

Multiobjective Optimization on a Limited Budget of Evaluations Using Model-Assisted \mathcal{S} -Metric Selection

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Abstract. Real-world optimization problems often require the consideration of multiple contradicting objectives. These multiobjective problems are even more challenging when facing a limited budget of evaluations due to expensive experiments or simulations. In these cases, a specific class of multiobjective optimization algorithms (MOOA) has to be applied. This paper provides a review of contemporary multiobjective approaches based on the singleobjective meta-model-assisted 'Efficient Global Optimization' (EGO) procedure and describes their main concepts. Additionally, a new EGO-based MOOA is introduced, which utilizes the \mathcal{S} -metric or hypervolume contribution to decide which solution is evaluated next. A benchmark on recently proposed test functions is performed allowing a budget of 130 evaluations. The results point out that the maximization of the hypervolume contribution within a real multiobjective optimization is superior to straightforward adaptations of EGO making our new approach capable of approximating the Pareto front of common problems within the allowed budget of evaluations.

Keywords: Efficient Global Optimization, \mathcal{S} -metric, Design and Analysis of Computer Experiments, Multiobjective Optimization, Real-World Problems.

1 Introduction

Modern industrial processes become more and more complex. They consist of multiple stages, each configurable by several parameters. Thus, the determination of adequate parameter settings is a recurring task. It is especially challenging in case of expensive experiments or numerical computer simulations, where every realization involves high personnel or material expenses or requires immense calculation time. In these cases it is essential to obtain the desired outcome within a small number of evaluations.

This task becomes even more challenging in case of multiple, potentially contradicting objectives, such as product quality and cost. For these multiobjective optimization problems (MOP), the target is to find Pareto-optimal solutions, i.e., solutions where an objective cannot be improved without deteriorating at least one other. The challenges involved in solving a MOP are to converge towards Pareto-optimal solutions and generate a well distributed solution set, which covers the entire Pareto front [1].

In order to apply MOOA to most real-world problems, these challenges have to be mastered efficiently within a minimum number of objective evaluations [2,3]. Thus, in this paper we present a review of recent MOOA for these problems and introduce a new enhanced approach called '*S*-Metric-Selection-based Efficient Global Optimization' (SMS-EGO). In particular, two state-of-the-art approaches – Knowles' ParEGO [2] and a MOOA presented by Jeong and Obayashi [4] – are reviewed and compared to SMS-EGO. All these methods compensate the limited amount of information by using approximate meta-models of the objective functions, on which a comprehensive optimization is performed to determine the next solution for evaluation on the actual problem. Since the actual objective evaluations are expensive, only a few iterations of the MOOA can be performed. Thus, the runtime of the optimization approach itself is not a critical issue. The restriction to a limited amount of evaluations is motivation as well as prerequisite.

In the next section, the state of the art in meta-model-assisted multiobjective optimization is presented. The EGO approach, which represents one of the most famous meta-model-based singleobjective optimization algorithms, is described in section 3. This approach allows solving common singleobjective problems with up to six dimensions on a budget of about 100 evaluations [5]. Subsequently, recent concepts to transfer EGO to multiple objectives are presented, and the new SMS-EGO is introduced. The implementation of the evaluated algorithms, the benchmark test functions, which are used to analyze whether the performance of EGO can be transferred to MOP, as well as the experimental results are described in section 4. Finally, the findings are summarized in section 5.

2 State-of-the-Art

A common approach to solve optimization tasks in case of expensive evaluations is to introduce an intermediate modeling step [6]. In this study, we focus on 'Design and Analysis of Computer Experiments' (DACE) [7]. DACE is a famous meta-modeling approach, which utilizes the assumption of close solutions being more likely to have similar objective values. This approach is widely accepted as a meta-model for deterministic non-linear functions. Furthermore, a recent study [3] supports its application also to problems with noisy evaluations. In the following we denote these kinds of meta-models as DACE models or DACE approximation.

Most papers on DACE-model-assisted MOOA are purely application oriented [8,9]. These algorithms simply apply the approximation as a surrogate function to reduce expensive evaluations. No comparable benchmark results are available. Furthermore, some MOOA additionally use the uncertainty of predictions to balance between local and global search. Emmerich et al. [10,11,12] use local DACE models to determine lower and upper confidence bounds for a prescreening of solutions within classical multiobjective evolutionary algorithms (MOEA, EMOA), such as NSGA-II, ε -MOEA, and SMS-EMOA. They report successful results on test functions and real-world problems. However, the confidence bounds are only used to evaluate solutions which are generated within the evolution. No criterion for a specific optimization has been developed.

Recent approaches [2,4,13] transfer concepts of the popular EGO approach to multiple objectives and are described and reviewed in the next sections.

3 Efficient Global Optimization

The EGO approach by Jones et al. [5] is the most famous DACE-model-based optimization algorithm. The prediction of DACE models is based on the n already evaluated solutions $\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(n)}$ by modeling the corresponding error $\epsilon(\mathbf{x})$ to a constant regression model $y(\mathbf{x}) = \mu + \epsilon(\mathbf{x})$. In this μ denotes the mean of the observations and $\epsilon(\mathbf{x})$ is assumed to have a mean of zero and covariance $Cov(\epsilon(\mathbf{x}), \epsilon(\mathbf{x}^{(j)})) = \sigma^2 R$ between $\epsilon(\mathbf{x})$ and each observed error $\epsilon(\mathbf{x}^{(j)})$ according to the measured process variance σ^2 and the correlation model $R(\mathbf{x}, \mathbf{x}^{(j)}, \theta, \mathbf{p}) = \prod_{i=1}^d \exp(-\theta_i |x_i - x_i^{(j)}|^{p_i})$, $j = 1, \dots, n$, with d being the dimension in decision space. The modeling parameter $p_i \in]0, 2]$ controls the smoothness of the approximated function, and the parameter $\theta_i > 0$ specifies the activity in dimension i . Both are determined via maximum likelihood estimation.

A key feature of DACE models is the approximation of the corresponding uncertainty of a prediction. Using this information, the 'Expected Improvement' (EI) measures the expected value of improvement compared to the currently found minimum f_{min} . It can be calculated based on the predicted function value \hat{y} and standard deviation \hat{s}

$$E[I(x)] = (f_{min} - \hat{y})\Phi(u) + \hat{s}\phi(u), \quad u = \frac{f_{min} - \hat{y}}{\hat{s}}, \quad (1)$$

where Φ and ϕ denote the normal cumulative distribution function and the normal probability distribution function, respectively. In EGO the maximization of the EI provides the 'infill sampling criterion' [14] to determine the next point for evaluation. Due to the unknown correlation parameters and the resultant undervaluation of \hat{s} , this approach may lead to an undesired local search. However, approaches have been developed to overcome this drawback [14,15].

3.1 Adaptations of EGO for Multiobjective Problems

In case of m concurrent objectives, a separate model can be built for each objective dimension. Thereby, vectors of predicted values and estimated uncertainties are available. The calculation of the EI with respect to multiple objectives has been formerly derived by Keane [13]. He avoids the problem of selecting an appropriate reference vector \mathbf{f}_{min} (cf. eq. 1) by computing the probability of augmenting the current Pareto front or dominating at least one of its solutions. Afterwards, the centroid of the distribution of the corresponding probability density can be used as expected solution to calculate an indicator of improvement to the current Pareto front. For $m > 2$, both tasks incorporate a numerically demanding partitioning of the objective space, for which no free implementations are available. Thus, this approach could not be benchmarked within our study. Additionally, two straightforward solutions to this problem have been published, which are described in the following subsections.

Multiobjective EI Optimization. Jeong and Obayashi [4] present an approach which directly uses the EI in each objective separately as fitness vector in a multiobjective

optimization. For each objective they generate a DACE model and determine the best solution found at that time. Subsequently, the EI of a solution can be calculated for an optimization based on MOEA. Since MOEA usually obtain large sets of solutions, a small, yet representative sample of the population has to be obtained. To accomplish this, Jeong and Obayashi choose the m solutions having the highest EI values on each separate DACE model. Additionally, they keep the solution located closest to the center of the area, which is spanned by the final MOEA population in objective space.

Multiple Singleobjective EI Sampling. ParEGO [2] developed by Knowles reverses the processing steps of model building and objective integration. It obviates the necessity of considering a multiobjective EI by first reducing the MOP to a singleobjective problem via an augmented Tchebycheff aggregation. In order to find solutions covering the whole Pareto front, the corresponding weight vector is randomly changed per iteration. The possible weight vectors are a priori calculated and evenly distributed. After combining the objectives, the scheme of EGO can be applied accordingly. Knowles seems to be the only author, who provides comparative results on established test problems with respect to a limited amount of evaluations [2,16]. He successfully compared ParEGO with random search, NSGA-II [17] as well as a binary-search-tree-based low-budget variant of MSOPS [16]. Nevertheless, a comparison to algorithms, which also use DACE meta-models, has not been performed.

\mathcal{S} -Metric Selection-based Efficient Global Optimization (SMS-EGO). The fundamental target of any MOEA consists in the improvement of the internal Pareto front approximation. Emmerich et al. [12] provide techniques to use common MOEA selection principles based on vectors of predicted values $\hat{\mathbf{y}}$ and estimated uncertainties $\hat{\mathbf{s}}$. They report best results using the lower confidence bound (LCB) $\hat{\mathbf{y}}_{pot} = \hat{\mathbf{y}} - \alpha \hat{\mathbf{s}}$ for a given confidence level $p_\alpha = (1 - 2\Phi(\alpha))^m$, which follows the non-error principle [10] to avoid the non-consideration of potentially promising solutions.

In our SMS-EGO approach, the idea of Emmerich et al. [11] to calculate the \mathcal{S} -metric [18] or hypervolume contribution of $\hat{\mathbf{y}}_{pot}$ to the current Pareto front approximation is extended to an independent infill criterion. The \mathcal{S} -metric contribution is chosen since it requires no normalization of the objective space [19] and holds some desired theoretical properties [20]. Wagner et al. [21] showed that a selection routine based on this contribution is superior to popular MOEA and also scales well with the number of objectives. As aforementioned, the problem of its computational complexity can be disregarded for the class of problems focused on.

Due to the use of the LCB, potential solutions can be predicted slightly beyond the real objective space. In order to tackle this problem as well as to support a good distribution, additive ε -dominance [20] is applied. The assignment of the vector ε is managed by introducing an adaptive scheme, which aims on a maximum number of individuals in the Pareto front approximation $\varepsilon = \frac{\Delta\Lambda}{|\Lambda|} + c \cdot n_{left}$, $\Delta\Lambda = \max(\Lambda) - \min(\Lambda)$, where Λ refers to the current Pareto front approximation, n_{left} denotes the number of remaining evaluations, and $c = 1 - 1/(2^m)$ is a correction factor, which constitutes the idealized probability for a remaining solution of being non-dominated [21].

In the calculation of the internal fitness value, three cases are considered. In the first case of a non- ε -dominated solution, its contribution to the \mathcal{S} -metric is calculated by

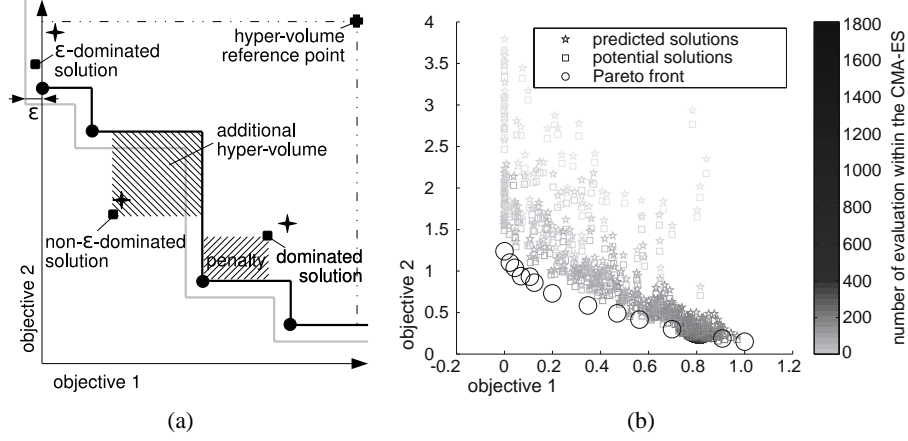


Fig. 1. (a) Graphical explanation of the evaluation of solutions within SMS-EGO. (b) An exemplary run of the model-based internal optimization on the ZDT1 test function. The grayscales express the sequence of evaluations performed by the CMA-ES. Consequently, a potential solution filling the gap in the Pareto front around $(0.8, 0.2)^T$ has been found.

$f = S(\Lambda) - S(\hat{\mathbf{y}}_{pot} \cap \Lambda)$. The reference point needed for this calculation is defined by $\max(\Lambda) + \mathbf{1}$ according to Emmerich et al. [22]. Second, in the case of a dominated solution, a penalty p is added for each dominating point. To keep the penalty close to the S -metric, the differences in each of the m objective dimensions are multiplied. Additionally, a slight transformation is performed to assure that a positive penalty is assigned to weakly dominated solutions

$$p = \sum_{\mathbf{y}^{(i)} \in \Lambda} \begin{cases} -1 + \prod_{j=1}^m \left(1 + (\hat{y}_{pot,j} - y_j^{(i)})\right) & \left| \mathbf{y}^{(i)} \preceq \hat{\mathbf{y}}_{pot} \right. \\ 0 & \text{otherwise} \end{cases} . \quad (2)$$

In the third case of ε -dominated solutions, which are not dominated in the strict sense, the penalty is limited to the objectives that are inferior with respect to the considered Pareto front solution.

All three cases are visualized in Fig. 1 for $m = 2$. The preferred values of this fitness function are negative since new, non-dominated solutions increase the hypervolume of the current Pareto front approximation. In areas of dominated solutions, the search is guided towards non-dominated solutions by means of the penalty term. This measure can be minimized by any global singleobjective optimizer. Corresponding to the EGO procedure, only the solution achieving the minimum of this criterion is selected to be evaluated on the actual problem. Afterwards, the models are updated based on the new observation in order to utilize as much information as possible.

4 Experiments

In this section a comprehensive analysis of the results, which can be achieved on a budget of 130 function evaluations, is provided. To accomplish this, the approaches of

Jeong and Obayashi [4], Knowles' ParEGO [2], and the newly proposed SMS-EGO are benchmarked on established test functions.

Pre-experimental planning: Based on recent suggestions for performance assessment [23], five test functions are selected. More precisely, R_ZDT1 (biobjective, unimodal), R_ZDT4 (biobjective, multimodal), and two R_DTLZ2 variants with three and five objectives (scalability) [24] are chosen. The decision space dimension d is decreased to six in order to facilitate the modeling and to accord with typical numbers of process parameters in real-world processes [3]. Furthermore, the domain of R_ZDT4 has been reduced to three variables and $x_2, x_3 \in [-1, 1]$ to obtain a manageable number of only 20 local optima. This relaxed version is denoted as R_ZDT4_{relax}. Additionally, the OKA2 [25] test function is considered since it provides a challenging Pareto set in terms of shape and distribution.

Setup: All algorithms are implemented in MATLAB®. As suggested by Knowles, they start with an initial sampling of $n_{init} = 11d - 1$ solutions based on a Latin hypercube design (LHD) within the given box constraints [2]. This kind of random design is appropriate for real-world applications since in most cases the interesting parameter region is identified in a screening and then sampled by some kind of space-filling design. Furthermore, LHD have been proven to be suited for the generation of DACE models [5,7]. The design is evaluated, and the parameters of the DACE models are calculated by maximum likelihood estimation using Hansen's CMA-ES [26] implementation¹. Whenever the CMA-ES is applied, the default values are chosen for all parameters, and three stopping criteria, i.e., a maximum number of $4000d$ evaluations and the convergence of the population in the objective or decision space, are set up. For each test function, an amount of 130 evaluations on the actual test function is allowed. To speed up the Pareto front calculation, external C-code programed by Yi Cao is applied².

Jeong's approach is implemented using code of NSGA-II³ for the internal multiobjective EI optimization. According to Jeong's suggestions, the population size and the number of generations are set to 512 and 100, respectively [4]. The center solution is determined as minimizer of the uniformly weighted augmented Tchebycheff aggregation of the normalized Pareto front solutions. Also in ParEGO, the augmented Tchebycheff aggregation is implemented according to Knowles using $\rho = 0.05$ and normalized objective values [2]. Within SMS-EGO the \mathcal{S} -metric calculation is performed by a C implementation of Fonseca et al. [27]. The factor of the estimated uncertainty is set to $\alpha = \Phi^{-1}(0.5 + \frac{1}{2^m})$. The infill criteria of ParEGO and SMS-EGO are maximized using the CMA-ES.

The PISA test environment is applied for the evaluation of the results. As performance measures, the unary hypervolume indicator [18], Hansen and Jaszkiewicz's R2 indicator [28], and the unary epsilon indicator [20] are used. These indicators are suggested for multiobjective performance assessment and evaluate both, convergence and distribution [20]. Additionally, the mean distance of the approximated Pareto front to the real one is calculated analytically on R_DTLZ2 to allow the separated consideration of the convergence. For each algorithm and each test function, five runs are performed.

¹ http://www.bionik.tu-berlin.de/user/niko/cmaes_inmatlab.html

² <http://www.mathworks.com/matlabcentral/fileexchange/loadFile.do?objectId=17251>

³ <http://www.mathworks.com/matlabcentral/fileexchange/loadFile.do?objectId=10429>

Table 1. The table shows the median and worst-case results of the hypervolume, R_2, and ε -indicator on OKA2, R_ZDT1, R_ZDT4_{relax} and R_DTLZ2 (with three and five objectives). The smallest and highest value in each group are printed in bold and italics, respectively. The letters in brackets indicate whether the difference of the median value is statistically significant compared to Jeong (J), ParEGO (P), and SMS-EGO (S) based on a one-sided Kruskal Wallis test ($p < 0.01$).

test function m / d	indicator	algorithm					
		Jeong		ParEGO		SMS-EGO	
		median	max	median	max	median	max
OKA2 2 / 3	S -metric	<i>3.41e-1</i> (-,-)	<i>4.01e-1</i>	2.47e-1 (-,-)	3.35e-1	1.40e-1 (-,-)	1.42e-1
	R_2	8.94e-2 (-,S)	1.37e-1	2.42e-2 (J,S)	7.00e-2	<i>1.66e-1</i> (-,-)	<i>1.67e-1</i>
	ε	3.48e-1 (-,S)	4.07e-1	2.87e-1 (J,S)	3.59e-1	<i>4.96e-1</i> (-,-)	<i>4.98e-1</i>
R_ZDT1 2 / 6	S -metric	<i>2.60e-1</i> (-,-)	<i>2.75e-1</i>	1.21e-1 (J,-)	1.55e-1	2.38e-2 (J,P)	7.03e-2
	R_2	3.48e-3 (-,-)	5.82e-3	9.22e-3 (-,-)	1.50e-2	7.30e-3 (-,-)	2.74e-2
	ε	<i>3.23e-1</i> (-,-)	<i>3.60e-1</i>	1.49e-1 (J,-)	1.59e-1	4.00e-2 (J,P)	7.34e-2
R_ZDT4 _{relax} 2 / 3	S -metric	<i>2.27e-1</i> (-,-)	<i>3.04e-1</i>	3.19e-1 (-,-)	3.68e-1	7.58e-2 (J,P)	1.16e-1
	R_2	2.22e-2 (-,-)	4.42e-2	<i>4.87e-2</i> (-,-)	<i>1.33e-1</i>	2.25e-2 (-,-)	4.24e-2
	ε	2.27e-1 (-,-)	3.45e-1	<i>3.33e-1</i> (-,-)	<i>3.80e-1</i>	1.04e-1 (J,P)	1.41e-1
R_DTLZ2 3 / 6	S -metric	<i>9.31e-2</i> (-,-)	<i>1.09e-1</i>	6.79e-2 (J,-)	7.62e-2	1.90e-2 (J,P)	2.12e-2
	R_2	5.15e-5 (-,-)	5.36e-5	<i>6.11e-5</i> (-,-)	<i>7.63e-5</i>	1.10e-5 (J,P)	1.43e-5
	ε	<i>1.97e-1</i> (-,-)	<i>2.03e-1</i>	1.58e-1 (J,-)	1.67e-1	8.05e-2 (J,P)	9.35e-2
R_DTLZ2 5 / 6	S -metric	<i>2.60e-2</i> (-,-)	<i>1.36e-1</i>	<i>5.31e-2</i> (-,-)	<i>8.26e-2</i>	1.22e-2 (J,P)	1.76e-2
	R_2	2.31e-5 (-,-)	5.19e-4	<i>8.16e-5</i> (-,-)	<i>1.14e-4</i>	5.68e-7 (-,-)	9.93e-7
	ε	1.69e-1 (-,-)	3.05e-1	<i>2.56e-1</i> (-,-)	<i>3.36e-1</i>	1.44e-1 (J,P)	1.66e-1

Experimentation/Visualization: The results of the experiments are summarized in Table 1. The distribution of solutions within the median Pareto front approximation is exemplarily visualized in Fig. 2. In Fig. 3, boxplots of the mean distance to the Pareto front are shown for R_DTLZ2 with three and five objectives.

Observations: SMS-EGO performs significantly better than ParEGO and Jeong with respect to the ε - and hypervolume indicator on R_ZDT1, R_ZDT4_{relax}, and

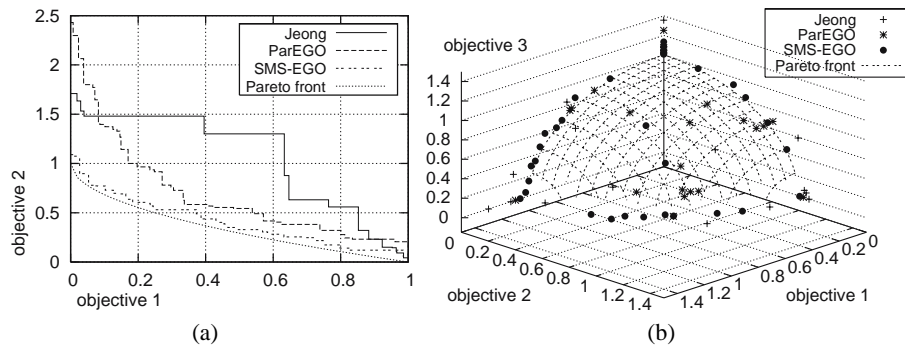


Fig. 2. (a) The median attainment surfaces of all algorithms on ZDT1. (b) The distribution of solutions in the objective space of DTLZ2 with three objectives. Exemplarily, the runs are chosen which achieved the median result with respect to hypervolume indicator.

R_DTLZ2 with five objectives while being worse on OKA2 for the R_2 and ε measure. When three objectives are considered, SMS-EGO outperforms all other algorithms for all metrics. On this R_DTLZ2 instance, on R_ZDT1, and on OKA2, ParEGO also outperforms Jeong regarding the ε - and hypervolume indicator.

Discussion: Whereas the concepts of the hypervolume and the ε -indicator are directly considered within SMS-EGO, the R_2 metric and ParEGO are both based on augmented Tchebycheff aggregation. Thus, it is particularly surprising that SMS-EGO significantly outperforms ParEGO with respect to this metric on the threeobjective R_DTLZ2 test function. Furthermore, the results on the test functions, which feature more than two objectives, show that SMS-EGO copes best to increasing objective dimensions. This fact is visualized in the boxplots showing the distributions of the mean distance to the Pareto front on R_DTLZ2 with five objectives in Fig. 3 (b). The inferior results on OKA2 can be explained by the difficulty of this test function. SMS-EGO obtains one extremal solution with high accuracy ($\approx 10^{-9}$). Other solutions are neglected since a comparable accuracy is necessary to provide further non-dominated solutions due to the steep ridges around the optimal area. Jeong and ParEGO are forced towards other solutions by their selection principles. Thus, they provide a better distribution, which results in significantly better indicator values. Nevertheless, they fail to provide close to optimal solutions. Consequently, OKA2-like problems with steep ridges cannot be solved within a reduced budget of just 130 evaluations using the proposed model-based approaches. The superior results of SMS-EGO on R_ZDT4_{relax} indicate that the use of the LCB solution does not disregard global exploration compared to the EI used in ParEGO and Jeong.

In order to further analyze the distribution and the convergence behavior of the algorithms, Fig. 2 visualizes the median Pareto front approximations in the objective space and Fig. 3 shows boxplots of the mean distance to the Pareto front on both variants of R_DTLZ2. Jeong and Obayashi's approach covers only the boundaries of the Pareto front with a competitive accuracy, which leads to the worst distance values of all algorithms. This behavior may be caused by the dimension-based reference values for the

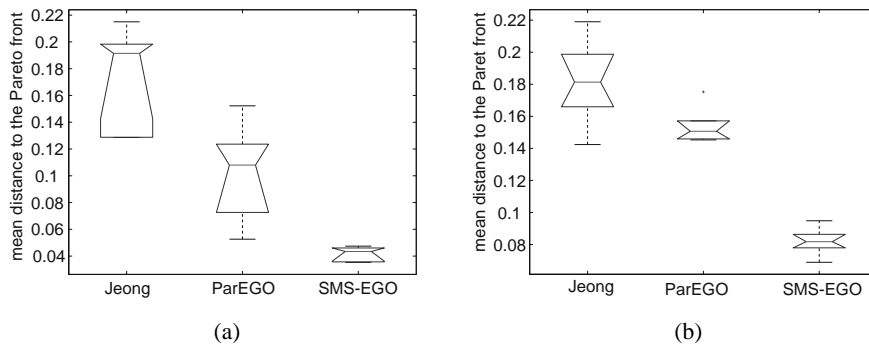


Fig. 3. Box plots of the mean distance to the Pareto front over five runs on DTLZ2 with three (a) and five objectives (b). The box extends from the lower quartile to the upper quartile, and a line is drawn at the median value. The spread of the sample is indicated by the whiskers. The notches represent a robust estimate of the uncertainty of the measured median for box to box comparison.

computation of the EI. ParEGO performs slightly better, but explores the boundaries of the Pareto front to a lesser extend. This problem of aggregation-based approaches using sets of weight vectors has already been observed by Wagner et al. [21]. SMS-EGO is the only MOOA that is able to approximately attain the complete Pareto fronts of R_ZDT1 and R_DTLZ2 with three and five objectives within the allowed budget of 130 evaluations, which is just slightly beyond the initial population size of most common MOEA (cf. Fig. 2 (a) and Fig. 3).

5 Conclusions

The optimization of most real-world problems requires an efficient use of evaluations. Thus, recent approaches, which transfer the singleobjective meta-model-assisted EGO approach to MOP, are presented and a new enhanced algorithm based on the \mathcal{S} -metric or hypervolume contribution (SMS-EGO) is introduced. A comprehensive benchmark is performed to analyze the results, which can be obtained on a budget of 130 evaluations. The SMS-EGO introduced in this paper performs significantly better on all considered R_ZDT and R_DTLZ2 instances. It is the only approach that is able to approximately attain the Pareto front of these problems under the given conditions while achieving both aims of multiobjective optimization, convergence and a good distribution of solutions.

The method of Keane [13] may show comparable results to SMS-EGO. However, his proposed improvement metric heavily depends on the scaling of the objectives. Since the use of the lower confidence bound for computing the hypervolume contribution in SMS-EGO also leads to some undesired side effects, such as the occurrence of dominated solutions, the implementation of his approach for formally determining the expected objective vector in arbitrary dimensions and the combination with the infill criterion of SMS-EGO are aspired.

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