Decision Space Diversity Can Be Essential for Solving Multiobjective Real-World Problems

Mike Preuss, Christoph Kausch, Claude Bouvy, and Frank Henrich

Abstract It has recently been argued that standard multiobjective algorithms like NSGA-II, SPEA2, and SMS-EMOA, are not well suited for solving problems with symmetries and/or multimodal single objective functions due to their concentration onto one Pareto set part. We here deliver a real-world application that shows such properties and is thus hard to solve by standard approaches. As direct tuning of the algorithms is too costly, we attempt it via constructive modeling (algorithm-based validation), but succeed only partly in improving performance, which emphasizes the need to integrate special operators for boosting decision space diversity in future algorithms.

Keywords Evolutionary multi-criterial optimization · Decision space diversity · Constructive surrogate modeling

1 Introduction

Within the last years, a number of *evolutionary multiobjective optimization algorithms* (EMOAs) have been established as a viable alternative to classical methods for multicriterial decision problems. NSGA-II (Deb et al. 2000) and SPEA2 (Zitzler et al. 2002) belong to this group, accompanied by newer methods as e.g., the SMS-EMOA (Emmerich et al. 2005). They have proven their ability to approximate Pareto fronts reasonably well in a single run due to their inherent population concept, which makes them a-posteriori techniques according to common definitions (Miettinen 1999).

In order to stretch the population over large parts of the Pareto front, EMOAs use diversification techniques like crowding or $\mathcal{S}$-metric based selection which are mostly applied in the objective space only. However, the Pareto set, as the set of

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preimages of points on the Pareto front, is usually implicitly assumed to be compact. For simple model test cases, it has recently been argued that this assumption is likely to be wrong if at least one of the treated objective functions is multimodal (Preuss et al. 2006). It goes without saying, that for real-world problems, there is no guarantee for unimodality in either objective as they usually represent rather complex systems. Thus, the Pareto sets may be scattered into different clusters throughout the search space. Despite their integrated diversification techniques, standard EMOAs have difficulties with detecting such clusters and keeping them in the focus of the search (Rudolph et al. 2007). In consequence, the obvious conjecture is that EMOAs – as many other algorithms for multicriterial decision making – do not cope too well with a large fraction of multiobjective real-world problems, namely the ones that embed multimodal singleobjective problems. Note that this means that it is not only hard to achieve a good approximation of the entire Pareto front, but also the missing ability to detect alternative equivalent or nearly equivalent fronts which may be very interesting for the practical implementation of an agreed solution.

Unfortunately, there is a current lack of investigations of other than simple test problems under this aspect. In this work, we perform such an investigation on a chemical process engineering problem where the task is to find an inexpensive distillation plant layout that additionally achieves a low energy consumption. Next to analyzing the obtained Pareto fronts and sets and taking into account the available results for the singleobjective case (Henrich et al. 2008), we employ an algorithm-based validation approach (Beielstein et al. 2003) via constructive modeling. Thereby, we strive to strengthen our understanding of the problem structure and at the same time increase the performance of the chosen EMOA. This method is in principle applicable to any other optimization problem with unknown features, as it bypasses the need for extensive testing that would render a purely exploratory approach infeasible due to immense computational cost.

The paper obeys the following scheme: Section 2 concretizes the aims pursued, Sect. 3 describes the treated real-world problem, Sect. 4 its graphical analysis, and Sect. 5 the attempts to improve the standard EMOAs performance.

2 Aims and Methods

The overall task of this work is to demonstrate that real-world problems of *type III* (partitioned Pareto set, a single front) as postulated in (Rudolph et al. 2007) indeed exist and to investigate how a standard EMOA copes with such a problem.

The second, related aim is to find out more about the nature of our real-world problem and to answer the question whether one of the detected disjoint Pareto sets is on its own sufficient to cover the whole Pareto front. In order to adapt the EMOA better to the problem, we employ a constructive modeling approach, supported by *sequential parameter optimization* (SPO) (Bartz-Beielstein 2006).

3 Real-world Distillation Plant Layout Problem

In general the modeling of process engineering tasks is a highly complex problem, which has been the focus of a great deal of research in the past decades. Naturally, the planning and design phase of such tasks have become more and more dominated by optimization tasks involving the layout and operation of plants or parts thereof. These optimization problems all involve economic criteria directly (e.g., investment sum, overall yearly costs) or indirectly (e.g., product quality, plant output) with ecological factors (e.g., yearly CO_2 emissions, yearly primary energy consumption) becoming increasingly important, often resulting in conflicting criteria if more than one factor has to be taken into account. In this work we investigate a separation task, where the layout and operation of a general distillation sequence featuring the separation of multi-component feed streams into multi-component products using non-sharp splits is addressed. Specifications for the streams and utilities are given in Table 1. A superstructure concept is used to model different structural alternatives including blending and stream bypassing, the number and sequence of splits as well as sharp and non-sharp splits (the latter of which are shown in Fig. 1). If multi-component products are desired, costs for energy and equipment can often be saved because the complete separation of the components with subsequent remixing is unnecessary if non-sharp splits are utilized (Henrich et al. 2008). The superstructure and operational variables are optimized using EAs and EMOAs.

The detailed modeling and thermodynamically rigorous simulation is accomplished by the combination with the ASPEN PLUS™ simulation system, thus ensuring that all boundary conditions are met and that a proposed structural alternative is in fact thermodynamically sound. For a detailed description of the approach and a discussion of published methods used to address this and related *mixed integer nonlinear programming* (MINLP) optimization problems refer to (Henrich et al. 2008).

Our approach enables investigating diverse structural alternatives and modes of operation, resulting in highly complex search topologies including multi-modalities and non-convexities. In order to simplify demonstrating our findings, we fix some of the structural alternatives so that for the example discussed in this paper, the optimization reduces to a *nonlinear programming* (NLP) problem (the optimization variables and their ranges are given in Table 2). The ξ_j^i denote the key component recoveries j of either the light (LK) or the heavy key (HK) components in distillation column i (the key component recoveries describe the fraction of the mole-flow

Table 1 Incoming feed structure and desired mixtures: mole flows for components A (Propane), B (iso-Butane) and C (n-Butane); available utilities

	$\dot{n}_{\mathrm{ges}}$	$\dot{n}_{\mathrm{A}}$	$\dot{n}_{\mathrm{B}}$	$\dot{n}_{\mathrm{C}}$
Stream	kmol/h	kmol/h	kmol/h	kmol/h
Feed	300	100	100	100
Product 1	110	30	50	30
Product 2	190	70	50	70

Steam:	@ 343 kPa, 3.6 USD/ t
Brine:	@ 258 K, $\Delta T = 15$ K, 0.12 \$/ t

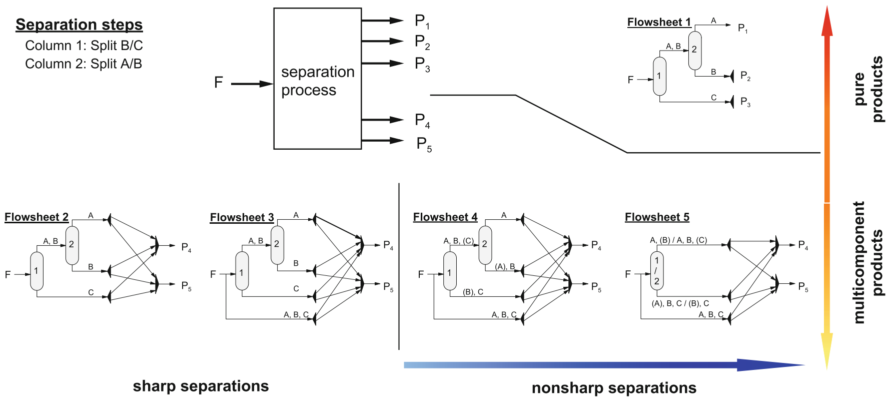

Fig. 1 Structural alternatives for separation of 3-component feed: complete separation (flowsheet 1) or fractionation into mixtures using sharp (flowsheets 2 and 3) or non-sharp (flowsheets 4 and 5) splits

Table 2 Optimization variables and allowed ranges

Variables	$\xi_{LK}^{A/B}$	$\xi_{LK}^{B/C}$	$\xi_{HK}^{A/B}$	$\xi_{HK}^{B/C}$	$x_{By,P1}$	$x_{By,P2}$	$x_{PFS1,P1}$	$x_{PFS2,P1}$	$x_{PFS3,P1}$
Number	1	2	3	4	5	6	7	8	9
Range	[0.5, 1]	[0.5, 1]	[0, 0.5]	[0, 0.5]	[0, 0.3]	[0, 0.5]	[0, 1]	[0, 1]	[0, 1]

of a component in the distillate stream compared to the mole-flow in the feed stream, e.g., in Flowsheet 4 of Fig. 1 for split B/C, i.e., column 1, the light key component is B the heavy key component is C). The $x_{By,k}$ stand for the bypass fractions to product k (i.e., the fraction of the feed stream which does not pass through a column and is directly mixed to form product k) and $x_{PFS,P1}$ mean the fraction of an output stream which is mixed to form product 1. The problem structure is similar to that shown in Flowsheet 4 of Fig. 1 except that we have chosen the split sequence A/B followed by B/C.

Table 2 contains the variables subject to optimization and their allowed ranges. We here investigate the investment cost for such a distillation sequence vs. the exergy loss. The exergy loss may be interpreted as an ecological criterion describing the grade of energy depreciation involved in a process (cf. Wozny et al. 1983a,b; Le Goff et al. 1996; Sattler 2001; Lucas 2004).

4 First Assessment of the Problem Structure

Due to the time needed to perform a single evaluation (by simulating the plant layout specified by concrete values for the variables in Table 2) which is on the order of seconds, we allowed a maximum of 10.000 target function calls. An optimization run thus takes about 25 hours on an average PC. Note that we varied the allowed tolerance on the output mixtures from 2 % (low) to 5 % (high) in order to simplify the problem. In a production environment, 2 % is already at the upper limit of desired product qualities. The reasoning behind is to first make the optimization algorithm run successfully on a simpler problem and then to adapt it to the harder one.

The first test runs conducted with an SMS-EMOA under default parameters (except for a smaller population size 20, motivated by the need to converge fast) revealed a number of rather unexpected problem features.

- The attained Pareto sets mostly concentrate on very small areas of the decision space, and these are usually disjoint ones for subsequent runs.
- The EMOA often gets stuck for a long time just before entering a valid region, and the needed effort for getting there can be very different.
- Even after reaching a valid region, very few valid search points are detected (around $5-10\%$ for the high tolerance, $\approx 2\%$ for the low tolerance).

The resulting complex structures of decision and objective spaces are visualized in Figs. 2 and 3. We plot about available 5.000 valid evaluations collected from several runs to give an idea of the distribution of valid regions. The chosen variables are the heavy component recoveries of column A/B and B/C, depicted in combination with their objective criteria values, the exergy loss and the investment cost respectively. In these variables, the valid regions clearly form islands as for most of the possible variable combinations.

The variable space of this problem shows clearly the non-convex and multimodal structure referred to above. Through the boundary conditions in the form

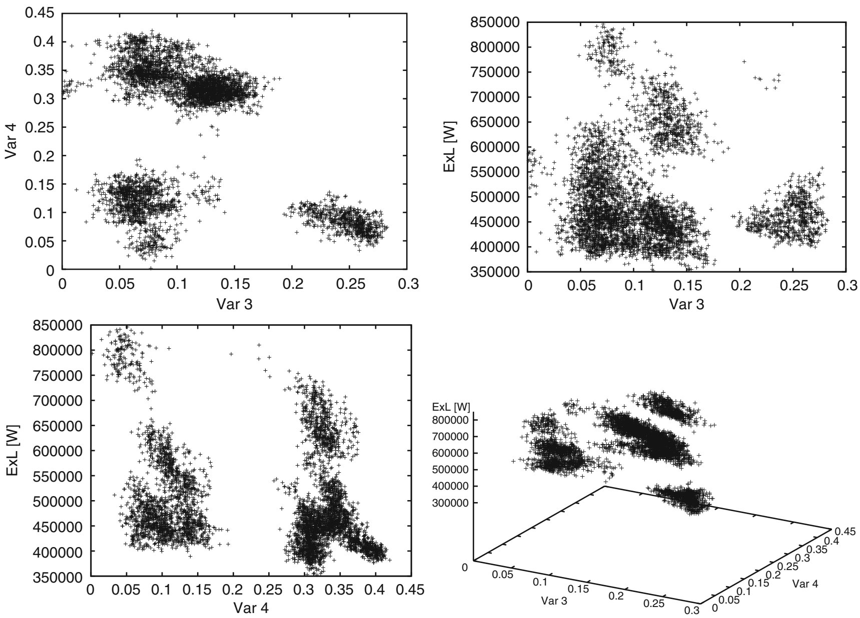

Fig. 2 Heavy key recoveries of split A/B and B/C (variables 3 and 4) against the exergy loss, all $\approx$5.000 valid solutions of several runs plotted to reveal the valid decision space structure

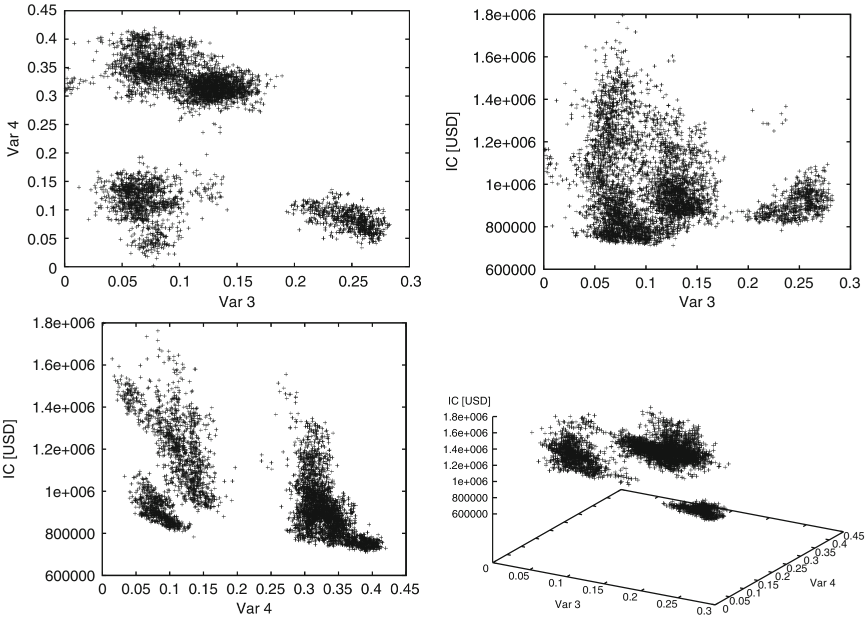

Fig. 3 Heavy key recoveries of split A/B and B/C (variables 3 and 4) against the investment cost, note that for both criteria (see Fig. 2), the valid decision space area is the same

of the mass balances and the thermodynamic principles involved in the rigorous simulation of the distillation columns (MESH-equations), valid evaluations are only found in certain areas showing a highly irregular structure with in general no clear correlations to problem variables being possible.

Figure 4 (bottom left) depicts the objective function values obtained by the 5.000 valid individuals as used above. The "optimal" Pareto front is located near the first axis with a step around investment costs of about 900.000 USD. If these two criteria are the basis for the design decision, we have a clear indicator for a distillation structure decision allowing for the reduction of exergy losses at low additional investment cost at the step. The top left diagram extracts the fronts of only 5 best runs to enhance visibility. The figure on the right side shows the matching Pareto sets, which clearly have a strong concentration on a small region each. From the figures, we conclude that the problem is of mixed type III (separate Pareto set parts of equal quality) and IV (separate sets and fronts).

5 Tuning via Constructive Modeling

With the first insight into the problem structure and the difficulties of EMOAs to converge to the Pareto front in mind (Sect. 4), it becomes clear that we would like to enhance their performance, e.g., by parameter tuning. However, direct tuning is

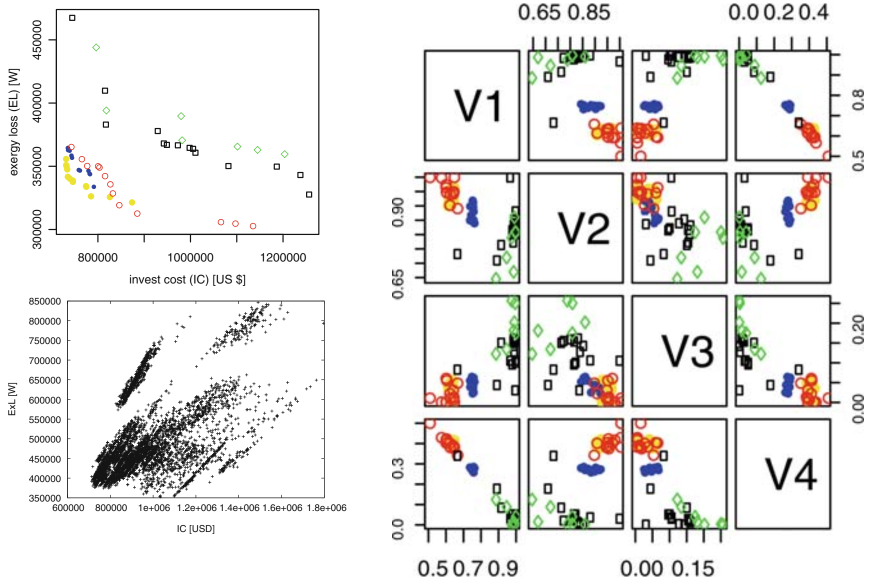

Fig. 4 Exergy loss and investment cost Pareto fronts of the best 5 runs (upper left), all valid individuals of several runs (bottom left), and pair plots of the Pareto sets of the best 5 runs over variables 1–4 (right)

not applicable here as only few runs can be spent due to the immense computational cost. We thus attempt an indirect approach by utilizing the available problem knowledge for constructing a simple model, on which the tuning method can operate. This resembles an algorithm-based validation approach similar to the one employed in (Henrich et al. 2008), only that here, no simplified target function is available.

The problem properties we orient our construction at are: An island-like structure, and the existence of plateaus or very flat regions near the valid regions. Furthermore, it is assumed for reasons of simplification that a separable model suffices, and that complete Pareto sets are available within each island. With respect to the multimodality, we chose the cosine as a base function, and redefine it where it reaches values below 0.5 (minimization). At this level, we model the invalid-valid transition by a large plateau that comprises of a fraction of w, the halved distance between two maxima. In the remaining inner (valid) space, we employ two quadratic functions, one for each target function. f_0 has its minimum at $\frac{1}{3}$ of the valid region, f_1 at $\frac{2}{3}$. A complete Pareto front may thus be attained by reaching the connecting line between a minimum of f_0 and of f_1, respectively, given that these are located in the same valley of the consine function (see Fig. 5). Several model parameters have been adapted to – if treated with the same EMOA as above – give similar results as for the original problem. As measures like the hypervolume are incomparable between original problem and model, we relied on auxiliary indicators, namely the number of valid individuals attained during one run, and the number of evaluations needed until a first valid solution is reached. The model's parameters are chosen according to the attained problem knowledge:

- We set the number of dimensions to 6, as the latter 3 of our 9 original variables show a strong concentration to very few discrete values.
- The number of valleys for each dimension is set to 4 to approximately resemble the visual impression provided by Figs. 2 and 3.
- According to the attained fraction of valid individuals, we adjust the plateau size w to 10% for the high tolerance case, and to 20% for the low (2%) tolerance case.

Concerning the two indicators named above, the EMOA behavior on model and original problem is largely comparable with the chosen model parameters. However, there is a significant difference, as for the original problem, the resulting front of one run nearly always consists of very similar solutions, whereas this is not the case for the model. Therefore, it proved to be necessary to add another constraint to integrate this behavior into the model by enforcing that a solution may only be valid if for each dimension, the same or a neighboring valley is chosen. Surprisingly, this suppresses mixed Pareto sets almost completely. Although this constraint is straightforward, it is by no means unique. The same behavior may be induced by choosing another one that somehow restricts the permitted combination of valleys. In the following, we experimentally evaluate if tuning on the model functions is helpful for improving EMOA behavior on the original problem.

Experiment: Is tuning the EMOA by means of a constructive model effective?
Pre-experimental planning. The model parameters have been adjusted via comparisons of the two indicators as described above, and a separate SPO run was executed for the 5% and the 2% tolerance case (see Table 3). Allowed parameter ranges are given in the top row.

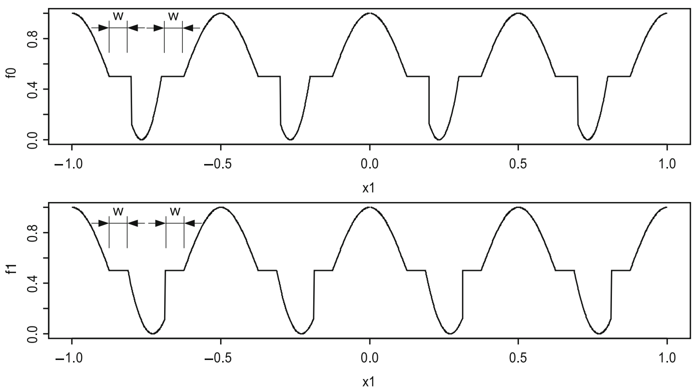

Fig. 5 Stepwise defined model functions f_0 and f_1 in each dimension, the plateau width is controlled by variable w. A part of the Pareto set is located in between the two minima of the parabola in each valley

Table 3 Parameter values and measured performances for different configurations, on the original problem and the model (M/P). Note that other than for the problem, model S-metric values are bound from above by 9

	M/P	tol.	popul.	p_{reco}	η_{reco}	η_{mut}	S-metric	#valid	front	runs
allowed ranges	–	–	2 : 100	0 : 1	1 : 100	1 : 100				
first runs	P	5%	20	0.5	20	15	3.09E+13	696	7	8
default parameters	P	2%	20	0.5	20	15	2.92E+13	85	5.09	22
model, default par.	M	5%	20	0.5	20	15	8.46	136	8.03	30
SPO optimized	M	5%	77	0.22	53.0	92.6	8.81	3740	55.6	30
model, default par.	M	2%	20	0.5	20	15	8.50	63	6.3	30
SPO optimized	M	2%	61	0.65	35.2	96.5	8.79	3762	60.9	30
SPO optimized	P	2%	61	0.65	35.2	96.5	2.92E+13	945	4.29	21

Task. We want to check if we have obtained a better EMOA configuration by using the model-optimized parameters, resulting in better S-metric values, larger final Pareto fronts, and a larger number of valid individuals. If so, we can state that our model fits the problem well with regard to the optimization algorithm.

Setup. We employ the parameter settings retrieved on the model for the original problem with 2% tolerance, performing 21 runs. All non-specified parameters are kept at default values. These are to be compared to the outcome achieved by default parameters (row 3).

Results. Table 3 contains the result of the optimized parameters (last row).

Observations. It is obvious that the S-metric performance has not changed between the default and the optimized parameters. However, the number of valid individuals has dramatically improved. Front sizes are slightly smaller than for the default values. In both cases, the whole attained fronts are located in very small regions in the decision space. Two more observations can be made: a) the variances of the mean S-metric values are quite large (around $10^{1}2$), and b) the default configuration leads to fast progress in the beginning, but stagnates in the end, whether the runs with optimized parameters still improve at 10.000 evaluations, this may be a turning point.

Discussion. Whereas the optimized parameters improve the EMOA behavior on the model, they are only of limited use for the original problem. However, the increase in valid individuals is enormous, which is a clear advantage concerning the empirical analysis of the problem. This is probably due to the reduced step sizes during recombination and mutation (η_{reco} and η_{mut}). It seems that parts of the problem properties are mapped rightly into the model, but others are not. Our understanding of the problem nature is thus not entirely wrong, but may still be improved. However, as the nature of the problem is quite unusual compared to standard test problems, it may not be possible to increase performance much further without additional means like special operators, multistart or niching mechanisms.

6 Conclusions

From the visualizations given in Sect. 4, we know that for the treated real-world problem, the valid regions of the decision space are separated into disjoint islands in several variables. The Pareto fronts and sets obtained by application of a standard EMOA suggest that the problem is of mixed type III (separate Pareto set parts of equal quality) and IV (separate sets and fronts). We can thus expect that standard EMOA are not very well suited for solving this problem reliably, which is demonstrated in the only partly successful attempt to adapt an EMOA to it (Sect. 5). To integrate specific operators (e.g., niching, multistart) into standard EMOAs therefore appears to be a promising task for future work.

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