. Furthermore, all $\preccurlyeq^i_{\text{part}}$ are preorders. Applying Theorem 2.7 leads to the above statement. For minpart, it can even be shown that $\preccurlyeq^{\text{minpart}[l+1]}$ is a refinement of $\preccurlyeq^{\text{minpart}[l]}$ for all $l > 0$.

In the following, we will mainly consider the set partitioning function minpart and refer to it as minimum elements partitioning (or nondominated sorting in the case of Pareto dominance). It induces a natural partitioning into sets of minimal elements where the partitions are linearly ordered according to strict preferability. For reasons of simplicity, we may omit the l when refering to the partition-extended relation $\preccurlyeq^{\text{minpart}[l]}$; it is usually set equal to the population size of the evolutionary algorithm used.

D. Combined Preference Relations

The issue of preferred (dominated) solutions in a set $A \in \Psi$ can not only be addressed by means of set partitioning functions, but also by using multiple indicators in sequence. For instance, one could use the hypervolumen indicator I_H (to assess the minimal elements in A) in combination with a diversity indicator I_D (to assess the non-minimal elements in A); according to Theorem 2.7, the set preference relation $\preccurlyeq_{H,D}$ given by the sequence $(\preccurlyeq_H, \preccurlyeq_D)$ is a proper refinement of weak Pareto dominance since $\preccurlyeq_H$ is a refinement (see above) and $\preccurlyeq_D$ is a preorder. Thus, such combinations can be useful to increase the sensitivity of a relation (meaning that the number of unidirectional edges $A \prec B$ is increased); however, there are several further reasons for combining indicators:

1) to embed indicators which induce only a weak refinement or no refinement at all into set preference relations representing refinements;
2) to reduce computation effort: for instance, the hypervolume indicator is expensive to compute; by using it only occasionally at the end of a sequence of indicators, a considerable amount of computation time may be saved;
3) to include heuristic information to guide the search: a set preference relation that reflects the user preferences not necessarily provides information for an effective search; therefore, it may be augmented by optimization-related aspects like diversity through additional dedicated indicators.

In the following, we present some examples for combined set preference relations that illustrate different application scenarios. All these relations are refinements of the set preference relation $\preccurlyeq_{\text{par}}$.

1) The first combination is based on the unary epsilon indicator $I_{\epsilon 1}$ with a reference set R in objective space which is defined as $I_{\epsilon 1}(A) = E(A, R)$ with

$$E(A, R) = \max_{r \in R} \min_{a \in A} \epsilon(a, r)$$

where

$$\epsilon(a, r) = \max\{f_i(a) - r_i \mid 1 \le i \le n\}$$

and r_i is the ith component of the objective vector r. Since this indicator induces only a weak refinement of the weak Pareto dominance relation $\preccurlyeq_{\text{par}}$, we will use the hypervolume indicator to distinguish between sets indifferent with respect $I_{\epsilon 1}$. The resulting set preference relation is denoted as $\preccurlyeq_{\epsilon 1,H}$; it is a refinement of $\preccurlyeq_{\text{par}}$.

2) The second combination uses the R_2 indicator proposed in [20] for which the following definition is used here:

$$I_{R2}(A) = R_2(A, R) = \frac{\sum_{\lambda \in \Lambda} u^*(\lambda, R) - u^*(\lambda, f(A))}{|\Lambda|}$$

where the function u^* is a utility function based on the weighted Tchebycheff function

$$u^*(\lambda, T) = -\min_{z \in T} \max_{1 \le j \le n} \lambda_j |z_j^* - z_j|$$

and Λ is a set of weight vectors $\lambda \in \mathbb{R}^n$, $R \subset \mathcal{Z}$ is a reference set, and $z^* \in \mathcal{Z}$ is a reference point. In this paper, we will set $R = \{z^*\}$. Also the R_2 indicator provides only a weak refinement; as before, the hypervolume indicator is added in order to achieve a refinement. This set preference relation will be denoted as $\preccurlyeq_{R2,H}$.

3) The next set preference relation can be regarded as a variation of the above relation $\preccurlyeq_{R2,H}$. It allows a detailed modeling of preferences by means of a set of reference points $r^{(i)} \in R$ with individual scaling factors $\rho^{(i)}$ and individual sets of weight vectors $\Lambda^{(i)}$. As a starting point, we define the generalized epsilon-distance between a solution $a \in \mathcal{X}$ and a reference point $r \in \mathcal{Z}$ as

$$F_\epsilon^\lambda(a, r) = \max_{1 \le i \le n} \lambda_i \cdot (f_i(a) - r_i)$$

with the weight vector $\lambda \in \mathbb{R}^n$ where $\lambda_i > 0$ for $1 \le i \le n$. In contrast to the usual epsilon-distance given, the coordinates of the objective space are weighted which allows choosing a preference direction.

The P indicator for a single reference point r can now be described as

$$I_P(A, r, \Lambda) = \sum_{\lambda \in \Lambda} \min_{a \in A} F_\epsilon^\lambda(a, r)$$

where Λ is a potentially large set of different weight vectors. The minimum operator selects for each weight vector λ the solution a with minimal generalized epsilon-distance. Finally, all these distances are summed up. In order to achieve a broad distribution of solutions and a sensitive indicator, the cardinality of $|\Lambda|$ should be large, i.e., larger than the expected number of minimum elements in A. For example, Λ may contain a large set of random vectors on a unit sphere, i.e., vectors with length 1. One may also scale the weight vectors to different lengths in order to express the preference for an unequal density of solutions.

If we have a set of reference points $r^{(i)} \in R$ with individual sets of weight vectors $\Lambda^{(i)}$ and scaling factors $\rho^{(i)} > 0$, we can simply add the individual P indicator values as follows:

$$I_P(A) = \sum_{r^{(i)} \in R} \rho^{(i)} \cdot I_P(A, r^{(i)}, \Lambda^{(i)}).$$

Of course, we may choose equal sets $\Lambda^{(i)}$ for each reference point. In this case, the scaling factors $\rho^{(i)}$ can be used to give preference to specific reference points.

The P indicator as defined above provides only a weak refinement; as before, the hypervolume indicator is added in order to achieve a refinement. This set preference relation will be denoted as $\preccurlyeq_{P,H}$.

4) The previous three indicator combinations will be used together with a set partitioning function. To demonstrate that the partitioning can also be accomplished by indicators, we propose the following sequence of indicators $S = (I_H, I_C, I_D)$ where I_C measures the largest distance of a solution to the closest minimal element in a set and I_D reflects the diversity of the solutions in the

objective space. The latter two indicators, which both do not induce weak refinements of $\preccurlyeq_{\text{par}}$, are defined as follows:

$$I_C(A) = \max_{a \in A} \min_{b \in \text{Min}(A, \preceq)} dist(f(a), f(b))$$

and

$$I_D(A) = \max_{a \in A} \left(\frac{1}{nn_1(a, A \setminus \{a\})} + \frac{1}{nn_2(a, A \setminus \{a\})} \right)$$

with

$$nn_1(a, B) = \min_{b \in B} dist(f(a), f(b))$$

$$nn_2(a, B) = \max_{c \in B} \min_{b \in B \setminus \{c\}} dist(f(a), f(b))$$

where $nn_1(a, B)$ gives the smallest and $nn_2(a, B)$ the second smallest distance of a to any solution in B. For the distance function $dist(z^1, z^2)$, Euclidean distance is used here, i.e., $dist(z^1, z^2) = \sqrt{\sum_{1 \le i \le n} (z_i^1 - z_i^2)^2}$. The I_C indicator resembles the generational distance measure proposed in [32] and I_D resembles the nearest neighbor niching mechanism in SPEA2 [37]. We will refer to the overall set preference relation as $\preccurlyeq_{H,C,D}$. According to Theorem 2.7, $\preccurlyeq_{H,C,D}$ is a refinement of $\preccurlyeq_{\text{par}}$.

It is worth mentioning that it is also possible to combine a non-total preorder such as $\preccurlyeq_{\text{par}}$ with total orders differently to the principle suggested in Definition 2.6. As has been pointed out, see e.g., Fig. 7, convergence may not be achievable if an optimization is not based on a preorder or if the underlying preorder is not a refinement. The following example illustrates why density-based MOEAs such as NSGA-II and SPEA2 show cyclic behavior, see [27], in particular when the population mainly contains incomparable solutions, e.g., when being close to the tradeoff surface.

For instance, let I be a unary indicator, then one may define a set preference relation $\preccurlyeq_{\text{par},I}$ as follows with $A, B \in \Psi$:

$$A \preccurlyeq_{\text{par},I} B \;\; :\Leftrightarrow (A \preccurlyeq_{\text{par}} B) \vee ((A \,||_{\text{par}}\, B) \wedge (A \preccurlyeq_I B)).$$

Now, consider a unary diversity indicator, e.g., I_D as defined above; this type of indicator usually does not induce a weak refinement. The resulting set preference relation $\preccurlyeq_{\text{par},I}$ is not a proper preorder as Fig. 13 demonstrates: transitivity is violated, i.e., $A \preccurlyeq_{\text{par},I} B$ and $B \preccurlyeq_{\text{par},I} C$, but $A \not\preccurlyeq_{\text{par},I} C$. The relation graph of $\preccurlyeq_{\text{par},I}$ contains cycles. However, if I stands for the hypervolume indicator I_H, then $\preccurlyeq_{\text{par},I}$ is a set preference relation refining $\preccurlyeq_{\text{par}}$; this combination could be useful to reduce computation effort.

IV. Multiobjective Optimization Using Set Preference Relations

The previous two sections discussed how to design set preference relations so that the concept of Pareto dominance is preserved while different types of user preferences are included. This section presents a corresponding generalized multiobjective optimizer that makes use of such set preference relations in order to search for promising solution sets. Section IV-A describes the algorithm, while Section IV-B discusses theoretical aspects of the algorithm, in particular convergence properties.

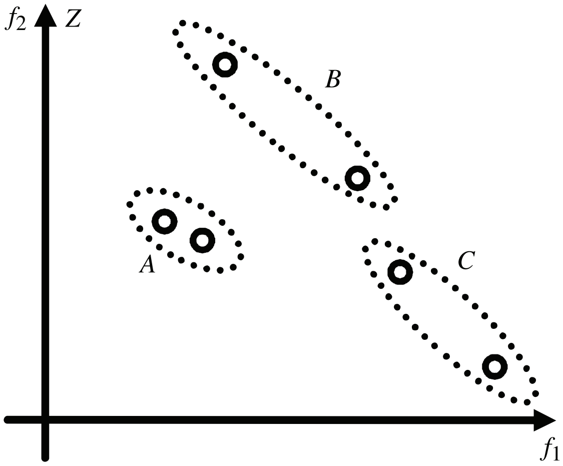


Fig. 13. Three sets are shown in the objective space where $A \preccurlyeq_{\text{par}} B$, $A \,||_{\text{par}}\, C$ and $B \,||_{\text{par}}\, C$. Using a combination of Pareto dominance and diversity results in a cyclic relation $\preccurlyeq_{\text{par},I}$ with $A \prec_{\text{par},I} B$, $B \prec_{\text{par},I} C$, and $C \prec_{\text{par},I} A$.

*A. **SPAM**—**S**et **P**reference **A**lgorithm for **M**ultiobjective Optimization*

The main part of the SPAM is given by Algorithm 1. It resembles a standard hill climber with the difference that two new elements of the search space Ψ are created using two types of mutation operators. The termination criterion can be any standard stopping condition like maximum number of iterations or no improvement over a given number of iterations; we will not discuss this critical issue here in detail and instead refer to the corresponding literature, see e.g. [7]. However, for the convergence proof provided later, we will assume that the algorithm loops forever, i.e., the termination criterion is *False*.

Algorithm 1 first creates a random initial set $P \in \Psi_m$ of size m and then employs a random mutation operator to generate another set P'. This operator should be designed such that every element in Ψ could be possibly generated, i.e., the neighborhood is in principle the entire search space. In practice, the operator will usually have little effect on the optimization process; however, its property of exhaustiveness is important from a theoretical perspective, in particular to show convergence, cf. Section IV-B.

Second, a heuristic mutation operator is employed. This operator mimics the mating selection, variation, and environmental selection steps as used in most MOEAs. The goal of this operator is to create a third set $P'' \in \Psi$ that is better than P in the context of a predefined set preference relation $\preccurlyeq$. However, since it is heuristic it cannot guarantee to improve P; there may be situations where it is not able to escape local optima of the landscape of the underlying set problem. Finally, P is replaced by P'', if the latter is weakly preferable to the former; otherwise, P is either replaced by P' (if $P' \preccurlyeq P$) or remains unchanged. Note that in the last step, weak preferability ($\preccurlyeq$) and not preferability ($\prec$) needs to be considered in order to allow the algorithm to cross landscape plateaus, cf. [5].

Algorithm 1 SPAM Main Loop

```
Require: set preference relation $\preccurlyeq$
1: generate initial set $P$ of size $m$, i.e., randomly choose $A \in \Psi_m$ and set $P \leftarrow A$
2: while termination criterion not fulfilled do
3:     $P' \leftarrow randomSetMutation(P)$
4:     $P'' \leftarrow heuristicSetMutation(P)$
5:     if $P'' \preccurlyeq P$ then
6:         $P \leftarrow P''$
7:     else if $P' \preccurlyeq P$ then
8:         $P \leftarrow P'$
9: return $P$
```

Algorithm 2 Random Set Mutation

```
1: procedure $randomSetMutation(P)$
2:     randomly choose $r_1, \ldots, r_k \in \mathcal{X}$ with $r_i \neq r_j$
3:     randomly select $p_1, \ldots, p_k$ from $P$ with $p_i \neq p_j$
4:     $P' \leftarrow P \setminus \{p_1, \ldots, p_k\} \cup \{r_1, \ldots, r_k\}$
5:     return $P'$
```

For the mutation operators, we propose Algorithms 2 and 3. Algorithm 2 (random set mutation) randomly chooses k decision vectors from $\mathcal{X}$ and uses them to replace k elements in P.[5] Algorithm 3 (heuristic set mutation) generalizes the iterative truncation procedures used in NSGA-II [8], SPEA2 [37], and others. First, k new solutions are created based on P; this corresponds to mating selection plus variation in a standard MOEA. While the variation is problem-specific, for mating selection either uniform random selection (used in the following) or fitness-based selection can be used (using the fitness values computed by Algorithm 4 resp. 5). Then, these k solutions are added to P, and finally the resulting set of size $m + k$ is iteratively truncated to size m by removing the solution with the worst fitness values in each step. Here, the fitness value of $a \in P$ reflects the loss in quality for the entire set P if a is deleted: the lower the fitness, the larger the loss.

To estimate how useful a particular solution $a \in P$ is, Algorithm 4 compares all sets $A_i \subset P$ with $|A_i| = |P| - 1$ to $P \setminus \{a\}$ using the predefined set preference relation $\preccurlyeq$. The fewer sets A_i are weakly preferable to $P \setminus \{a\}$, the better the set $P \setminus \{a\}$ and the less important is a. This procedure has a runtime complexity of $\mathcal{O}((m + k)g)$, where g stands for the runtime needed to compute the preference relation comparisons which usually depends on $m + k$ and the number of objective functions. If unary indicators are used, then fitness assignment can be done faster. Algorithm 5 gives an example where $\preccurlyeq$ is defined by a single unary indicator I; the loss in quality is simply the difference in the indicator value caused by the removal of a. The last scheme is used, e.g., in [14], [22], [25], [35] in combination with the hypervolume indicator; Fig. 14 illustrates the working principles.

Finally, note that Algorithm 3 is heuristic in nature, in particular the truncation method realized by the while loop at Step 4. Before entering the loop at Step 4, P'' contains exactly $m + k$ solutions. Ideally, that subset $A \subseteq P''$ with $|A| = m$ would be chosen that is weakly preferred by the lowest number of m-element subsets $A_i \subseteq P''$. However, computing the optimal subset A is usually computationally expensive and therefore the iterative truncation procedure represents a greedy strategy to obtain a good approximation of A in reasonable time.

Algorithm 3 Heuristic Set Mutation

```
1: procedure $heuristicSetMutation(P)$
2:     generate $r_1, \ldots, r_k \in \mathcal{X}$ based on $P$
3:     $P'' \leftarrow P \cup \{r_1, \ldots, r_k\}$
4:     while $|P''| > m$ do
5:         for all $a \in P''$ do
6:             $\delta_a \leftarrow fitnessAssignment(a, P'')$
7:         choose $p \in P''$ with $\delta_p = \min_{a \in P''} \delta_a$
8:         $P'' \leftarrow P'' \setminus \{p\}$
9:     return $P''$
```

Algorithm 4 Fitness Assignment (General Version)

```
1: procedure $fitnessAssignment(a, P'')$
2:     $\delta_a \leftarrow 0$
3:     for all $b \in P''$ do
4:         if $P'' \setminus \{b\} \preccurlyeq P'' \setminus \{a\}$ then
5:             $\delta_a \leftarrow \delta_a + 1$
6:     return $\delta_a$
```

B. Convergence Results

The main advantage of SPAM, as presented above, with respect to existing multiobjective randomized search algorithms is its flexibility. In principle, it can be used with any set relation; however, it will be effective only when the set preference relation $\preccurlyeq$ is reasonably designed as discussed in Sections II and III.

First, it is important that $\preccurlyeq$ represents a preorder and a refinement according to Definition 2.4. These properties ensure that 1) no cyclic behavior as reported for NSGA-II and SPEA2 in [27] can occur and that 2) under mild assumptions SPAM actually converges to an optimal subset of the Pareto-optimal set (see below). To our best knowledge, the latter property has only been shown for theory-oriented algorithms, e.g., [19], [29], but not for popular multiobjective evolutionary algorithms used in practice. The construction principle presented in Definition 2.6 provides a tool to design preorders and refinements as shown by Theorem 2.7. Furthermore, $\preccurlyeq$ should be a total preorder and it should be highly sensitive to changes in the sets in order to enable SPAM to search efficiently. A total set preference relation guarantees that SPAM has full information whether to accept or to reject a newly generated set. Section III explains in detail how total preorders can be constructed using quality indicators and how it can be ensured that the resulting preorders are still refinements, cf. Theorem 3.2. The issue of sensitivity led to the idea of set partitionings as presented in Section III-C—only this extension makes the use of single quality indicators for search effective. This discussion illustrates why the proper design of $\preccurlyeq$ is

[5] Note that for both mutation operators the same k is used here, although they can be chosen independently. The safe version ($k = m$) for the random mutation operator means that a random walk is carried out on Ψ.

Algorithm 5 Fitness Assignment (Unary Indicator Version)

```
procedure fitnessAssigment($a$, $P''$)
    $\delta_a \leftarrow I(P'' \setminus \{a\}) - I(P'')$
    return $\delta_a$
```

crucial for SPAM and any other set-oriented multiobjective optimizer and why the corresponding theoretical foundations presented in Sections II and III are of high importance in practice.

Next, we will focus on the theoretical convergence properties of SPAM, i.e., whether and under what conditions it converges to the optimum given infinite running time resources. Although convergence alone does not necessarily imply that the algorithm is fast and efficient in practice, it is an important and desirable property; in the EMO field, several convergence results are available to date, most notably [19], [27], [29], [33].

Here, we are interested in the properties of the set mutation operators that guarantee convergence of SPAM; in particular, we will investigate the influence of the parameter k that determines the number of newly created solutions per set mutation. Convergence in this paper refers to the limit behavior of an optimization algorithm. The line of arguments follows most closely the investigations of Rudolph *et al.* in [29].

In order to simplify the discussion, let us suppose that the set of solutions $\mathcal{X}$ is finite and that only random set mutation is used, i.e., *heuristicSetMutation*(P) always returns P for the time being. In addition, we have available a preference relation $\preccurlyeq$ on the set Ψ_m of sets containing not more than m solutions, see Section II.

Then, SPAM is called convergent the probability that the resulting set P is not minimal, i.e., $P \notin \text{Min}(\Psi_m, \preccurlyeq)$, approaches 0 for $N \to \infty$ where N denotes the number of iterations of the while loop in Algorithm 1. If we can now guarantee the convergence of SPAM, then this simple hill-climbing strategy would be able to solve any multiobjective optimization problem as stated in Section II-B in case of finite but unbounded computation time.

Given Ψ_m, let us consider the underlying set preference relation $\preccurlyeq$ and, in particular, the corresponding relation graph where there is an edge (A, B) for each pair $A, B \in \Psi_m$ with $A \preccurlyeq B$. As $\preccurlyeq$ is a preorder, there is a directed path from any minimal element $P^* \in \text{Min}(\Psi_m, \preccurlyeq)$ to any node P. In order to be able to reach such an optimal set using SPAM, the chosen preference relation as well as the set mutation operator need to satisfy certain constraints. They both must enable such paths under the condition that each set mutation replaces at most k elements from the current set P in order to generate P'. Note that the optimizer traverses a path in reverse direction as there is an edge from A to B if $A \preccurlyeq B$.

Let $(P^1, P^2, \ldots, P^i)$ denote the sequence of sets generated by SPAM where P^i denotes the contents of P at the beginning of the ith iteration of the while loop in Algorithm 1. In addition, r^i_j and p^i_j, $1 \le j \le k$ denote the elements randomly created resp. selected for removal in Algorithm 2. In particular, P^i is mutated by removing $p^i_1, \ldots, p^i_k$ and adding $r^i_1, \ldots, r^i_k$.

Definition 4.1: Let us now suppose that for any initial set P^1 there exists a number N of iterations and p^i_j and r^i_j, $1 \le j \le k$, $1 \le i \le N$ such that 1) $P^N \in \text{Min}(\Psi_m, \preccurlyeq)$ and 2) $P^{i+1} \preccurlyeq P^i$ for all $1 \le i \le N-1$. Then we say that the given set preference relation $\preccurlyeq$ is k-greedy.

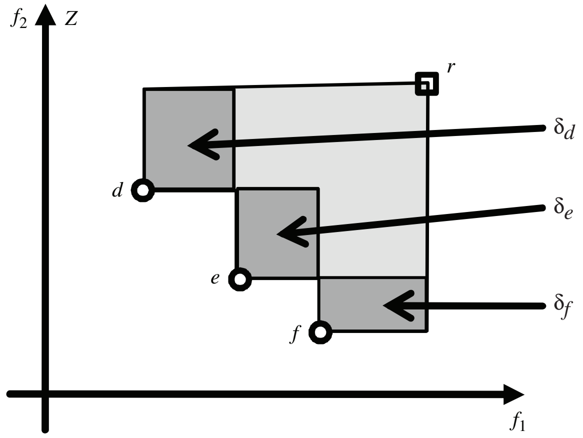


Fig. 14. Figure depicting the fitness values computed according to Algorithms 4 and 5 when using the hypervolume indicator. The light shaded area stands for the volume of the entire three-elements set, the dark shaded areas reflects the volume contributions (fitness values) of the distinct solutions.

The above property states that if the given set preference relation $\preccurlyeq$ is k-greedy, then there exists a sequence of sets with cardinality not larger than m that starts from any set in Ψ_m and ends at an optimal set in Ψ where at most k elements differ from one set to the next. Therefore, this path could be found by SPAM, if the *randomSetMutation* operator does exactly the requested replacements of elements. In order to make this argument more formal, we need to define properties of the set mutation operator. For example, if elements of some optimal set P^* cannot be generated, this set will never be reached.

Definition 4.2: Given any k different solutions $s_j \in \mathcal{X}$ and any k different solutions $\hat{p}_j$ in P where $1 \le j \le k$. If for an execution of the *randomSetMutation* operator the probability is larger than zero that 1) the selected elements satisfy $p_j = \hat{p}_j$ and 2) the randomly generated elements satisfy $r_j = s_j$ for all $1 \le j \le k$, then the *randomSetMutation* operator is called exhaustive.

In other words, an exhaustive *randomSetMutation* operator replaces any k elements of the current set P by any k elements from $\mathcal{X}$ with a finite probability. Therefore, if the set mutation operator is concatenated sufficiently often for an arbitrary initial set (e.g., *randomSetMutation*(*randomSetMutation*(P)))), then any possible set in Ψ_m can be generated. Based on the above results and using a straightforward extension of the work previously done in [29], we obtain the following theorem:

Theorem 4.3: If the given set preference relation $\preccurlyeq$ is k-greedy and the given *randomSetMutation* operator is exhaustive, then the SPAM optimization algorithm converges provided that the while-loop never terminates.

Proof: Consider a graph whose nodes correspond to all sets $Q \subseteq \mathcal{X}$ with size $|Q| = m$ and the edges of which correspond to all possible executions of the *randomSetMutation* operator. If we remove all edges (i, j) with $Q^j \not\preccurlyeq Q^i$, then each path in the graph corresponds to a feasible execution of SPAM. If the set preference relation $\preccurlyeq$ is k-greedy and the

TABLE II
OVERVIEW OF THE SET PREFERENCE RELATIONS USED IN THE EXPERIMENTAL STUDIES; FOR DETAILS, SEE SECTION III

$\preccurlyeq^{\text{minpart}}_{H}$	hypervolume indicator I_H with reference point $(12, 12)$ resp. $(12, 12, 12, 12, 12)$ and minimum elements partitioning
$\preccurlyeq^{\text{minpart}}_{P1,H}$	preference-based quality indicator I_P with two reference points $r^{(1)} = (0.2, 0.9)$ resp. $(0.2, 0.9, 0.9, 0.9, 0.9)$, $r^{(2)} = (0.8, 0.5)$ resp. $(0.8, 0.5, 0.5, 0.5, 0.5)$ with scaling factors $\rho^{(1)} = 1/3$ and $\rho^{(2)} = 2/3$, followed by the hypervolume indicator I_H with reference point $(12, 12)$ resp. $(12, 12, 12, 12, 12)$; in addition, minimum elements partitioning is used. For I_P, the same $1,000$ weights λ are used for all reference points; the weights are (once) uniformly randomly drawn from $\{(\lambda_1, \ldots, \lambda_n) \in \mathbb{R}^n \mid \lambda_i > 0 \text{ for } 1 \leq i \leq n,\ \|(\lambda_1, \ldots, \lambda_n)\| = 1\}$
$\preccurlyeq_{H,C,D}$	unary hypervolume indicator I_H with reference point $(12, 12)$ resp. $(12, 12, 12, 12, 12)$ followed by the distance-to-front indicator I_C (maximum distance of any solution to the closest front member) and the diversity indicator I_D (kth-nearest neighbor approach)
$\preccurlyeq^{\text{minpart}}_{R2,H}$	R_2 indicator I_{R2} with reference set $B = \{(0, 0)\}$ and $\Lambda = \{(0, 1), (0.01, 0.99), \ldots, (0.3, 0.7), (0.7, 0.3), (0.71, 0.29), \ldots, (1, 0)\}$ in the case of two objectives[a] ($\lvert\Lambda\rvert = 62$), followed by hypervolume indicator I_H with reference point $(12, 12)$ resp. $(12, 12, 12, 12, 12)$; in addition, minimum elements partitioning is used
$\preccurlyeq^{\text{minpart}}_{\epsilon 1,H}$	unary (additive) epsilon indicator $I_{\epsilon 1}$ with reference set $B = \{(k \cdot 0.002, 0.8 - k \cdot 0.004)\,;\, k \in \{0, 1, \ldots, 100\}\}$ resp. $B = \{(k \cdot 0.002, 0.8 - k \cdot 0.004, 0.8 - k \cdot 0.004, 0.8 - k \cdot 0.004, 0.8 - k \cdot 0.004)\,;\, k \in \{0, 1, \ldots, 100\}\}$, followed by the hypervolume indicator I_H with reference point $(12, 12)$ resp. $(12, 12, 12, 12, 12)$; in addition, minimum elements partitioning is used
$\preccurlyeq^{\text{minpart}}_{P0,H}$	preference-based quality indicator I_P with reference point $r^{(1)} = (0, 0)$ resp. $(0, 0, 0, 0, 0)$, followed by the hypervolume indicator I_H with reference point $(12, 12)$ resp. $(12, 12, 12, 12, 12)$; in addition, minimum elements partitioning is used. The same weights λ as in $\preccurlyeq^{\text{minpart}}_{P1,H}$ are used by I_P.
$\preccurlyeq^{\text{minpart}}_{D}$	diversity indicator I_D (kth-nearest neighbor approach) combined with minimum elements partitioning

[a] The weight combinations used for the five-objective problem instances are provided in the Appendix; in this case, the considered reference set was $B = \{(0, 0, 0, 0, 0)\}$.

randomSetMutation operator is exhaustive, then there exists a path with finite probability from any node to a node with $Q \in \text{Min}(\Psi_m, \preccurlyeq)$.

Because of the finiteness of $\mathcal{X}$, SPAM will not converge iff for some execution we have $P^i \equiv P^{i+1}$ and $P^* \prec P^{i+1}$ for all $i \geq K$ with some constant K and for some minimal element $P^* \in \text{Min}(\Psi_m, \preccurlyeq)$. During such an execution, a subset of nodes is visited infinitely often. Let us now suppose that SPAM does not converge. Then none of the infinitely visited nodes has an outgoing edge (i, j) with $Q^j \prec Q^i$. This contradicts the assumption that there exists a path with finite probability from any node to an optimal node Q with $Q \in \text{Min}(\Psi_m, \preccurlyeq)$. ■

Theorem 4.4: Every set preference relation $\preccurlyeq$ is m-greedy where m denotes the maximum size of the sets of solutions, i.e., Ψ_m is the universe of the sets under consideration.

Proof: The set preference relation $\preccurlyeq$ is a preorder. Therefore, there exists a path from any initial set P^1 to an optimal set P^N in Definition 4.1. The intermediate populations $P^2, \ldots, P^N$ can be generated by exchanging at most all m solutions from one set to the next. As the set preference relation is m-greedy, the elements p^i_j and r^i_j can be chosen correspondingly. ■

The last theorem leads to the fact that SPAM can be used with any set preference relation resp. quality indicator inducing a preorder if we use $k = m$. Whereas this statement may be of theoretical value, SPAM will be of no practical use for large m if only the *randomSetMutation* operator is applied; the reason is that the probability to determine a better set by exchanging randomly a large number of elements will be very small. Therefore, the *heursticSetMutation* operator is used in order to obtain improved sets with a high probability; however, this operator *in general* is not exhaustive, i.e., it may not possible to follow a path to an optimal set $P^* \in \text{Min}(\Psi_m, \preccurlyeq)$. Therefore, if the used *randomSetMutation* operator is exhaustive, i.e., it generates any possible k-neighbor with a finite probability, then SPAM converges to an optimal solution.

Finally, one may ask whether smaller values for k with $k < m$ are possible while still guaranteeing convergence. This may be desirable from a practical perspective since the generation of new solutions in $\mathcal{X}$ would thereby be tighter linked to the update of P; several indicator-based MOEAs basically use set mutation operators where k equals 1 [14], [22]. The answer clearly depends on the set preference relation under consideration. It can be shown that the set preference relations induced by the epsilon indicator and the hypervolume indicator are in general not 1-greedy; the proofs can be found in the appendix.

Corollary 4.5: The set preference relation $\preccurlyeq_{\epsilon 1}$ induced by the unary epsilon indicator $I_{\epsilon 1}$ is not 1-greedy.

Corollary 4.6: The set preference relation $\preccurlyeq_H$ induced by the hypervolume indicator I_H is not 1-greedy.

That means whenever these indicators are used within a set preference relation incorporated in SPAM, then there are cases where SPAM will not convergence if $k = 1$; this also holds for any other MOEA that replaces only a single solution in the current population and is based on these indicators. Whether other values for k with $1 < k < m$ are sufficient to guarantee convergence for these indicators is an open research issue.

V. Experimental Validation

This section investigates the practicability of the proposed approach. The main questions are: 1) can different user preferences be expressed in terms of set preference relations; 2) is it feasible to use a general search algorithm for arbitrary set preference relations, i.e., is SPAM effective in finding appropriate sets; and 3) how well are set preference relations suited to guide the optimization process? However, the purpose is not to carry out a performance comparison of SPAM to existing MOEAs; the separation of user preferences and search algorithm is the focus of our study.

A. Comparison Methodology

In the following, we consider different set preference relations for integration in SPAM; they have been discussed in Section III and are listed in Table II. All of them except of the last one are refinements of the set dominance relation $\preccurlyeq_{\text{par}}$; the relation $\preccurlyeq_D^{\text{minpart}}$ is just used for the purpose of mimicking the behavior of dominance and density-based MOEAs such as NSGA-II and SPEA2. As reference algorithms, NSGA-II [8] and IBEA[6] [36] are used; in the visual comparisons also SPEA2 [37] is included.

In order to make statements about the effectiveness of the algorithms considered, one needs to assess the generated Pareto-set approximations with regard to the set preference relation under consideration. We suggest the use of the Mann–Whitney U test to compare multiple outcomes of one algorithm with multiple outcomes of another algorithm. This is possible since all set preference relations considered in this paper are total preorders; otherwise, the approach proposed in [26] can be applied. Thereby, one can obtain statements about whether either algorithm yields significantly better results for a specified set preference relation.

In detail, the statistical testing is carried as follows. Assuming two optimizers OA and OB, first all Pareto-set approximations generated by OA are pairwisely compared to all Pareto-set approximations generated by OB. If, e.g., 30 runs have been performed for each algorithm, then overall 900 comparisons are made. Now, let A and B be two Pareto-set approximations resulting from OA respectively OB; then, we consider set A as better than set B with respect to the set preference relation $\preccurlyeq$, if $A \prec B$ holds. By counting the number of comparisons where the set of OA is better than the corresponding set of OB, one obtains the test statistics U; doing the same for OB gives U' which reflects the number of cases where OB yields a better outcome. The bigger U is compared to U', the better algorithm OA is geared toward the test relation $\preccurlyeq$ regarding OB.

As long as the entirety of the considered sets can be regarded as a large sample (e.g., 30 runs per algorithm), one can use the one-tailed normal approximation to calculate the significance of the test statistics U, correcting the variance for ties. Furthermore, multiple testing issues need to be taken into account when comparing multiple algorithms with each other; here, the significance levels are Bonferroni-corrected.

TABLE III

Parameter Settings Used in Section V-B

Parameter	Value
Set size/population size m	20*, 50**
Newly created solutions/offspring individuals k	20*, 50**
Number of iterations/generations	1000
Mutation probability	1
Swap probability	0.5
Recombination probability	1
η-Mutation	20
η-Recombination	20
Symmetric recombination	False
Scaling	False
Tournament size	2
Mating selection	Uniform

* Visual comparision, ** Statistical testing.

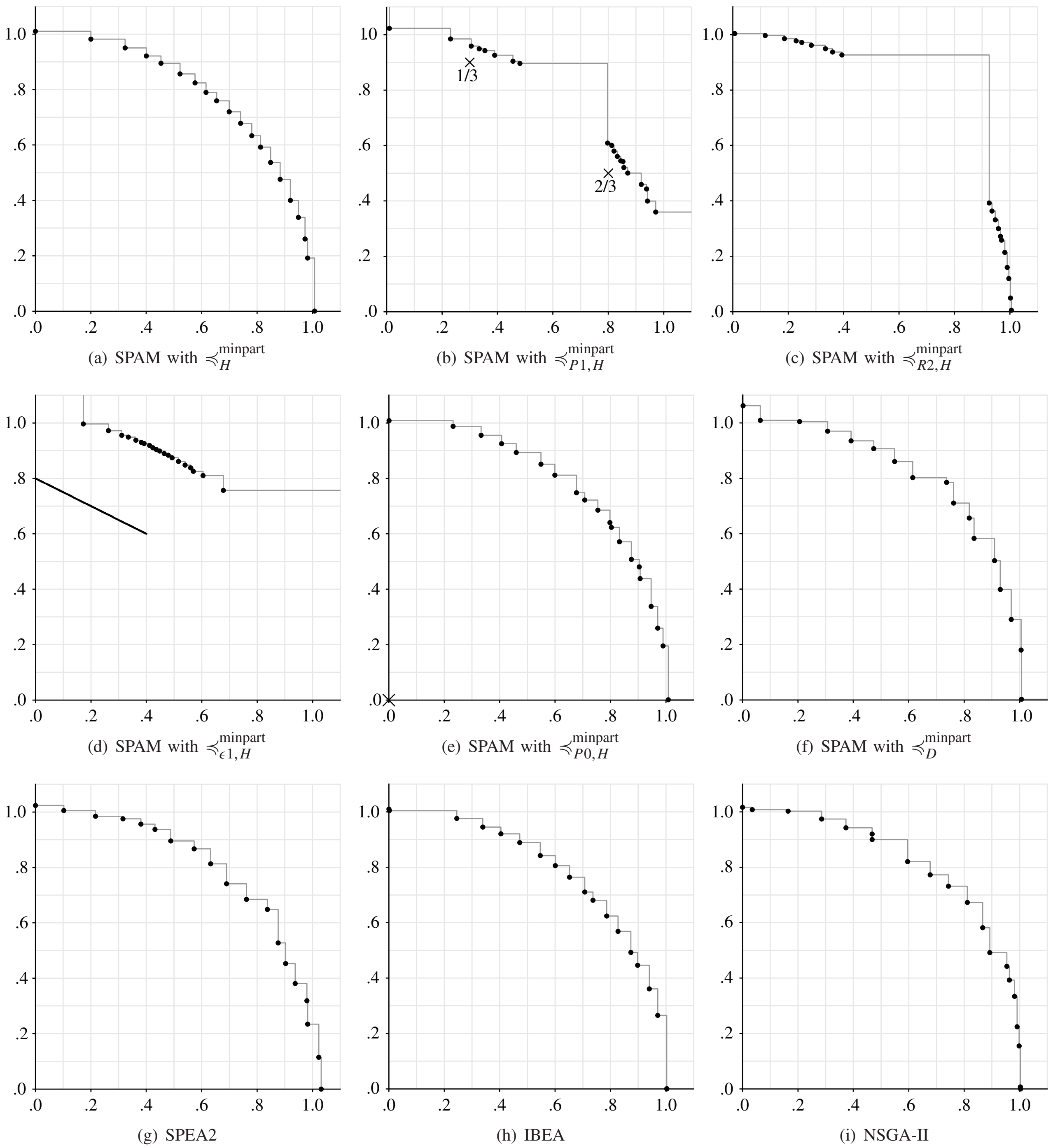
Finally, the SPAM implementation used for the following experimental studies does not include the random set mutation operator, i.e., lines 3, 7, and 8 in Algorithm 1 were omitted. The reason is that every set comparison is computationally expensive—especially when the hypervolume indicator is involved—and that in practice it is extremely unlikely that random set mutation according to Algorithm 2 yields a set that is superior to the one generated by the heuristic set mutation operator. Nevertheless, a set mutation operator that in principle can generate any set in Ψ is important to guarantee theoretical convergence. One may think of more effective operators than Algorithm 2 which preserves the convergence property; however, this topic is subject to future work and not investigated in this paper.

One may also ask whether the if statement at line 5 of Algorithm 1 is actually of practical relevance. Testing SPAM with three set preference relations, namely $\preccurlyeq_{P0,H}^{\text{minpart}}$, $\preccurlyeq_{P1,H}^{\text{minpart}}$, and $\preccurlyeq_{H,D}$, on a three-objective DTLZ5 problem instance indicates that on average every 50th generation (using $\preccurlyeq_{P0,H}^{\text{minpart}}$) and 100th generation (using $\preccurlyeq_{P1,H}^{\text{minpart}}$ and $\preccurlyeq_{H,D}$) the set produced by heuristic mutation is worse than the current set, i.e., the current set is not replaced. One can expect and observe, though, that this situation arises especially when being close to or on the Pareto front (all set members are incomparable) and less frequently at the early phase of the search process. Overall, no significant differences between the quality of the outcomes could be measured when running SPAM with and without the check at line 5; on average, the computation time increased by 12% ($\preccurlyeq_{P0,H}^{\text{minpart}}$ and $\preccurlyeq_{P1,H}^{\text{minpart}}$) and 8% ($\preccurlyeq_{H,D}$). Nevertheless, we recommend to keep this additional check because it represents a crucial aspect of a hill climber and prevents cycling behavior which is theoretically possible whenever worse sets are accepted.

B. Results

This section provides experimental results for two test problems, namely DTLZ2 and DTLZ5 [12] with 20 decision

[6] With parameters $\kappa = 0.05$ and $\rho = 1.1$.



(a) SPAM with $\preccurlyeq_{H}^{\text{minpart}}$

(b) SPAM with $\preccurlyeq_{P1,H}^{\text{minpart}}$

(c) SPAM with $\preccurlyeq_{R2,H}^{\text{minpart}}$

(d) SPAM with $\preccurlyeq_{\epsilon 1,H}^{\text{minpart}}$

(e) SPAM with $\preccurlyeq_{P0,H}^{\text{minpart}}$

(f) SPAM with $\preccurlyeq_{D}^{\text{minpart}}$

(g) SPEA2

(h) IBEA

(i) NSGA-II

Fig. 15. Pareto-set approximations found after 1000 generations on a biobjective DTLZ2 problem for a set size/population size of $m = 20$. All algorithms were started with the same initial set/population.

variables for two and five objectives. On one hand, we will provide visual comparisons in order to verify to which extent the formalized user preferences have been achieved. On the other hand, statistical tests are applied to investigate which search strategy is best suited to optimize which user preferences; for each optimizer, 30 runs have been carried out. The general parameters used in the optimization algorithms are given in Table III.

1) Visual comparisons: Fig. 15 shows the Pareto-set approximations generated by SPAM with the aforementioned set preference relations and by the reference algorithms for the biobjective DTLZ2 problem. The plots well reflect the chosen user preferences: (a) a set maximizing hypervolume, (b) a divided set close to two reference points, (c) focus on the extremes using corresponding weight combinations, (d) closeness to a given reference set, (e) a set minimizing the weighted epsilon-distance to the origin for a uniformly distributed set of weight combinations, and (f) a uniformly distributed set of solutions. This demonstrates that SPAM is in principle capable of optimizing toward the user preferences

TABLE IV

PAIRWISE STATISTICAL COMPARISON OF 30 RUNS PER ALGORITHM AFTER 1000 GENERATIONS. IN THE NOTATION $U : U'$, U (RESP. U') STANDS FOR THE NUMBER OF TIMES A SET GENERATED BY ALGORITHM A (RESP. B) BEATS A SET OF ALGORITHM B (RESP. A) WITH REGARD TO THE TEST RELATION ASSOCIATED WITH THE CORRESPONDING ROW. A STAR NEXT TO THESE NUMBERS INDICATES A SIGNIFICANT DIFFERENCE, THE FEW CASES WHERE THIS WAS NOT THE CASE ARE SHOWN IN BOLD

(a) 2-D DTLZ2

Alg B. / Alg. A		SPAM with set preference relation …							IBEA	NSGA-II	test relation
		$\preccurlyeq^{\text{minpart}}_{P1,H}$	$\preccurlyeq^{\text{minpart}}_{H}$	$\preccurlyeq^{\text{minpart}}_{R2,H}$	$\preccurlyeq^{\text{minpart}}_{\epsilon 1,H}$	$\preccurlyeq^{\text{minpart}}_{P0}$	$\preccurlyeq_{H,C,D}$	$\preccurlyeq^{\text{minpart}}_{D}$			
SPAM with set preference relation …	$\preccurlyeq^{\text{minpart}}_{P1,H}$	—	900: 0*	900: 0*	900: 0*	899: 1*	900: 0*	900: 0*	900: 0*	900: 0*	$\preccurlyeq_{P1,H}$
	$\preccurlyeq^{\text{minpart}}_{H}$	900: 0*	—	900: 0*	900: 0*	900: 0*	**456:444**	900: 0*	900: 0*	900: 0*	$\preccurlyeq_{H}$
	$\preccurlyeq^{\text{minpart}}_{R2,H}$	900: 0*	900: 0*	—	900: 0*	900: 0*	900: 0*	900: 0*	900: 0*	900: 0*	$\preccurlyeq_{R2,H}$
	$\preccurlyeq^{\text{minpart}}_{\epsilon 1,H}$	900: 0*	900: 0*	900: 0*	—	900: 0*	889: 1*	900: 0*	900: 0*	900: 0*	$\preccurlyeq_{\epsilon 1,H}$
	$\preccurlyeq^{\text{minpart}}_{P0,H}$	900: 0*	**60:840**	830: 70*	846: 54*	—	**75:835**	900: 0*	**134:766**	835: 75*	$\preccurlyeq_{P0,H}$
	$\preccurlyeq_{H,C,D}$	900: 0*	**444:456**	900: 0*	900: 0*	843: 57*	—	900: 0*	820: 80*	900: 0*	$\preccurlyeq_{H,C,D}$

* Preference is significant at the 0.001 level (1-tailed, Bonferroni-adjusted).

(b) 2-D DTLZ5

Alg B. / Alg. A		SPAM with set preference relation …							IBEA	NSGA-II	test relation
		$\preccurlyeq^{\text{minpart}}_{P1,H}$	$\preccurlyeq^{\text{minpart}}_{H}$	$\preccurlyeq^{\text{minpart}}_{R2,H}$	$\preccurlyeq^{\text{minpart}}_{\epsilon 1,H}$	$\preccurlyeq^{\text{minpart}}_{P0}$	$\preccurlyeq_{H,C,D}$	$\preccurlyeq^{\text{minpart}}_{D}$			
SPAM with set preference relation …	$\preccurlyeq^{\text{minpart}}_{P1,H}$	—	900: 0*	900: 0*	900: 0*	900: 0*	900: 0*	900: 0*	887: 13*	900: 0*	$\preccurlyeq_{P1,H}$
	$\preccurlyeq^{\text{minpart}}_{H}$	900: 0*	—	900: 0*	900: 0*	900: 0*	**445:455**	900: 0*	900: 0*	900: 0*	$\preccurlyeq_{H}$
	$\preccurlyeq^{\text{minpart}}_{R2,H}$	900: 0*	900: 0*	—	900: 0*	900: 0*	900: 0*	900: 0*	900: 0*	900: 0*	$\preccurlyeq_{R2,H}$
	$\preccurlyeq^{\text{minpart}}_{\epsilon 1,H}$	900: 0*	891: 9*	900: 0*	—	900: 0*	897: 3*	900: 0*	900: 0*	900: 0*	$\preccurlyeq_{\epsilon 1,H}$
	$\preccurlyeq^{\text{minpart}}_{P0}$	898: 2*	**22:878**	891: 9*	899: 1*	—	**12:888**	788:112*	**95:805**	885: 15*	$\preccurlyeq_{P0}$
	$\preccurlyeq_{H,C,D}$	900: 0*	**455:445**	900: 0*	900: 0*	795:105*	—	900: 0*	900: 0*	900: 0*	$\preccurlyeq_{H,C,D}$

* Preference is significant at the 0.001 level (1-tailed, Bonferroni-adjusted).

(c) Five-dimensional DTLZ2

Alg B. / Alg. A		SPAM with set preference relation …							IBEA	NSGA-II	test relation
		$\preccurlyeq^{\text{minpart}}_{P1,H}$	$\preccurlyeq^{\text{minpart}}_{H}$	$\preccurlyeq^{\text{minpart}}_{R2,H}$	$\preccurlyeq^{\text{minpart}}_{\epsilon 1,H}$	$\preccurlyeq^{\text{minpart}}_{P0}$	$\preccurlyeq_{H,C,D}$	$\preccurlyeq^{\text{minpart}}_{D}$			
SPAM with set preference relation …	$\preccurlyeq^{\text{minpart}}_{P1,H}$	—	820: 80*	820: 80*	805: 95*	838: 62*	820: 80*	900: 0*	820: 80*	900: 0*	$\preccurlyeq_{P1,H}$
	$\preccurlyeq^{\text{minpart}}_{H}$	900: 0*	—	900: 0*	900: 0*	900: 0*	**404:496**	900: 0*	895: 5*	900: 0*	$\preccurlyeq_{H}$
	$\preccurlyeq^{\text{minpart}}_{R2,H}$	900: 0*	900: 0*	—	900: 0*	900: 0*	900: 0*	900: 0*	900: 0*	900: 0*	$\preccurlyeq_{R2,H}$
	$\preccurlyeq^{\text{minpart}}_{\epsilon 1,H}$	900: 0*	895: 5*	870: 30*	—	894: 6*	895: 5*	900: 0*	895: 5*	900: 0*	$\preccurlyeq_{\epsilon 1,H}$
	$\preccurlyeq^{\text{minpart}}_{P0}$	880: 20*	810: 90*	871: 29*	899: 1*	—	900: 0*	898: 2*	**32:868**	900: 0*	$\preccurlyeq_{P0}$
	$\preccurlyeq_{H,C,D}$	900: 0*	**496:404**	900: 0*	900: 0*	843: 57*	—	900: 0*	900: 0*	900: 0*	$\preccurlyeq_{H,C,D}$

* Preference is significant at the 0.001 level (1-tailed, Bonferroni-adjusted).

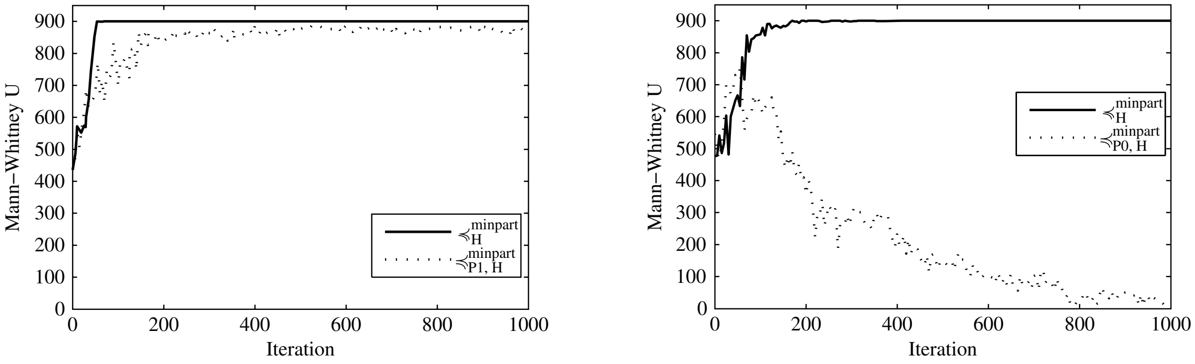
(d) Five-dimensional DTLZ5

Alg B. / Alg. A		SPAM with set preference relation …							IBEA	NSGA-II	test relation
		$\preccurlyeq^{\text{minpart}}_{P1,H}$	$\preccurlyeq^{\text{minpart}}_{H}$	$\preccurlyeq^{\text{minpart}}_{R2,H}$	$\preccurlyeq^{\text{minpart}}_{\epsilon 1,H}$	$\preccurlyeq^{\text{minpart}}_{P0}$	$\preccurlyeq_{H,C,D}$	$\preccurlyeq^{\text{minpart}}_{D}$			
SPAM with set preference relation …	$\preccurlyeq^{\text{minpart}}_{P1,H}$	—	877: 23*	900: 0*	900: 0*	900: 0*	**723:177**	900: 0*	874: 26*	900: 0*	$\preccurlyeq_{P1,H}$
	$\preccurlyeq^{\text{minpart}}_{H}$	900: 0*	—	900: 0*	900: 0*	900: 0*	**455:445**	900: 0*	900: 0*	900: 0*	$\preccurlyeq_{H}$
	$\preccurlyeq^{\text{minpart}}_{R2,H}$	900: 0*	900: 0*	—	900: 0*	900: 0*	900: 0*	900: 0*	900: 0*	900: 0*	$\preccurlyeq_{R2,H}$
	$\preccurlyeq^{\text{minpart}}_{\epsilon 1,H}$	892: 8*	**618:282**	900: 0*	—	900: 0*	**626:274**	900: 0*	893: 7*	900: 0*	$\preccurlyeq_{\epsilon 1,H}$
	$\preccurlyeq^{\text{minpart}}_{P0}$	900: 0*	841: 59*	819: 81*	873: 27*	—	752:148*	867: 33*	**121:779**	**547:453**	$\preccurlyeq_{P0}$
	$\preccurlyeq_{H,C,D}$	900: 0*	**445:455**	900: 0*	900: 0*	900: 0*	—	900: 0*	900: 0*	900: 0*	$\preccurlyeq_{H,C,D}$

* Preference is significant at the 0.001 level (1-tailed, Bonferroni-adjusted).

that are encoded in the corresponding set preference relation. It can also be seen that the density-based approaches by NSGA-II and SPEA2 can be imitated by using a corresponding diversity indicator—although this is not the goal of this paper.

2) Usefulness for Search: After having seen the proof-of-principle results for single runs, we now investigate the question of how effective SPAM is in optimizing a given set preference relation $\preccurlyeq$, i.e., how specific the optimization process is. The hypothesis is that SPAM used in combination with a specific $\preccurlyeq_A$ (let us say SPAM-A) yields better Pareto-set approximations than if used with any other set preference relation $\preccurlyeq_B$ (let us say SPAM-B)—better here means with respect to $\preccurlyeq_A$. Ideally, for every set A generated by SPAM-A and every set B generated by SPAM-B, it would hold $A \preccurlyeq_A B$ or even $A \prec_A B$. Clearly, this describes an ideal situtation. A set preference relation that is well suited for representing certain preferences may not be well suited for search *per se*, cf. Section III-D; for instance, when using a



(a) SPAM using $\preccurlyeq_{P1,H}^{\text{minpart}}$ and $\preccurlyeq_{H}^{\text{minpart}}$

(b) SPAM using $\preccurlyeq_{P0,H}^{\text{minpart}}$ and $\preccurlyeq_{H}^{\text{minpart}}$

Fig. 16. Each figure compares two SPAM variants for the biobjective DTLZ2 problem: SPAM with $\preccurlyeq_{H}^{\text{minpart}}$ versus SPAM with $\preccurlyeq_{P1,H}^{\text{minpart}}$ (left) and SPAM with $\preccurlyeq_{H}^{\text{minpart}}$ versus SPAM with $\preccurlyeq_{P0,H}^{\text{minpart}}$. Per figure, both algorithms are compared with respect to both set preference relations (without set partitioning). The solid line on the left gives for each iteration, the number of cases (30 runs versus 30 runs) where SPAM with $\preccurlyeq_{H}^{\text{minpart}}$ is better than SPAM with $\preccurlyeq_{P1,H}^{\text{minpart}}$ with respect to $\preccurlyeq_{H}$. The dotted line on the left shows how often SPAM with $\preccurlyeq_{P1,H}^{\text{minpart}}$ is better than SPAM with $\preccurlyeq_{H}^{\text{minpart}}$ regarding $\preccurlyeq_{P1,H}$ over time. The right figure provides the same where $\preccurlyeq_{P1,H}$ is replaced by $\preccurlyeq_{P0,H}$.

TABLE V

AVERAGED RUNNING TIME IN SECONDS PER ITERATION FOR SPAM USING THE GENERAL FITNESS ASSIGNMENT PROCEDURE (ALGORITHM 4) AS WELL AS THE PROCEDURE DEDICATED TO UNARY INDICATORS (ALGORITHM 5). THE COMPARISON ARE PROVIDED FOR THE TWO SET PREFERENCE RELATIONS $\preccurlyeq_{\epsilon 1}^{\text{minpart}}$ AND $\preccurlyeq_{H}^{\text{minpart}}$

Algorithm	2d	5d
SPAM using Algorithm 4 and $\preccurlyeq_{\epsilon 1}^{\text{minpart}}$	0.0601 s	24.8660 s
SPAM using Algorithm 5 and $\preccurlyeq_{\epsilon 1}^{\text{minpart}}$	0.0055 s	0.2128 s
SPAM using Algorithm 4 and $\preccurlyeq_{H}^{\text{minpart}}$	0.0170 s	253.8699 s
SPAM using Algorithm 5 and $\preccurlyeq_{H}^{\text{minpart}}$	0.0097 s	1.9722 s

single indicator such as the hypervolume indicator refinement through set partitioning is important for effective search.

To this end, we statistically compare all algorithmic variants with each other with respect to the six refinements listed in Table II. Note that set partitioning is only used for search, not for the comparisons. The outcomes of the pairwise comparisons after Bonferroni correction are given in Table IV. With only a few exceptions, the above hypothesis is confirmed: using $\preccurlyeq_A$ in SPAM yields the best Pareto-set approximations with regard to $\preccurlyeq_A$, independently of the problem and the number of objectives under consideration. These results are highly significant at a significance level of 0.001.

Concerning the exceptions, first it can be noticed that there is no significant difference between $\preccurlyeq_{H}^{\text{minpart}}$ and $\preccurlyeq_{H,C,D}$ when used in SPAM—both times, the hypervolume indicator value is optimized. This actually confirms the assumption that set partitioning can be replaced by a corresponding sequence of quality indicators. Second, the algorithm based on the set preference relation $\preccurlyeq_{P0,H}^{\text{minpart}}$ using the I_P indicator with the origin as reference point performs worse than SPAM with $\preccurlyeq_{H}^{\text{minpart}}$ on DTL2; this is not suprising, as it actually can be regarded as an approximation of the hypervolume-based relation. However, it is suprising that SPAM with $\preccurlyeq_{P0,H}^{\text{minpart}}$ is outperformed by IBEA on both DTLZ2 and DTLZ5; it seems that IBEA is more effective in obtaining a well-distributed front. This result indicates the sensitivity of $\preccurlyeq_{P0,H}^{\text{minpart}}$ with respect to the distribution and the number of the weight combinations chosen. The problem can be resolved by selecting a larger number of weights as discussed in Section III-D.

To see how the differences develop over the course of time, Fig. 16 compares selected SPAM variants with each other and provides the test statistics for each iteration. As can be seen on the left, already after 150 iterations the differences become highly significant when comparing SPAM with $\preccurlyeq_{H}^{\text{minpart}}$ and SPAM with $\preccurlyeq_{P1,H}^{\text{minpart}}$. In Fig. 16 on the right, it can be observed that SPAM with $\preccurlyeq_{P0,H}^{\text{minpart}}$ is—after a competetive starting phase—soon overtaken by SPAM with the hypervolume indicator. As already mentioned, this reflects the dependency of $\preccurlyeq_{P1,H}^{\text{minpart}}$ from the number of weight combinations.

3) Running Time Issues: Last, we investigate the running time of SPAM where the absolute computation time is considered instead of the number of fitness evaluations. The question is how the choice of the set preference relation and the fitness assignment procedure (Algorithm 4 versus 5) affects the number of iterations that can be performed in a fixed time budget. Table V reveals that the average computation time per iteration heavily depends on the specific set preference relation. For instance, the hypervolume-based set preference relations induce considerably more computation time—especially in higher dimensions—than the relation based on the epsilon indicator. However, the influence of the fitness assignment algorithms is even stronger: the use of Algorithm 4 slows down the search by a factor of 100 in comparison to Algorithm 5.

VI. CONCLUSION

In this paper, we have discussed EMO from a single-objective perspective that is centered around set preference relations and based on the following three observations:

1) the result of an MOEA run is usually a set of trade-off solutions representing a Pareto set approximation;
2) most existing MOEAs can be regarded as hill climbers—usually (1, 1)-strategies—on set problems;
3) most existing MOEAs are (implicitly) based on set preference information.

When applying an evolutionary algorithm to the problem of approximating the Pareto-optimal set, the population itself can be regarded as the current Pareto-set approximation. The subsequent application of mating selection, variation, and environmental selection heuristically produces a new Pareto-set approximation that—in the ideal case—is better than the previous one. In the light of the underlying set problem, the population represents a single element of the search space which is in each iteration replaced by another element of the search space. Consequently, selection and variation can be regarded as a mutation operator on populations resp. sets. Somewhat simplified, one may say that a classical MOEA used to approximate the Pareto-optimal set is a (1, 1)-strategy on a set problem. Furthermore, MOEAs are usually not preference-free. The main advantage of generating methods such as MOEAs is that the objectives do not need to be aggregated or ranked *a priori*; but nevertheless preference information is required to guide the search, although it is usually weaker and less stringent. In the environmental selection step, for instance, an MOEA has to choose a subset of individuals from the parents and the offspring which constitutes the next Pareto-set approximation. To this end, the algorithm needs to know the criteria according to which the subset should be selected, in particular when all parents and children are incomparable, i.e., mutually nondominating. That means the generation of a new population usually relies on set preference information.

We here have tried to consequently take this line of thought further and to study how set preference information can be formalized such that a total order on the set of Pareto-set approximations results. To this end, we have shown how to construct set preference relations on the basis of quality indicators and provided various examples. Moreover, we have presented a general set preference algorithm for multiobjective optimization (SPAM), which is basically a hill climber and generalizes the concepts found in most modern MOEAs. SPAM can be used in combination with any type of set preference relation and thereby offers full flexibility for the decision maker; furthermore, it can be shown to converge under general conditions. As the experimental results indicate, set preference relations can be used to effectively guide the search as well as to evaluate the outcomes of multiobjective optimizers.

The new perspective that this paper offers is, roughly speaking, considering EMO as using evolutionary algorithms for single-objective set problems in the context of multiobjective optimization. Clearly, there are many open issues, e.g., the design of both specific and arbitrary set preference relations to integrate particular user preferences, especially local preferences. Furthermore, the design of fast search algorithms dedicated to particular set preference relations is of high interest; SPAM provides flexibility, but is rather a baseline algorithm that naturally cannot achieve maximum possible efficiency. And finally, one may think of using a true evolutionary algorithm for set-based multiobjective optimization, one that operates on populations of Pareto set approximations—whether this approach can be beneficial is an open research issue.

Appendix

In order to prove Theorem 2.7 we first need to state a set of smaller results:

Lemma A.1: If all preference relations $\preccurlyeq^j$, $1 \leq j \leq k$ in Definition 2.6 are preorders, then $\preccurlyeq_S$ is a preorder.

Proof: Reflexivity: As $A \preccurlyeq^i A$ holds for all $1 \leq i \leq k$ (since all $\preccurlyeq^i$ are preorders), we have $i = k$ in Definition 2.6 (i). Therefore, $(A \preccurlyeq_S A) \Leftrightarrow (A \preccurlyeq^i A)$ and the reflexivity holds. Transitivity: We prove transitivity by induction. We first need to show that transitivity holds for $k = 1$. In this case, we have $A \preccurlyeq_S B \Leftrightarrow A \preccurlyeq^1 B$ as $i = k$ in Definition 2.6 (i). Transitivity holds as $\preccurlyeq^1$ is a preorder. Now we have to show that transitivity holds for k if it holds for $k - 1$. Let us define the sequence of length $k - 1$ as S'. Then we can reformulate Definition 2.6 as follows:

$$(A \preccurlyeq_S B) \Leftrightarrow ((A \equiv_{S'} B) \wedge (A \preccurlyeq^k B)) \vee (A \prec_{S'} B). \quad (3)$$

Now, we can show that transitivity holds:

$$\begin{aligned}
&(A \preccurlyeq_S B) \wedge (B \preccurlyeq_S C) \Rightarrow\\
&\quad \Rightarrow [((A \equiv_{S'} B) \wedge (A \preccurlyeq^k B)) \vee (A \prec_{S'} B)] \wedge\\
&\quad\quad [((B \equiv_{S'} C) \wedge (B \preccurlyeq^k C)) \vee (B \prec_{S'} C)] \Rightarrow\\
&\quad \Rightarrow ((A \equiv_{S'} B) \wedge (B \equiv_{S'} C) \wedge (A \preccurlyeq^k B) \wedge (\preccurlyeq^k C)) \vee\\
&\quad\quad ((A \prec_{S'} B) \wedge (B \prec_{S'} C)) \Rightarrow\\
&\quad \Rightarrow ((A \equiv_{S'} C) \wedge (A \preccurlyeq^k C)) \vee (A \prec_{S'} C) \Rightarrow A \preccurlyeq_S C.
\end{aligned}$$

■

Lemma A.2: If all preference relations $\preccurlyeq^j$, $1 \leq j \leq k$ in Definition 2.6 are total preorders, then $\preccurlyeq_S$ is a total preorder.

Proof: A preorder $\preccurlyeq$ is called total if $(A \preccurlyeq B) \vee (B \preccurlyeq A)$ holds for all $A, B \in \Psi$. Using the same induction principle as in the proof of A.1 we can notice that for $k = 1$ we have $(A \preccurlyeq_S B) \Leftrightarrow (A \preccurlyeq^1 B)$ and therefore, $\preccurlyeq_S$ is total. For the induction we know that (3) holds. Therefore, we can conclude

$$\begin{aligned}
&(A \preccurlyeq_S B) \vee (B \preccurlyeq_S A) \Leftrightarrow\\
&\quad \Leftrightarrow ((A \equiv_{S'} B) \wedge (A \preccurlyeq^k B)) \vee ((B \equiv_{S'} A) \wedge (B \preccurlyeq^k A)) \vee\\
&\quad\quad (A \prec_{S'} B) \vee (B \prec_{S'} A) \Leftrightarrow\\
&\quad \Leftrightarrow (A \equiv_{S'} B) \vee (A \prec_{S'} B) \vee (B \prec_{S'} A) \Leftrightarrow \text{true}.
\end{aligned}$$

■

Lemma A.3: If $\preccurlyeq^k$ in Definition 2.6 is a refinement of a given preference relation $\preccurlyeq$ and all relations $\preccurlyeq^j$, $1 \leq j < k$ are weak refinements of $\preccurlyeq$, then $\preccurlyeq_S$ is a refinement of $\preccurlyeq$.

Proof: Let us suppose that $A \prec B$ holds for some $A, B \in \Psi$. We have to show that $A \prec_{S'} B$ holds. At first note, the $A \preccurlyeq^j B$ holds for all $1 \leq j < k$ as $\preccurlyeq^j$ are weak refinements and $A \prec^k B$ holds as $\preccurlyeq^k$ is a refinement. Let us now consider the sequence S' of length $k - 1$. Because all $\preccurlyeq^j$ are weak

TABLE VI
COUNTEREXAMPLE FOR 1-GREEDYNESS OF THE UNARY EPSILON INDICATOR

	r^1	r^2	r^3	r^4	$f(x^1)$	$f(x^2)$	$f(x^3)$	$f(x^4)$
1	4	0	6	3	6	2	0	3
2	0	4	3	6	2	6	0	3
3	6	6	2	2	4	4	6	2

refinements, either $A \equiv^j B$ or $A \prec^j B$ holds. Taking into account the construction of S' according to Definition 2.6 we can easily see that $A \preccurlyeq_{S'} B$ holds. Based on the fact that $\preccurlyeq_{S'}$ is a weak refinement, we will show that $A \prec_S B$ holds, i.e. $\prec_S$ is a refinement. To this end, we again use (3) to derive

$$\begin{aligned}(A \preccurlyeq_S B) \wedge (B \not\preccurlyeq_S A) \Leftrightarrow& \\ \Leftrightarrow[((A \equiv_{S'} B) \wedge (A \preccurlyeq^k B)) \vee (A \prec_{S'} B)]\wedge& \\ ((B \not\equiv_{S'} A) \vee (B \not\preccurlyeq^k A)) \wedge (A \not\preccurlyeq_{S'} B).& \qquad (4)\end{aligned}$$

As $\preccurlyeq_{S'}$ is a weak refinement, we need to consider two cases. If $A \equiv_{S'} B$ holds, then $A \not\preccurlyeq_{S'} B$ holds as well as $B \not\preccurlyeq_{S'} A$. In this case, the expression becomes $(A \preccurlyeq^k B) \wedge (B \not\preccurlyeq^k A)$ which yields true. If $A \prec_{S'} B$ holds, then $A \not\equiv_{S'} B$, $B \not\equiv_{S'} A$ and $B \not\preccurlyeq_{S'} A$ hold. The expression above becomes now $(A \prec_{S'} B) \wedge (B \not\preccurlyeq_{S'} A)$ which also yields true. ■

Now we can give the proof of Theorem 2.7.

Proof of Theorem 2.7: Because of Lemma A.3, we know that the sequence $S' = (\preccurlyeq^1, \preccurlyeq^2, \ldots, \preccurlyeq^{k'})$ leads to a refinement of $\preccurlyeq$. We just need to show that additional preference relations $\preccurlyeq^j$, $k' < j \leq k$ in the sequence do not destroy this property. We again use the same induction principle as in the previous proofs. Let us suppose that S' yields a refinement (as shown above) and S has one additional relation $\preccurlyeq^{k'+1}$, i.e. $k = k'+1$. Using again (3) we can derive the expression for $A \prec_S B$ as in (4). If we suppose that $A \prec B$ holds in the given preorder, and $\preccurlyeq_{S'}$ is a refinement, the relations $A \not\equiv_{S'} B$, $B \not\equiv_{S'} A$, $A \prec_{S'} A$, and $B \not\preccurlyeq_{S'} A$ hold. For the expression in (4) we get $(A \preccurlyeq^k B) \wedge (B \not\preccurlyeq^k A)$ which yields true. ■

Proof of Theorem 3.2: Suppose conditions 1 and 2 hold, and let $A, B \in \Psi$ be two arbitrary sets with $A \prec B$, i.e. $(A \preccurlyeq B) \wedge (B \not\preccurlyeq A)$. For the proof, we will apply the two local transformations in order to gradually change B to A and show that at each step the indicator value does not increase and there is at least one step where it decreases. First, we successively add the elements of B to A; since for each $b \in B$ it holds $A \preccurlyeq \{b\}$, according to condition 1 the indicator value remains constant after each step, i.e., $I(A) = I(A \cup B)$. Now, we successively add the elements of A to B; since $A \prec B$, there exists an element $a \in A$ such that $B \not\preccurlyeq \{a\}$ according to the conformance of $\preccurlyeq$ with $\preceq$. That means when adding the elements of A to B the indicator value either remains unchanged (condition 1) or decreases (and it will decrease at least once, namely for a, according to condition 2), and therefore $I(A \cup B) < I(B)$. Combining the two intermediate results, one obtains $I(A) = I(A \cup B) < I(B)$ which implies $A \preccurlyeq_I B$ and $B \not\preccurlyeq_I A$. Hence, $\preccurlyeq_I$ refines $\preccurlyeq$. For weak refinement, the proof is analogous.

TABLE VII
VALUES $\epsilon(z, r)$ FOR THE COUNTEREXAMPLE

	$f(x^1)$	$f(x^2)$	$f(x^3)$	$f(x^4)$
r^1	2	6	0	3
r^2	6	2	0	3
r^3	2	3	4	0
r^4	3	2	4	0

TABLE VIII
COUNTEREXAMPLE FOR 1-GREEDYNESS OF THE HYPERVOLUME INDICATOR

	r	$f(x^1)$	$f(x^2)$	$f(x^3)$	$f(x^4)$
1	10	1	6	5	7
2	7	6	2	3	1

To the prove that the second condition is a necessary condition, suppose $A \not\preccurlyeq \{b\}$. According to Definition 2.2, $(A \cup \{b\}) \prec A$ which implies that $(A \cup \{b\}) \preccurlyeq_I A$ (weak refinement) respectively $(A \cup \{b\}) \prec_I A$ (refinement). Hence, $I(A \cup \{b\}) \leq I(A)$ respectively $I(A \cup \{b\}) < I(A)$ according to (1). ■

Proof of Corollary 4.5: We will show that in the case of a 3-D objective space $\mathcal{Z} \subset \mathbb{R}^3$, the epsilon indicator $I_{\epsilon 1}(A) = I_\epsilon(A, R)$ is not 1-greedy.

The proof is done by providing a counterexample. We will give a scenario consisting of an objective space $\mathcal{Z} \subset \mathbb{R}^3$, reference set $R \subset \mathcal{Z}$, a maximum set size m and an initial set $P \in \Psi_m$. We will show that there is no path from the initial set P to an optimal set P^* such that every time only one element of the set is exchanged. In particular, we have $\mathcal{X} = \{x^1, x^2, x^3, x^4\}$, $R = \{r^1, r^2, r^3, r^4\}$, $m = 2$, $P = \{x^1, x^2\}$, $P^* = \{x^3, x^4\}$, and $f : \mathcal{X} \to \mathcal{Z}$ according to Table VI. With the values $\epsilon(z, r)$ shown in Table VII we obtain the epsilon indicator value for all possible sets as $I_\epsilon(\{x^1, x^2\}, R) = 2$, $I_\epsilon(\{x^1, x^3\}, R) = 3$, $I_\epsilon(\{x^1, x^4\}, R) = 3$, $I_\epsilon(\{x^2, x^3\}, R) = 3$, $I_\epsilon(\{x^2, x^4\}, R) = 3$ and $I_\epsilon(\{x^3, x^4\}, R) = 0$. Therefore, from the initial set $\{x^1, x^2\}$, every set mutation operator that exchanges one element only leads to a worse indicator value.

Finally, note that it can be shown that in $\mathbb{R}^2$ the epsilon indicator is 1-greedy. ■

Proof of Corollary 4.6: We will show that in the case of a 2-D objective space $\mathcal{Z} \subset \mathbb{R}^2$, the hypervolume indicator I_H is not 1-greedy.

The proof is done by providing a counterexample similar to the proof of the previous Corollary. Here we use again a decision space $\mathcal{X} = \{x^1, x^2, x^3, x^4\}$, a reference set $R = \{r\}$, an initial set $P = \{x^1, x^2\}$, an optimal set $P^* = \{x^3, x^4\}$, and $f : \mathcal{X} \to \mathcal{Z}$ according to Table VIII. Using this scenario, we obtain the hypervolume indicators for all possible populations as $I_H(\{x^1, x^2\}, R) = -25$, $I_H(\{x^1, x^3\}, R) = -24$, $I_H(\{x^1, x^4\}, R) = -24$, $I_H(\{x^2, x^3\}, R) = -24$,

$I_H(\{x^2, x^4\}, R) = -24$ and $I_H(\{x^3, x^4\}, R) = -26$. Therefore, from the initial set $\{x^1, x^2\}$, every set mutation operator that exchanges one element only leads to a worse indicator value. ■

Proof Weight combinations for $\preccurlyeq^{\text{minpart}}_{R2,H}$*:* In the case of five objectives, overall $32 \cdot 5$ weight combinations are used for the set preference relation $\preccurlyeq^{\text{minpart}}_{R2,H}$, cf. Table II. In detail, Λ is defined as follows:

$$\begin{aligned}
\Lambda \;=\; & \{ \\
& (0,0,0,0,1), \\
& (0.01/4, 0.01/4, 0.01/4, 0.01/4, 0.99), \\
& \ldots, \\
& (0.3/4, 0.3/4, 0.3/4, 0.3/4, 0.7) \\
& \} \\
\cup \\
& \{ \\
& (0,0,0,1,0), \\
& (0.01/4, 0.01/4, 0.01/4, 0.99, 0.01/4), \\
& \ldots, \\
& (0.3/4, 0.3/4, 0.3/4, 0.7, 0.3/4) \\
& \} \\
\cup \\
\ldots \\
\cup \\
& \{ \\
& (1,0,0,0,0), \\
& (0.99, 0.01/4, 0.01/4, 0.01/4, 0.01/4), \\
& \ldots, \\
& (0.7, 0.3/4, 0.3/4, 0.3/4, 0.3/4) \\
& \}
\end{aligned}$$ ■

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Eckart Zitzler received the Diploma degree in computer science from the University of Dortmund, Germany, and Doctor of Technical Sciences degree from Eidgenössische Technische Hochschule (ETH) Zürich, Switzerland.

Since 2003, he has been Assistant Professor for Systemsg Optimization in the Computer Engineering and Networks Laboratory, Department of Information Technology and Electrical Engineering, ETH Zürich, Switzerland. His research focuses on bioinspired computation, multiobjective optimization, computational biology, and computer engineering applications.

Prof. Zitzler was General Co-Chairman of the first three international conferences on evolutionary multi-criterion optimization (EMO 2001, EMO 2003, and EMO 2005).

Johannes Bader studied Information Technology and Electrical Engineering at the Eidgenössische Technische Hochschule (ETH) Zürich, and received the Master's degree in 2006. Since then, he has been a doctoral student in the Systems Optimization Group at the Computer Engineering and Networks Laboratory at the ETH Zürich, Switzerland.

His interest is focused on evolutionary multiobjective optimization.

Lothar Thiele was born in Aachen, Germany, on April 7, 1957. He received the Diplom-Ingenieur and Dr.-Ing. degrees in electrical engineering from the Technical University of Munich in 1981 and 1985, respectively. After completing his Habilitation thesis from the Institute of Network Theory and Circuit Design of the Technical University Munich, he joined the Information Systems Laboratory at Stanford University in 1987.

In 1988, he took up the Chair of Microelectronics at the Faculty of Engineering, University of Saarland, Saarbrucken, Germany. He joined Eidgenössische Technische Hochschule (ETH) Zürich, Switzerland, as a Full Professor of Computer Engineering, in 1994. Currently, He is leading the Computer Engineering and Networks Laboratory at the ETH Zürich, Switzerland. His research interests include models, methods, and software tools for the design of embedded systems, embedded software, and bioinspired optimization techniques.

Prof. Thiele received the "Dissertation Award" of the Technical University of Munich in 1986; the "Outstanding Young Author Award" of the IEEE Circuits and Systems Society in 1987; the Browder J. Thompson Memorial Award of the IEEE in 1988; and in 2000–2001, the "IBM Faculty Partnership Award." In 2004, he joined the German Academy of Natural Scientists Leopoldina. In 2005, he was the recipient of the Honorary Blaise Pascal Chair of University Leiden, The Netherlands.