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Pareto-, Aggregation-, and Indicator-based
Methods in Many-objective Optimization

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Pareto-, Aggregation-, and Indicator-based Methods in Many-objective Optimization

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Abstract. Research within the area of Evolutionary Multi-objective Optimization (EMO) focused on two- and three-dimensional objective functions, so far. Most algorithms have been developed for and tested on this limited application area. To broaden the insight in the behavior of EMO algorithms (EMOA) in higher dimensional objective spaces, a comprehensive benchmarking is presented, featuring several state-of-the-art EMOA, as well as an aggregative approach and a restart strategy on established scalable test problems with three to six objectives. It is demonstrated why the performance of well-established EMOA (NSGA-II, SPEA2) rapidly degrades with increasing dimension. Newer EMOA like ϵ -MOEA, MSOPS, IBEA and SMS-EMOA cope very well with high-dimensional objective spaces. Their specific advantages and drawbacks are illustrated, thus giving valuable hints for practitioners which EMOA to choose depending on the optimization scenario. Additionally, a new method for the generation of weight vectors usable in aggregation methods is presented.

1 Introduction

In the field of evolutionary multi-objective optimization, a lot of test problems and applications with two or three objectives have been studied. Problems with more than three objectives, which have been termed *many*-objective problems by Farina and Amato [1], have been tackled only rarely. Many techniques that work well for only a few objectives are anticipated to have difficulties in high-dimensional objective spaces. Thus, many-objective optimization is significantly more challenging than scenarios usually being analyzed.

Within multi-objective optimization, we consider d -dimensional vectors of objective values for a problem of d objective functions $\mathbf{f} = (f_1, \dots, f_d)$. Among these vectors, a partial order holds concerning the considered minimization problems. An individual p with decision vector \mathbf{x} *dominates* another p' with decision vector \mathbf{x}' , if and only if for the objective vectors $\mathbf{y} = \mathbf{f}(\mathbf{x})$ and $\mathbf{y}' = \mathbf{f}(\mathbf{x}')$ holds: $\forall i \in \{1, \dots, d\} : y_i \leq y'_i$ and $\mathbf{y} \neq \mathbf{y}'$. Within a set of individuals, individuals that are not dominated by other members are called *non-dominated*. The minimal elements of the partial order of the dominance relation, which are globally

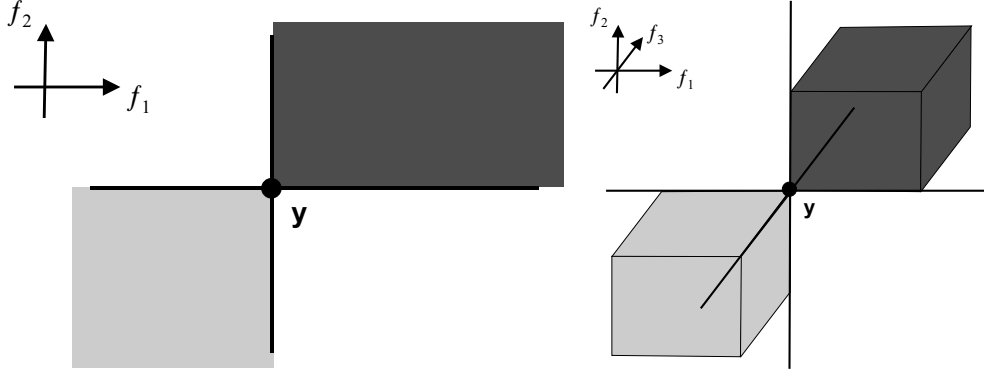


Fig. 1: A solution's comparable space in case of two (left) and three objectives (right). The region which is dominated by a point \mathbf{y} is marked dark gray and the region consisting of points dominating \mathbf{y} is shaded light gray. Only points in those areas are comparable to \mathbf{y} with respect to Pareto-dominance, whereas all other points are incomparable.

non-dominated are called *Pareto optimal*. The set of Pareto optimal decision vectors is called *Pareto set* and the corresponding set of Pareto optimal objective vectors is called *Pareto front*. The selection module of an EMO algorithm (EMOA) requires a mapping of an objective vector to a ranking criterion to establish a complete order among individuals. Popular EMOA usually consist of two selection operators. The primary selection operator is based on Pareto dominance and favors non-dominated solutions over dominated ones. The secondary operator is constituted diversity preserving and rates solutions incomparable concerning the primary operator. Whenever the set of solutions being equivalent concerning the primary operator is too large to be completely taken into the following population, the secondary operator is applied.

This concept of selection already documents the insight that Pareto dominance may not be sufficient as a sole selection operator, due to the large amount of possibly incomparable solutions. More precisely, a d -dimensional objective vector is only comparable with a fraction of $1/2^{d-1}$ of an (infinite) objective space, as stated by Farina and Amato [1]. This fact is depicted in Fig. 1. The importance of the secondary selection operator grows with increasing dimension of the objective space since the incomparability concerning the Pareto-based operator becomes the typical case.

Few previous studies on many-objective optimization by Purshouse and Fleming [2] and Hughes [3] focus to demonstrate the bad performance of NSGA-II by Deb et al. [4]. Hughes observed a simple single-objective restart strategy outperforming NSGA-II on a six-objective function in a two-dimensional decision space. Upon this, he implied a generalization to all Pareto-based techniques.

In contradiction, the work at hand includes positive results by demonstrating that some modern EMOA using Pareto-concepts cope very well with high-dimensional objective spaces. We ascribe the good performance of ε -MOEA,

IBEA, SMS-EMOA, and MSOPS to new concepts of aggregation and indicator functions and explain how and why these EMOA work successfully. A comprehensive benchmark is presented on the established test functions of the DTLZ function family, which feature a high dimensional decision and a scalable objective space. Moreover, a slight modification to NSGA-II is suggested, which causes a better performance. Our motivation is not to modify NSGA-II but to demonstrate which aspects of classic EMOA are responsible for the problems within many-objective optimization.

The aggregation method MSOPS by Hughes [3] which performs an optimization with respect to all objectives in parallel not harking back to the concept of Pareto dominance is studied more detailedly. The problems using aggregation are described and solution concepts are presented with a focus on suitable sets of weight vectors.

The insights are very interesting for practitioners who have to decide which algorithm is suitable to solve their problem effectively and efficiently. The discussed aspects of parameterization simplify the successful application of EMOA. For designers of algorithms, the study gives hints to possible improvements.

The considered test functions, performance measures and basic settings of the EMOA are described in the following section. Section 3 deals with the behavior of Pareto-based EMOA, Section 4 with aggregation methods, and Section 5 with methods utilizing indicator functions for selection. In these sections, algorithms are presented and their performances are described with help of the quality measures. Section 6 summarizes the findings and gives an outlook on how to further deepen insight in many-objective optimization.

2 Benchmark Settings

All algorithms, except otherwise mentioned, have been implemented within the PISA framework¹ [5] since an integrative framework simplifies comparisons. The same variation operators are used with exactly the same parameterization, which is chosen according to the studies of Deb et al. [6]. Simulated binary crossover (SBX) and polynomial mutation (PM) as described by Deb [7] are applied with mutation probability $p_m = 1/n$ per decision variable and recombination probability $p_c = 1$ per individual. The distribution indices $\eta_c = 15$ and $\eta_m = 20$ are used. If not otherwise stated, a $(\mu + \mu)$ strategy and a binary tournament for mating selection are applied. A number of 30.000 function evaluations is accomplished and the population size $\mu = 100$ is chosen. For each EMOA, besides SMS-EMOA, on each test function, 20 runs are performed. Due to the exponential runtime and the small standard deviation in the observed runs, SMS-EMOA is only repeated 5 times.

¹ PISA - Platform and Programming Language Independent Interface for Search Algorithms, ETH Zürich (www.tik.ee.ethz.ch/pisa/)

2.1 Test Functions

To benchmark the performance of the considered EMOA, the functions DTLZ1 and DTLZ2 of the DTLZ test function family [8] are invoked. These functions are scalable in the number of objectives and thus allow for a many-objective study. A bottom-up approach is used, which combines a parametric description of the Pareto front with a distance function. Therefore, the decision vector is divided into two subvectors. The first one of length $d - 1$ contains the parameters defining the position on the given surface while the second of length ν specifies the distance to the Pareto front. This results in dimension $d + \nu - 1$ of the decision space. According to Deb et al. [8], $\nu = 5$ is used in DTLZ1 and $\nu = 10$ is used in DTLZ2 respectively.

The Pareto front of DTLZ1 is a linear hyperplane ($\sum_{i=1}^d f_i(\mathbf{x}) = 0.5$). DTLZ2 features a Pareto front that corresponds to the positive part of the unit hypersphere ($|\mathbf{f}(\mathbf{x})| = 1$). Here, the interaction between objectives is nonlinear. The domain of all decision variables is $[0, 1]$. Due to different scaling constants in the distance function, the codomain of objective values for DTLZ1 is $[0, 1 + 225\nu]$ and $[0, 1 + 0.25\nu]$ for DTLZ2, respectively. The Pareto set of both test functions corresponds to $x_d, \dots, x_n = 0.5$ with arbitrary values for x_1, \dots, x_{d-1} .

2.2 Performance Assessment

For performance assessment, the \mathcal{S} -metric by Zitzler and Thiele [9] and the convergence measure [6] are considered. The \mathcal{S} -metric determines the size of the dominated hypervolume in objective space bounded by a reference point \mathbf{r} . In EMO research it is of outstanding importance due to its theoretical properties. The values depend on proximity to the Pareto front as well as on distribution of points. The maximal \mathcal{S} -metric value is reached by the Pareto front. The reference points $\mathbf{r} = 0.7^d$ for DTLZ1 and $\mathbf{r} = 1.1^d$ for DTLZ2 were used in previous studies [6, 10] and are close to the Pareto front in order to emphasize on the distribution of optimal solutions. Points that do not dominate the reference point are discarded for metric calculation. The metric values are normalized by calculating the fraction of the analytical optimal value. Note that exactly 100% are unreachable with a finite number of points.

The convergence measure describes the average distance of the approximation to the Pareto front in objective space. In contrast to the study of Deb et al. [6], the euclidean distance to the nearest optimal solution is determined analytically without using a reference set.

In analytic geometry, the distance of a point to a hyperplane can be calculated using the Hesse normal form. Given a parametric surface S defined by $n_1x_1 + \dots + n_dx_d = a$, the distance d_S of a point $(r_1, \dots, r_d)^T$ to S is

$$d_S = \left| \frac{n_1r_1 + \dots + n_dr_d - a}{\sqrt{n_1^2 + \dots + n_d^2}} \right|.$$

The DTLZ1 hyperplane possesses the normal vector $(n_1, \dots, n_d)^T = (1, \dots, 1)^T$ resulting in the distance

$$d_{DTLZ1}(\mathbf{x}) = |f_1(\mathbf{x}) + \dots + f_d(\mathbf{x}) - 0.5|$$

of a solution \mathbf{x} to the Pareto front.

On DTLZ2, the shortest way to the Pareto front is the line between the position vector of the solution and the origin of the objective coordinate system. Since the distance of the origin to each point of the Pareto front is 1, the distance of a solution \mathbf{x} to the Pareto front constitutes

$$d_{DTLZ2}(\mathbf{x}) = |\mathbf{f}(\mathbf{x})| - 1.$$

3 Pareto-based EMOA

As *Pareto-based* EMOA, we classify EMOA with selection criteria that are mainly based on the qualitative information of Pareto-dominance, Pareto-based ranking, or counting. Thus, NSGA-II, SPEA2, and ε -MOEA are considered here.

NSGA-II The *Elitist Non-dominated Sorting Genetic Algorithm* (NSGA-II) by Deb et al. [4] applies the rank assigned to each solution by non-dominated sorting as primary selection criterion. Non-dominated individuals are assigned rank one and the set of individuals with equal rank is called a front. Those individuals that are non-dominated if the first front was removed are assigned rank two. The third front is decided within the population discarding the first and the second front and so on. Individuals with equal ranks are evaluated using a secondary selection criterion called crowding distance. This subsumes the distances to the next higher and lower values in each dimension, respectively. Currently, the NSGA-II is supposed to be the best known and most frequently applied EMOA. Jensen [11] improves the non-dominated sorting algorithm, determining the overall runtime of NSGA-II, to run in $O(\mu \log^{d-1} \mu)$ per generation.

SPEA-2 The *Strength Pareto Evolutionary Algorithm* (SPEA2) by Zitzler et al. [12] uses two ranking criteria as well. It is an elitist algorithm with an archive of constant size, which is chosen to be the population size μ in the experiments at hand. As primary selection criterion, a strength value that gives the number of individuals in the population dominated by the current individual is assigned. Based on these values a raw fitness is computed as the sum of the strength values of every individual that dominates it. Thus, every non-dominated individual's raw fitness equals zero. In a second step, a density estimation is performed based on the euclidean distances between all individuals. The primary fitness value is the raw fitness plus the reciprocal of the sum of the distance to the k -nearest

neighbor [13]². To fill the archive for the next generation, the individuals with the best fitness are copied. In case of individuals with equal fitness, the distance to the k -nearest neighbor for increasing k is used as further criterion. Given $d \geq 3$, these methods require a runtime in $O(d\mu^2)$ per generation [11].

ε -MOEA Laumanns et al. [14] proposed the ε -MOEA to combine the convergence properties of an elitist MOEA like suggested by Rudolph and Agapie [15] with the need to preserve a diverse set of solutions. The objective space is divided into a grid of boxes, whose size can be adjusted by the choice of ε . Dominance is checked according to the boxes where the solutions are positioned. The archive \mathbf{E} holds one solution for each non-dominated box. If the box of a new solution dominates other boxes in the archive, the associated archive members are rejected. In case of two solutions belonging to the same box, Laumanns et al. decline the new solution except it dominates the old one. Later, Deb et al. [6] propose to select the solution, which is closer to the best corner of the box. They also administrate a co-evaluated population \mathbf{P} of constant size. If a new solution is not dominated by any member of the population, it replaces a randomly chosen member favoring dominated solutions. They also suggest a steady-state approach, where the offspring is generated by a parent from \mathbf{P} and a parent from \mathbf{E} . A binary tournament regarding the dominance relation is performed to choose the member of \mathbf{P} for mating. If two non-dominated solutions are chosen, a random decision will be applied. The parent from \mathbf{E} is chosen equiprobable. Because no further diversity measures need to be computed, the runtime of a generation of ε -MOEA is $O(d|\mathbf{E}|)$.

3.1 Experimental Results

The results of the experiments are presented in Tab. 1 and Tab. 2. Like the following tables, these consist of two parts. The left part provides the information which algorithm and how many objectives were used while the results are placed in the right part. The results themselves are split in two parts regarding the concerned problem. Here, the left and the right column of each part yield the most interesting information for investigation, i.e. the mean and the median of the resulting values received by all runs performed. Next to the averaged values, the standard deviation (std.dev.) of the averaged values is stated.

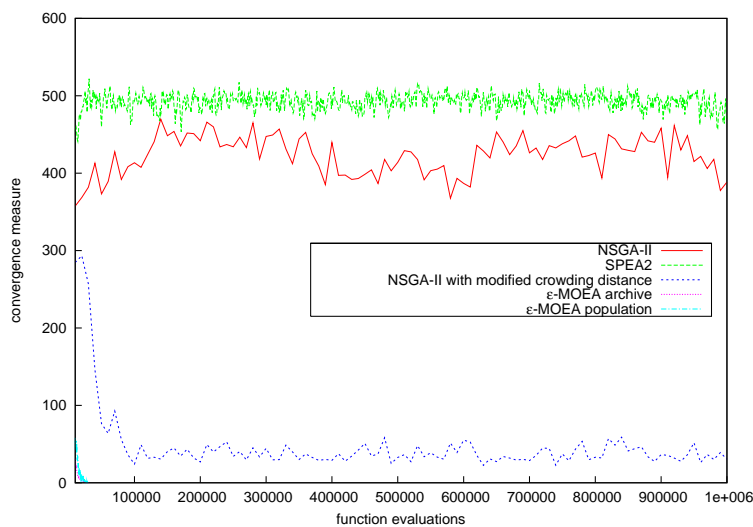
NSGA-II and SPEA2 rapidly decrease in quality with increasing dimension of objective space. If more than four objectives are considered, these algorithms do not converge to the Pareto set as indicated by the high distance values (cf. Tab. 1). With dimension greater than four, no relative hypervolume is measured because no point dominating the reference point is achieved (cf. Tab. 2). Further studies with these algorithms have been performed to exhibit if any convergence occurs with a higher number of function evaluations. As shown in Fig. 2, both algorithms increase the distance to the Pareto front in the first generations because the diversity based selection criteria favor higher distances

² In PISA k is chosen as 1.

Table 1: The convergence measure for the pareto dominance based algorithms.

obj.	algorithm	DTLZ1			DTLZ2		
		mean	std.dev	median	mean	std.dev	median
3	ϵ -MOEA	0.00614	0.00413	0.00484	0.00102	0.00022	0.00105
	NSGA-II	0.06333	0.15581	0.01002	0.01049	0.00162	0.01027
	SPEA2	0.06783	0.16435	0.00792	0.00801	0.00112	0.00806
4	ϵ -MOEA	0.15990	0.34073	0.01990	0.00129	0.00024	0.00126
	NSGA-II	1.70260	1.95260	0.69515	0.08522	0.02580	0.08060
	SPEA2	3.47990	4.78910	1.66910	0.08164	0.01676	0.08901
5	ϵ -MOEA	0.22348	0.41685	0.01941	0.02681	0.00120	0.02670
	NSGA-II	300.416	37.2461	317.506	1.06780	0.14504	1.07770
	SPEA2	358.818	25.0853	366.236	1.30970	0.15758	1.27760
6	ϵ -MOEA	0.97014	1.39920	0.27217	0.00272	0.00067	0.00266
	NSGA-II	393.674	17.6076	388.689	2.15610	0.09584	2.16910
	SPEA2	482.742	13.6757	479.577	2.32000	0.09617	2.36070

between solutions. Special emphasis is given to extremal solutions with values near zero in one or more objectives. These solutions remain non-dominated and the distance cannot be decreased thereafter.

**Fig. 2:** Convergence measure during the optimization run performing the median result on six-objective DTLZ1.

To confirm this assumptions and improve NSGA-II in the many-objective case, a slight modification of crowding distance is studied. Originally, an individual without a neighbor regarding one dimension of the objective space is assigned an infinite crowding distance. Instead of that, a value of zero is used, causing that non-dominated solutions with extremal values are rejected. Although this variant is not able to converge to the Pareto front, an improvement of the average distance within the first 100,000 function evaluations is obvious (Fig. 2). Then, most of the decision variables have reached their optimal value.

Only one or two of them remain in a local optimum. This experiment shows that a diversity measure with emphasis on a spread of the population can misguide the MOEA to deterioration and the loss of promising non-dominated solutions.

Table 2: The relative hypervolume for the pareto dominance based algorithms.

obj.	algorithm	DTLZ1, $r = 0.7^d$			DTLZ2, $r = 1.1^d$		
		mean	std.dev	median	mean	std.dev	median
3	ε -MOEA	0.94560	0.01005	0.94662	0.92858	0.00118	0.92836
	NSGA-II	0.94333	0.11423	0.96923	0.86913	0.00803	0.86918
	SPEA2	0.98010	0.00152	0.98068	0.90760	0.00350	0.90782
4	ε -MOEA	0.85493	0.18655	0.92697	0.87722	0.00186	0.87766
	NSGA-II	0.45730	0.40600	0.46204	0.71644	0.01971	0.71733
	SPEA2	0.62316	0.34319	0.72224	0.78461	0.01258	0.78202
5	ε -MOEA	0.82261	0.16668	0.86933	0.83847	0.00308	0.83809
	NSGA-II	0	0	0	0.11570	0.06842	0.11734
	SPEA2	0	0	0	0.12528	0.06942	0.12864
6	ε -MOEA	0.64563	0.38344	0.81552	0.85332	0.01434	0.85497
	NSGA-II	0	0	0	0	0	0
	SPEA2	0	0	0	0	0	0

The performance of ε -MOEA highly depends on the choice of ε . We choose it such that \mathbf{E} finally contains about 100 solutions³. The ε -MOEA is able to produce optimal solutions within the allowed number of function evaluations for all considered numbers of objectives. This is shown in the lower left part of figure 2. The active dominance-preserving function of the archive, combined with an utopia point distance criterion for non-dominated individuals in the same hyperbox avoids the effects of deterioration and thus ensures convergence even for the co-evolving set \mathbf{P} . Though, the hypergrid guarantees an uniform distribution of individuals, the obtained hypervolume values are only for DTLZ2 competitive with the best considered algorithms. This is due to the trend of the hyperbox method to avoid extremal solutions, as described by Deb et al. [6].

4 Aggregation-based EMOA

Basic aggregation methods are single-objective optimizers, which multiply the objective values with weights and accumulate them to a scalar value. The EMOA considered here, enhance aggregation concepts in order to produce a set of solutions. In contrast to the other EMOA considered, aggregation-based approaches require the a priori definition of relations between objective functions. This results in a certain focus during the optimization.

³ $d=3$, DTLZ1: $\varepsilon = (0.03, 0.03, 0.03)$, DTLZ2: $\varepsilon = (0.058, 0.058, 0.058)$.

$d=4$, DTLZ1: $\varepsilon = (0.047, 0.047, 0.047, 0.047)$, DTLZ2: $\varepsilon = (0.125, 0.125, 0.125, 0.125)$.

$d=5$, DTLZ1: $\varepsilon = (0.057, \dots, 0.057)$, DTLZ2, $\varepsilon = (0.18, \dots, 0.18)$.

$d=6$, DTLZ1: $\varepsilon = (0.066, \dots, 0.066)$, DTLZ2, $\varepsilon = (0.232, \dots, 0.232)$.

MSOPS *Multiple Single Objective Pareto Sampling* (MSOPS) does not feature Pareto methods, but handles all objectives in parallel. The decision maker has to choose T vectors of weights for every objective function to enable an aggregation. Hughes [16] recommends weighted *min-max* (MSOPS 1) and a combination of this approach with *Vector-Angle-Distance-Scaling* (VADS) called *dual optimisation* (MSOPS 2). Depending on the aggregation strategy, one receives a set of T or $2T$ aggregated scores per solution. The scores are held in a score matrix S , where each row belongs to a solution and each column represents an aggregated score. Each column of the matrix S is ranked, giving the best performing population member rank one. The rank values are stored in a matrix R . Each row of R is sorted ascending, allowing in a lexicographical order of the individuals. The runtime is in $O(\mu T d)$ for the computation of the aggregated scores, and in $O(\mu T \log T)$ and $O(T \mu \log \mu)$ respectively to perform the sort of the rows and columns. Thus, the runtime of MSOPS is $O(\mu T (d + \log T + \log \mu))$ per generation.

Obviously, the choice of weight vectors determines the distribution properties of MSOPS. Each weight vector $\mathbf{w} = (w_1, \dots, w_d)$ corresponds to a direction, analytically given by a target vector starting in the origin. The aim of the aggregation methods is to reach the point on the corresponding direction vector which is as close as possible to the origin. To this end, weighted *min-max* focuses on the distance to the origin, while VADS favors solutions whose position vector has a small intersecting angle with the target vector.

Since our comparative study aims at an approximation of the whole Pareto front in order to maximize the covered hypervolume, an appropriate set of weights has to be chosen. In Hughes [3] benchmarking '50 target vectors spread uniformly across the search space' are used. The target vectors $\mathbf{t} = (t_1, \dots, t_d)$ are created by calculating an initial number of steps $s = \lfloor \sqrt[d]{T} \rfloor$ and constructing each possible vector containing multiples of $1/s$ between 0 and 1. Afterward, these target vectors are normalized and doubles are removed. If the number of targets is lower as desired, s is incremented and the procedure is repeated. At the end, a next neighbor technique is used to prune the set of target vectors to the desired size. Because the PISA implementation of MSOPS uses weight vectors, a transformation of the target vectors into weights is necessary. The authors recommend – deviant from Hughes [3] – the following procedure for transformation, that can also be used to transform a set of utopia or reference points into weights and avoids numerically unstable calculations in many cases.

From the aggregation methods can be referred that a weight vector for a specified target fulfills the following $d - 1$ conditions:

$$w_1 \cdot t_1 = w_2 \cdot t_2, \quad w_2 \cdot t_2 = w_3 \cdot t_3, \quad \dots \quad w_{d-1} \cdot t_{d-1} = w_d \cdot t_d$$

The normalizing condition $w_1 + \dots + w_d = 1$ is added in order to obtain a completely defined system of equations. Thus, the components of the corresponding weight vector can be computed as follows:

$$w_i = \frac{\prod_{j \neq i} t_j}{\sum_{k=1}^d \prod_{j \neq k} t_j} (i = 1, \dots, d) \quad (1)$$

To extremal solutions with value 0 in $d - 1$ objectives, a small ε needs to be added to allow the above calculation. Hughes [16] generally recommends to use a number of target vectors that is lower than the population size. Besides, he states that the number of target vectors has to be increased for more objectives. To cover both needs, three different sets of target vectors are used. The first contains 50 vectors, the second 100 vectors, and the third 200 vectors.

RSO A restart strategy of a conventional single-objective evolutionary optimizer is applied as well and abbreviated *RSO (Repeated Single Objective)* according to Hughes [3]. Here, a single-objective run is performed for each of the 100 weight vectors. Thus, the number of function evaluations has to be divided among them, resulting in only 300 evaluations per run. The derandomized mutation operator by Ostermeier et al. [17] is applied in a (1, 10)-evolution strategy. This operator was a first step towards the popular Covariance Matrix Adaptation (CMA) operator by Hansen and Ostermeier [18], which is known to produce good results within limited function evaluations [19]. To handle multiple objectives in a single-objective EA, the weighted *min-max* approach was chosen like in MSOPS.

4.1 Experimental Results

The methods using aggregation show an obvious convergence in all scenarios considered because they benefit from the property of the *min-max* method to minimize all objectives at once. While MSOPS obtains very promising results, RSO does not succeed in reaching the Pareto front. This is due to a too small number of function evaluations per run and the loss of information with every restart. Confirming the observations of Hughes [3], RSO outperforms NSGA-II and SPEA2 in case of five and six objectives.

Almost all variants of MSOPS attain very low average distances indicating that only optimal solutions have been found. Only for five or six objectives, variants using a lower number of target vectors fail to converge to the Pareto front in some of the runs. In the table, this behavior can be inferred from a high standard deviation and high differences between the mean and the median value.

From the obtained hypervolume can be concluded that the distribution properties can be slightly improved by the supporting use of VADS. Hughes assumption that the number of target vectors should be increased if more objectives are concerned is confirmed. For three objectives, the variants of MSOPS using 50 target vectors obtain the maximal hypervolume among the aggregation methods. With increasing objectives, the best values can be obtained with a higher number of target vectors. In general, the results show that the method used to design the target vectors is able to generate well distributed Pareto front approximations. Even for three objectives, NSGA-II and ε -MOEA (DTLZ1), respectively NSGA-II and SPEA2 (DTLZ2) can be outperformed regarding the \mathcal{S} -metric. Note that the given method to generate the target vectors only performs well on continuous Pareto fronts. As observed by Hughes [16], a refinement of the

Table 3: The convergence measure for the aggregation algorithms.

obj.	algorithm	DTLZ1			DTLZ2		
		mean	std.dev	median	mean	std.dev	median
3	MSOPS 1 50	0.00276	0.00235	0.00185	0.00013	0.00014	$9.0 \cdot 10^{-5}$
	MSOPS 1 100	0.00278	0.00241	0.00244	0.00015	0.00010	0.00015
	MSOPS 1 200	0.00234	0.00156	0.00210	0.00080	0.00020	0.00076
	MSOPS 2 50	0.00214	0.00221	0.00161	$9.0 \cdot 10^{-5}$	$5.9 \cdot 10^{-5}$	$8.4 \cdot 10^{-5}$
	MSOPS 2 100	0.00222	0.00172	0.00191	0.00037	0.00013	0.00035
	MSOPS 2 200	0.00128	0.00074	0.00116	0.00168	0.00034	0.00168
	RSO	62.9990	15.2960	59.7140	0.26753	0.04901	0.26776
4	MSOPS 1 50	0.00392	0.00451	0.00269	0.00023	0.00023	0.00012
	MSOPS 1 100	0.00292	0.00252	0.00231	0.00024	0.00039	0.00013
	MSOPS 1 200	0.00365	0.00319	0.00264	0.00072	0.00028	0.00067
	MSOPS 2 50	0.00246	0.00216	0.00182	0.00016	0.00010	0.00012
	MSOPS 2 100	0.00849	0.02369	0.00282	0.00074	0.00024	0.00072
	MSOPS 2 200	0.00439	0.00378	0.00260	0.00203	0.00047	0.00195
	RSO	118.260	33.4420	121.190	0.56473	0.07953	0.57386
5	MSOPS 1 50	0.08016	0.31475	0.00814	0.00059	0.00027	0.00060
	MSOPS 1 100	0.05667	0.23459	0.00337	0.00017	0.00023	$7.1 \cdot 10^{-5}$
	MSOPS 1 200	0.00779	0.00556	0.00651	0.00096	0.00033	0.00092
	MSOPS 2 50	0.13676	0.26271	0.01882	0.00113	0.00038	0.00097
	MSOPS 2 100	0.03308	0.11179	0.00614	0.00138	0.00065	0.00119
	MSOPS 2 200	0.00870	0.01079	0.00535	0.00231	0.00059	0.00233
	RSO	111.960	35.1240	112.140	0.73556	0.15491	0.72211
6	MSOPS 1 50	0.02207	0.06509	0.00604	0.00044	0.00030	0.00044
	MSOPS 1 100	0.00936	0.01579	0.00406	0.00012	$8.7 \cdot 10^{-5}$	$9.7 \cdot 10^{-5}$
	MSOPS 1 200	0.00734	0.00420	0.00712	0.00048	0.00028	0.00039
	MSOPS 2 50	0.27890	0.63926	0.02603	0.00091	0.00058	0.00069
	MSOPS 2 100	0.18106	0.32499	0.02496	0.00190	0.00097	0.00180
	MSOPS 2 200	0.01344	0.01134	0.01026	0.00118	0.00056	0.00116
	RSO	110.910	42.7920	113.600	0.67628	0.13970	0.69903

targets is necessary for more complicated problems. Discontinuous Pareto fronts lead to an approximation of the '*objective front*'[16], i.e. the intersection of the target vectors with the domain of objectives. Thus, the approximation reached with wide spread target vectors can obtain solutions that are not optimal in sense of Pareto optimality. An evaluation of the aggregated values reached by the individuals in the final population is necessary to identify target vectors that support these solutions and accordingly refine the set of target vectors⁴.

⁴ In real-world applications with unknown Pareto fronts, the above approach can be helpful to find discontinuities and other informations about the shape of the Pareto front. But, it has to be kept in mind that a refinement is necessary to find optimal trade-offs.

Table 4: The relative hypervolume of the aggregation algorithms.

obj.	algorithm	DTLZ1, $r = 0.7^d$			DTLZ2, $r = 1.1^d$		
		mean	std.dev	median	mean	std.dev	median
3	MSOPS 1 50	0.97142	0.00127	0.97184	0.89663	0.00717	0.89817
	MSOPS 1 100	0.96484	0.00171	0.96537	0.88344	0.00208	0.88341
	MSOPS 1 200	0.96180	0.00955	0.96625	0.88752	0.02681	0.88490
	MSOPS 2 50	0.97278	0.00111	0.97317	0.89822	0.00054	0.89799
	MSOPS 2 100	0.96719	0.00623	0.96776	0.91774	0.01203	0.92105
	MSOPS 2 200	0.95744	0.00965	0.96020	0.91117	0.00775	0.91253
	RSO	0	0	0	0.67735	0.03730	0.68188
4	MSOPS 1 50	0.96590	0.00107	0.96623	0.84765	0.01438	0.85238
	MSOPS 1 100	0.94724	0.00573	0.94887	0.72575	0.03761	0.73177
	MSOPS 1 200	0.94764	0.01187	0.94968	0.81489	0.03289	0.82292
	MSOPS 2 50	0.96726	0.00062	0.96730	0.85284	0.00049	0.85273
	MSOPS 2 100	0.96908	0.00258	0.96955	0.86206	0.00609	0.86445
	MSOPS 2 200	0.95605	0.00561	0.95742	0.85938	0.01289	0.86395
	RSO	0	0	0	0.39649	0.02363	0.39435
5	MSOPS 1 50	0.97740	0.00614	0.97956	0.78971	0.05479	0.80668
	MSOPS 1 100	0.96312	0.01848	0.97160	0.48432	0.32422	0.72034
	MSOPS 1 200	0.97749	0.00584	0.97694	0.82177	0.01404	0.82490
	MSOPS 2 50	0.93235	0.16743	0.98387	0.81037	0.00915	0.80863
	MSOPS 2 100	0.98743	0.00119	0.98762	0.86497	0.00606	0.86565
	MSOPS 2 200	0.97966	0.00296	0.97987	0.84002	0.01467	0.84609
	RSO	0	0	0	0.04960	0.03184	0.05873
6	MSOPS 1 50	0.98688	0.00469	0.98770	0.70669	0.18905	0.76654
	MSOPS 1 100	0.95343	0.02840	0.96312	0.63285	0.13323	0.68515
	MSOPS 1 200	0.99046	0.00169	0.99056	0.81435	0.03071	0.81964
	MSOPS 2 50	0.92549	0.18116	0.99355	0.84659	0.00215	0.84627
	MSOPS 2 100	0.96533	0.06398	0.98592	0.79881	0.01918	0.79436
	MSOPS 2 200	0.99122	0.00160	0.99154	0.81208	0.11049	0.83925
	RSO	0	0	0	0.16333	0.03440	0.15121

5 Indicator-based EMOA

The term *indicator-based EA (IBEA)* was introduced by Zitzler and Künzli [20] for EMOA guided by a general preference information. The EMOA's selection operator uses a preference function (indicator) as a single-objective substitute for the d -dimensional objective function. In contrast to the aggregation methods, this preference information describes a general aim. No specification of weights or targets is needed. As already stated in Sec. 1, classic EMOA use two ranking criteria: one regarding the dominance relation and the other for distribution aspects. Here, a single indicator is used to optimize a desired property of the approximation set.

IBEA In Zitzler's and Künzli's [20] IBEA framework, binary performance metrics that map an ordered pair of individuals to a scalar value are suggested as

indicator functions. Each individual is compared with all others, thus $O(\mu^2)$ indicator values must be calculated. A suitable indicator has to be *dominance preserving* [20], which sloppily means that the indicator must not evaluate a vector better than another that dominates it. Two efficiently computable indicators have been suggested in [20]. The additive ϵ -indicator subsumes the translations in each dimension of objective space that are necessary to create a weakly dominated solution. The hypervolume indicator measures the dominated hypervolume that is only dominated by one vector and not by the other. Both indicators can be computed in linear time regarding the dimension of the objective space. This results in a runtime $O(\mu^2 d)$ per generation. For both indicators, negative values mean that the first individual of the argument pair dominates the other. For each individual, its indicator values are charged in a sum of an exponential function to get a fitness value

$$F(\mathbf{x}^{(1)}) = \sum_{\mathbf{x}^{(2)} \in P \setminus \{\mathbf{x}^{(1)}\}} -e^{-I(\mathbf{x}^{(2)}, \mathbf{x}^{(1)})/\kappa}. \quad (2)$$

A positive scaling constant is invoked, which is chosen as $\kappa = 0.05$ as recommended in [20] for the applied adaptive variant of IBEA, which works on normalized indicator values. For dominance preserving indicators holds that the fitness value of a vector is worse than the fitness value of a vector that dominates it.

SMS-EMOA The *S-metric Selection-EMOA* (SMS-EMOA) by Emmerich et al. [21, 10] aims at maximizing the \mathcal{S} -metric value of the population. This optimization aim rewards progression toward the Pareto front as well as a good distribution of individuals. The maximal \mathcal{S} -metric value is reached by the Pareto front. Thus, optimizing the \mathcal{S} -metric value is a very general purpose. Contrary to most other EMOA, a steady-state selection scheme and an equiprobable mating selection are applied. SMS-EMOA invokes the non-dominated sorting procedure as primary selection criterion and the selection occurs among the members of the worst ranked front. The secondary criterion applied to the last front is the hypervolume contribution, which is defined as the exclusively dominated hypervolume of an objective vector. The individual with the lowest hypervolume contribution is discarded. Experiments show that the non-dominated sorting can alternatively be omitted, which hardly influences the algorithms performance. The runtime of a generation of SMS-EMOA is $O(\mu^{d/2+1})$ as described by Beume and Rudolph [22].

5.1 Experimental Results

As can be inferred from the convergence measure, both IBEA variants reach the Pareto front of DTLZ2. On DTLZ1, only IBEA $_{\epsilon+}$ converges towards the Pareto front for all dimensions. IBEA $_{HD}$ reaches a very good distance value on DTLZ1 with three dimensions but fails in case of more objectives. This is due to the

Table 5: The convergence measure of the indicator-based EMOA.

obj.	algorithm	DTLZ1			DTLZ2		
		mean	std.dev.	median	mean	std.dev.	median
3	IBEA $_{\epsilon+}$	0.04399	0.17481	0.00057	0.00015	$5.0 \cdot 10^{-5}$	0.00014
	IBEA $_{HD}$	0.00137	0.00337	0.00029	$1.3 \cdot 10^{-5}$	$5.3 \cdot 10^{-6}$	$1.2 \cdot 10^{-5}$
	SMS-EMOA	0.00110	0.00148	0.00039	$3.4 \cdot 10^{-6}$	$1.2 \cdot 10^{-6}$	$2.8 \cdot 10^{-6}$
4	IBEA $_{\epsilon+}$	0.01790	0.02940	0.00096	0.00071	0.00012	0.00069
	IBEA $_{HD}$	76.1230	119.550	0.00136	$4.5 \cdot 10^{-5}$	$1.3 \cdot 10^{-5}$	$4.2 \cdot 10^{-5}$
	SMS-EMOA	0.00193	0.00176	0.00100	$1.4 \cdot 10^{-5}$	$5.0 \cdot 10^{-6}$	$1.2 \cdot 10^{-5}$
5	IBEA $_{\epsilon+}$	0.02056	0.06678	0.00129	0.00115	0.00019	0.00112
	IBEA $_{HD}$	151.310	131.820	215.000	0.00013	0.00014	0.00010
	SMS-EMOA	0.00333	0.00215	0.00351	$3.7 \cdot 10^{-5}$	$9.2 \cdot 10^{-6}$	$3.8 \cdot 10^{-5}$
6	IBEA $_{\epsilon+}$	0.00467	0.00450	0.00256	0.00187	0.00031	0.00184
	IBEA $_{HD}$	82.1580	116.410	0.00182	0.00015	$5.6 \cdot 10^{-5}$	0.00014
	SMS-EMOA	0.10278	0.22310	0.00444	$5.4 \cdot 10^{-5}$	$1.1 \cdot 10^{-5}$	$5.2 \cdot 10^{-5}$

normalization of objective values to $[0, 1]$, tending the hypervolume indicator to favor extremal solutions, which hinder the progression.

Surprisingly, the IBEA $_{\epsilon+}$ using the additive ϵ -indicator reaches better \mathcal{S} -metric values than the IBEA $_{HD}$ invoking the hypervolume indicator. The consideration of translation lengths in the additive ϵ -indicator causes a good distribution of solutions. Contrary, the approximation of the hypervolume contribution through the binary hypervolume indicator tends to spiral downward with increasing dimension of objective space. Both adaptive IBEA fail to produce a good distribution on DTLZ1, which we ascribe to the high-scaled co-domain and the resulting difficulties in the scaling of the fitness values.

Table 6: The relative hypervolume of the indicator-based algorithms.

obj.	algorithm	DTLZ1, $\mathbf{r} = 0.7^d$			DTLZ2, $\mathbf{r} = 1.1^d$		
		mean	std.dev.	median	mean	std.dev.	median
3	IBEA $_{\epsilon+}$	0.77693	0.03182	0.78033	0.92991	0.00075	0.93002
	IBEA $_{HD}$	0.73929	0.03144	0.74208	0.92023	0.00071	0.92008
	SMS-EMOA	0.98352	0.00071	0.98387	0.93870	$6.3 \cdot 10^{-5}$	0.93873
4	IBEA $_{\epsilon+}$	0.82920	0.02445	0.83425	0.89477	0.00059	0.89484
	IBEA $_{HD}$	0.51417	0.35620	0.70647	0.88633	0.00090	0.88619
	SMS-EMOA	0.97612	0.00034	0.97627	0.90370	$6.4 \cdot 10^{-5}$	0.90368
5	IBEA $_{\epsilon+}$	0.87018	0.02777	0.86961	0.88571	0.00097	0.88584
	IBEA $_{HD}$	0.26292	0.33673	0	0.88250	0.00122	0.88259
	SMS-EMOA	0.99182	0.00019	0.99182	0.89619	$9.5 \cdot 10^{-5}$	0.89624
6	IBEA $_{\epsilon+}$	0.89146	0.03569	0.90029	0.89283	0.00130	0.89322
	IBEA $_{HD}$	0.40153	0.30853	0.53634	0.88431	0.02231	0.89124
	SMS-EMOA	0.96688	0.06741	0.99698	0.90483	0.00014	0.90481

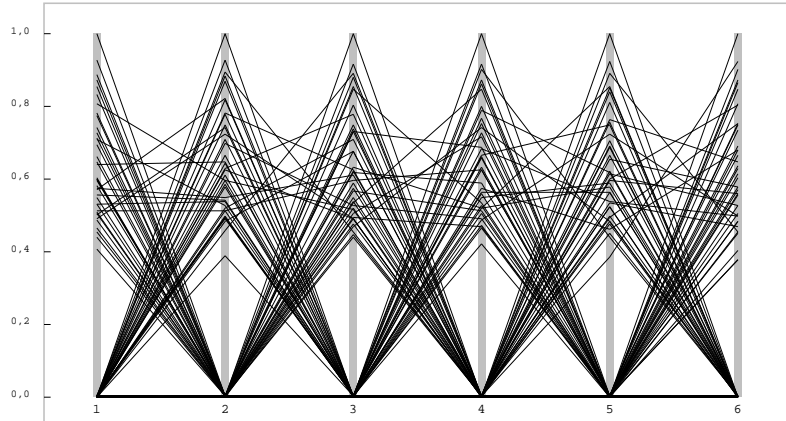


Fig. 3: Results of one run of SMS-EMOA on six-objective DTLZ2. In the parallel plot, each column corresponds to one objective.

SMS-EMOA reaches the best \mathcal{S} -metric values of all considered algorithms. The distance values are very good as well and all runs except one reached the Pareto front. This run on six-objective DTLZ1 stagnated since one decision variable—which defines the distance—remains static at a non-optimal value due to an unusual loss of diversity in decision space in the beginning of the optimization process. Since the selector modules in PISA only decide regarding the objective values, this effect cannot be blamed to the selection properties of SMS-EMOA. Figure 3 exemplarily pictures the distribution of an usual six-objective result set of SMS-EMOA in a parallel plot. Every objective is covered and the structure of the set is almost symmetric, indicating a uniformly spread distribution of solutions over the whole Pareto front.

6 Summary and Outlook

The bad performance of early Pareto-based methods like NSGA-II and SPEA2 observed by Hughes [3] and Purshouse and Fleming [2] is confirmed. They show a rapid degradation with increasing number of objectives. Some additional studies show that they do not converge to the Pareto front at all and stagnate far away from it. The performance of ε -MOEA refutes the hypothesis of Hughes that a Pareto-based approach cannot succeed on many-objective problem instances. Instead, favoring extremal solutions has been shown to hinder the progression in many-objective spaces, which is also obviously for IBEA.

It is shown that more recent EMOA using indicators, which feature more than just distribution aspects, perform very well in many-objective optimization. Especially, SMS-EMOA, which optimizes the population's dominated hypervolume, outperforms the other algorithms on all considered test functions. Moreover, an aggregation-based EMOA, namely MSOPS, performs well with respect to convergence aspects. A sophisticated scheme for the generation of weight vectors

is introduced and also produces well distributed solution sets. In comparison to the simple restart strategy RSO, MSOPS benefits from structural equalities of good solutions by optimizing all weight vectors in parallel.

Future research will deepen the insights in the behavior of indicator-based algorithms in particular. Theoretical statements are aspired for the convergence of the MOEA showing promising results in this study. Statistically guided parameter studies should be performed to obtain suitable parametrizations for many-objective problems. Especially, the size of the population and the offspring are to be studied. Furthermore, relations between the Pareto front and the Pareto set are studied all together resulting in new optimization techniques. These feature good convergence and distribution properties in objective space as well as in decision space.

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References

1. Farina, M., Amato, P.: On the optimal solution definition for many-criteria optimization problems. In Keller, J., Nasraoui, O., eds.: Proc. of the NAFIPS-FLINT Int'l Conf. 2002, IEEE Press, Piscataway NJ (2002) 233–238
2. Purshouse, R.C., Fleming, P.J.: Evolutionary Multi-Objective Optimisation: An Exploratory Analysis. In: Proc. of the 2003 Congress on Evolutionary Computation (CEC'2003). Volume 3., Canberra, Australia, IEEE Press (2003) 2066–2073
3. Hughes, E.J.: Evolutionary Many-Objective Optimisation: Many Once or One Many? In: Evolutionary Computation 'Congress (CEC'05), Edinburgh, UK. Volume 1., IEEE Press, Piscataway NJ (2005) 222–227
4. Deb, K., Pratap, A., Agarwal, S., Meyarivan, T.: A Fast and Elitist Multiobjective Genetic Algorithm: NSGA-II. *IEEE Transactions on Evolutionary Computation* **6**(2) (2002) 182–197
5. Bleuler, S., Laumanns, M., Thiele, L., Zitzler, E.: PISA — a platform and programming language independent interface for search algorithms. In Fonseca, C.M., et al., eds.: Evolutionary Multi-Criterion Optimization, 2nd Int'l Conf. (EMO 2003). LNCS 2632, Springer, Berlin (2003) 494 – 508
6. Deb, K., Mohan, M., Mishra, S.: A Fast Multi-objective Evolutionary Algorithm for Finding Well-Spread Pareto-Optimal Solutions. KanGAL report 2003002, Indian Institute of Technology, Kanpur, India (2003)
7. Deb, K.: Multi-Objective Optimization using Evolutionary Algorithms. Wiley, Chichester, UK (2001)
8. Deb, K., Thiele, L., Laumanns, M., Zitzler, E.: Scalable Multi-objective Optimization Test Problems. In: Proc. of the 2002 Congress on Evolutionary Computation (CEC 2002). Volume 1., IEEE Press, Piscataway NJ (2002) 825–830

9. Zitzler, E., Thiele, L.: Multiobjective Optimization Using Evolutionary Algorithms—A Comparative Case Study. In Eiben, A.E., ed.: *Parallel Problem Solving from Nature V*. LNCS 1498, Springer, Berlin (1998) 292–301
10. Naujoks, B., Beume, N., Emmerich, M.: Multi-objective optimisation using S-metric selection: Application to three-dimensional solution spaces. In: *Evolutionary Computation Congress (CEC'05)*, Edinburgh, UK. Volume 2., Piscataway NJ, IEEE Press (2005) 1282–1289
11. Jensen, M.T.: Reducing the run-time complexity of multiobjective EAs: The NSGA-II and other algorithms. *IEEE Transactions On Evolutionary Computation* **7**(5) (2003) 503–515
12. Zitzler, E., Laumanns, M., Thiele, L.: SPEA2: Improving the Strength Pareto Evolutionary Algorithm. Technical Report 103, Computer Engineering and Networks Laboratory (TIK), Swiss Federal Institute of Technology (ETH) Zürich, Switzerland (2001)
13. Silverman, B.W.: *Density estimation for statistics and data analysis*. Chapman and Hall, London (1986)
14. Laumanns, M., Thiele, L., Deb, K., Zitzler, E.: Combining convergence and diversity in evolutionary multi-objective optimization. *Evolutionary Computation* **10**(3) (2002) 263–282
15. Rudolph, G., Agapie, A.: Convergence properties of some multi-objective evolutionary algorithms. In Zalzalá, A., Eberhart, R., eds.: *Congress on Evolutionary Computation (CEC2000)*. Volume 2., Piscataway NJ, IEEE Press (2000) 1010–1016
16. Hughes, E.J.: Multiple Single Objective Pareto Sampling. In: *Congress on Evolutionary Computation (CEC'03)*, IEEE Press, Piscataway NJ (2003)
17. Ostermeier, A., Gawelczyk, A., Hansen, N.: Step-size adaptation based on non-local use of selection information. In Davidor, Y., et al., eds.: *Parallel Problem Solving from Nature (PPSN 1994)*. LNCS 866, Springer, Berlin (1994) 189–198
18. Hansen, N., Ostermeier, A.: Completely Derandomized Self-Adaptation in Evolution Strategies. *IEEE Computational Intelligence Magazine* **9**(2) (2001) 159–195
19. Naujoks, B., Willmes, L., Haase, W., Bäck, T., Schütz, M.: Multi-point airfoil optimization using evolution strategies. In: *European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS'00)* (CD-Rom and Book of Abstracts), Center for Numerical Methods in Engineering (CIMNE), Barcelona, Spain (2000) 948
20. Zitzler, E., Künzli, S.: Indicator-based selection in multiobjective search. In Yao, X., et al., eds.: *8th Int'l Conf. on Parallel Problem Solving from Nature (PPSN VIII)*, UK, Springer (2004) 832–842
21. Emmerich, M., Beume, N., Naujoks, B.: An EMO algorithm using the hypervolume measure as selection criterion. In Coello, C.A.C., et al., eds.: *Evolutionary Multi-Criterion Optimization: 3rd Int'l Conf. (EMO 2005)*, Springer, Berlin (2005) 62–76
22. Beume, N., Rudolph, G.: Faster S-Metric Calculation by Considering Dominated Hypervolume as Klee's Measure Problem. In: *International Conference on Computational Intelligence (CI 2006)*. (2006) (in print).