Scalability of Multi-Objective Evolutionary Algorithms for Solving Real-World Complex Optimization Problems

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Abstract. The use Multi-Objective Evolutionary Algorithms (MOEAs) to solve real-world multi-objective optimization problems often finds a problem designated by the curse of dimensionality. This is mainly because the progression of the algorithm along successive generations is based on non-dominance relations that practically do not exist when the number of objectives is high. Also, the existence of many objectives makes the choice of a solution to the problem under study very difficult. Several methods have been proposed in the literature to reduce the number of objectives to use during the optimization process. In the present work, a methodology to reduce the number of objectives is proposed. This method is based on DAMICORE (DAta MIning of COde REpositories), a machine-learning algorithm proposed by the authors. A theoretical comparison with a similar machine learning approach is made, pointing out some advantages of using the proposed algorithm using a benchmark problem designated by DTLZ5. Also, a real problem is used to show the effectiveness of the methodology.

Keywords: Objectives Reduction, Data Mining, MOEAs, Many Objectives.

1 Introduction

Real-world optimization problems have very often many objectives that must be satisfied simultaneously. Multi-Objective Evolutionary Algorithms (MOEAs) showed to be very efficient in solving this type of problems. However, the use of MOEAs to tackle these problems suffers from a difficulty designated by the curse of dimensionality, in which the increase of the number of objectives makes the progression towards the Pareto-Optimal Frontier (POF) very challenging [1-4]. Also, the existence of many objectives makes the visualization of the POF almost impossible, which puts difficult to help the decision maker in selecting a solution and, more importantly, to explain his decision. Associated with this, often the decision space is also of large size, which, additionally, worsens the difficulties for the MOEAs [5]. Therefore, a scalability problem arises, not only due to the high number of decision variables and/or objectives but also due to the complex interrelations existent between the decision variables, between the objectives, and between the decision variables and the objectives.

To deal with the curse of dimensionally due to the high number of objectives several methodologies to reduce the number of objectives during the optimization have been

proposed in the literature. This is a challenging problem in which a balance must be made between the requirement of preserving the original (with all objectives) problem characteristics and the possibility of obtaining acceptable solutions when the number of objectives used during the optimization is reduced.

Another important question is to know if the individual objectives are relevant during the entire optimization process (along the generations), i.e., it is important to know if it is possible to start the optimization using some objectives and during the successive generations change the objectives used. This is, as the solutions approach the POF the complex structure between the decision variables and the objectives can change.

The objective of this work is to study the applicability of MOEAs to complex real problems based on objectives reduction using a data mining technique, and not to compare the performance of different methodologies. Thus, using the data mining methodology proposed the aim is to be able to use the existing complex relations inside the problem to help the optimization process. However, must be clear that the aim is not to obtain a reduced objective set which represents the original set without errors, but the reduced set will be a very good approximation to the originally defined set of objectives with a reduced error. This will be very useful for real problems in which it is not possible to reduce the number of objectives due to the strong interaction between these same objectives, but that makes it possible to facilitate the search and help the DM to understand the considered process. In fact, real problems often have some characteristics that are not present in benchmark problems. In such real problems, there is a complexity associated with the relations between the decision variables and the objectives that are not present in benchmark test problems, where those relations are placed on purpose [5].

This text is organized as follows: in section 2 a state-of-the-art related to objectives reduction will be made, in section 3 the data mining technique used will be presented and discussed, in section 4 the real-world problem to study is presented, in section 5 the results are presented and discussed, and in section 6 the conclusions and some suggestion for further work will be stated.

2 Related Work with Objectives Reduction

Brockoff and Zitzler [1, 2] proposed two different algorithms for objectives reduction based on the definition of two types of problems, the first, to obtain the minimum objective subset that produces a certain error, and the second, to obtain an objective subset of a predefined size with the minimum possible error. Deb and Saxena [3, 4] based on principal component analysis proposed a method for reducing the number of objectives by maintaining the objectives that can explain most of the variance in the objective space, but without explaining clearly how the objective reduction alters the dominance structure. Jaimes et al. [6] proposed two algorithms to address the two problems identified by Brockoff and Zitzler above based on a feature selection method. The algorithms were validated by comparing the results with the algorithms of Brockoff and Zitzler. Saxena et al. [7] presented a framework for using both linear and nonlinear objective reduction algorithms. The authors proposed to develop a general framework,

taking into account the possibility of the data being noisy, to reduce the number of algorithms parameters and to propose an error measure. The algorithms were applied to a broad range of problems and the results were compared with others in the literature. Sinha et al. [8] proposed a methodology to reduce the objectives before presenting the solutions to the decision maker that iteratively chose the best solutions. The methodology was applied to solve some real world problems. Finally, Duro et al. [9] proposed a machine learning methodology with the aim of learning the preference-structure different objectives present in the problem in order to obtain the smallest set of objectives that can originate the same POF, the smallest objective set corresponding to a minimum pre-defined error and the objective sets of a certain size that originates a minimum error. The characteristics of this methodology were compared with the one proposed in the present paper at the end of the next section.

3 Approach Based on Data Mining

3.1 Data Mining Methodology Adopted - FS-OPA

Main concepts. First introduced by Sanches et al. [10], DAMICORE, borrowed from Theory, Complex Networks, and Phylogenetic Inference, aiming at revealing the hidden hierarchical relationship of objects from an unstructured (raw) dataset. It uses three principal steps: S1) given a metric of similarity, build a distance matrix comparing every two objects; S2) convert the matrix into a phylogenetic tree by connecting close objects according to hierarchical levels of similarity; S3) apply a community detection process to group close subtrees into clusters. Figure 1 shows a set of objects *xi*, the elements d_{ij} of the distance matrix correspond to a measure of dissimilarities between objects x_i and x_j, according to some given metric. The matrix is broken down into a tree, where the distance between any two objects (leaves) corresponds to the sum of the lengths of the branches connecting them. Finally, the third step groups the objects that are strongly connected (according to the tree topology) into a community, generating a set of distinguishable similarity clusters. The original DAMICORE method selects three specific algorithms for the Steps S1, S2, and S3 (Figure 1), respectively, Normalized Compression Distance (NCD) [12, 13] (since it works with any data type and mixed types); Neighbor Joining [14] (NJ) (widely employed in bioinformatics), and Fast Newman (FN) (that constructs a graph partition by a greedy algorithm that uses a bottom-up strategy to maximize the graph modularity function [15]).

The pipeline with NCD, NJ, possesses relevant properties. NCD makes DAMICORE a data-type agnostic method, in the sense that it works with any kind of object (texts, images, audio, etc.) and mixed data types. Moreover, DAMICORE can be used without any data pre-processing, such as filtering, outlier detection, feature extraction, parameter setup and knowledge of the problem domain. DAMICORE requires no parameters setup to run (although some execution options may improve its performance). DAMICORE has been successfully employed in a variety of fields, for example, software-hardware co-design [16, 17, 18], compiler optimization [19, 20], student profiling in e-learning environments [21, 22], identification of phytopathology from sensor data

[18], systematic literature review, identification of cross-cut concerns [23], electrical distribution systems [24], and novel methods in bioinformatics [25].

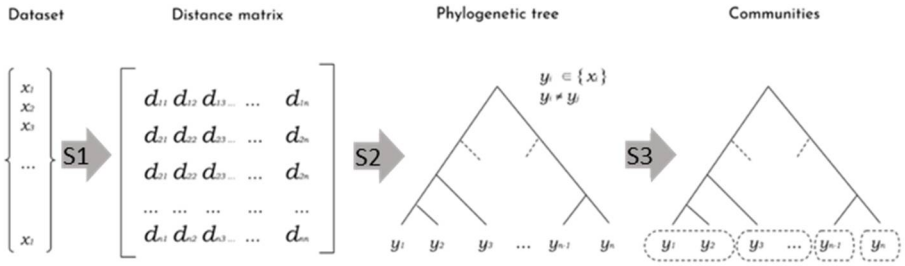


Fig. 1. The tree-steps pipeline called DAMICORE (reproduced with permission from [11].

Feature Sensitivity Analysis. A Feature Sensitivity (FS) analysis aims at salienting the principal features of a problem, taking into account common real-world challenges (such as the quality of data acquired and the database consistency and representativeness), its feature interactions, and their contribution to a target or objective. Such a scope differs from those where the standard feature selection algorithms have succeeded. In other words, an FS strategy is expected to benefit the learning of a problem from scratch. Such learning can induce a model for optimization algorithms (such as Estimation of Distribution Algorithms). We use phylogram-based models since they can work with small datasets and there is an optimization approach prepared to use such models: Optimization based on Phylogram Analysis (OPA).

Figure 2 shows a diagram synthesizing OPA with the use of the FS analysis by it; such a combination is called FS-OPA. The two principal FS steps are: *A*) Salienting Samples (SS) according to a criterion; and *B*) applying DAMICORE to construct a phylogram-based model. SS ranks the samples according to each of the *M* criteria (or non-dominated fronts), producing the sets of selected samples (Figure 3), denoted BC1 (the samples in the best quantile according to Criterion 1), BC2, …, BCM. DAMICORE (Section 3.1.1) constructs a phylogram (a rough model) from BCi, *i*=1, …, *M*, generating *M* models (BC1-based model, …, BCM-based model). Then, a consensus strategy produces a unified phylogram-based model. An OPA cycle completes when the unified model generates new samples.

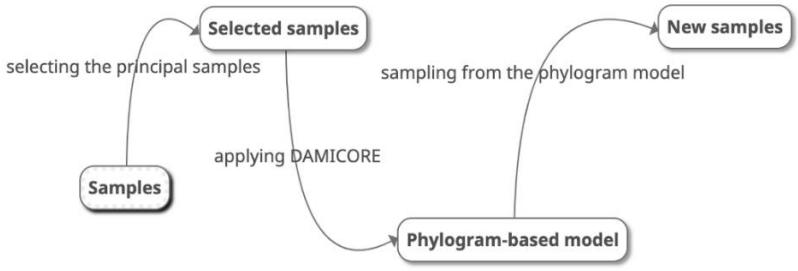


Fig. 2. Diagram of the Optimization based on Phylogram Analysis - OPA.

This paper instantiates the procedures from Steps *A* and *B* for the modelling of polymer extrusion (Section 4). The learned model is expected to benefit the optimization problem associated with polymer extrusion. However, the sampling from the unified model (the last OPA step) is not performed, thus, not a complete optimization cycle is run.

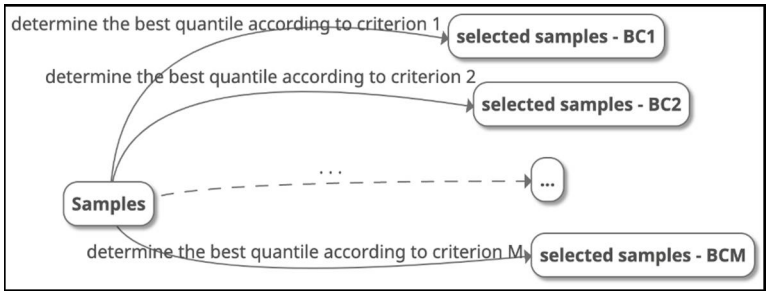


Fig. 3. SS procedure that obtains the selected samples shown in Figure 2.

Soares et al. [24] and Martins et al. [18] show some experimental results and proofs related to the performance of OPA for challenging combinatorial mono- and multi-objective optimization problems. The main mechanisms of FS-OPA, relevant to the scope of a data-driven design of an extruder concentrated on the DAMICORE method, are introduced in Section 3.2.

3.2 Comparison of FS-OPA with NL-MVU-PCA for MaOPs data-driven structural learning

NL-MVU-PCA (Non Linear – Maximum Variance Unfolding - Principal Component Analysis) is the main method investigated for MaOPs by [9]. The non-linear (NL) approach performs the optimization of the Kernel (Gram) matrix values by minimizing the Maximum Variance Unfolding (MVU) to find the best mapping (that preserves the geometric properties of local neighbourhoods; while linear methods aim at keeping the Euclidean distances between all pairs of data points). Table 1 summarizes the relevant properties of both NL-MVU-PCA and FS-OPA for MaOPs. The latter investigates three types of associations: variable-variable (producing results similar to the Gibbs measure for Ising Models, or Markov Random fields [26]), objective-objective (the dissimilarities when found can favour the construction of (non-dominated) front distributions [25]), and the variable-objective (that may benefit inference as Markov Blankets [27]). The former only works on the objective space for the exclusive purpose of space reduction to determine *the essential objective set* [9]. Moreover, the FS-OPA preserves the original variable space, which favours non-expert human interpretability (relevant for some classes of real-world problems); it also has a relatively low-time complexity and has shown beneficial results when applied to small datasets [10,16-23].

The Feature Sensitivity (FS) analysis of FS-OPA aims at finding the variable and/or objective interactions that benefit inferences through structural (graph-based) and prob-

abilistic modelling. Probabilistic results are fundamental due to the odds of bias in observed data or small-data sampling. Interpretability is fundamental for some classes of real-world problems, mainly involving decisions by experts from an application domain. Variable-variable and variable-objective interactions also benefit practitioners' comprehension of founds (The Why), increasing their confidence in a decision.

Table 1. NL-MVU-PCA and DAMICORE for multidimensional data-driven structural learning applied to MaOPs.

Category	Types		NL-MVU-PCA	FS-OPA
Analyses	Objective-objective		X	X
	Variable-variable			X
	Variable-objective			X
	Objective space reduction		X	
	Sensitivity			X
Priors	Kernel function choice		X	Not necessary
	Parameter optimization		X	Not necessary
Interpretability - The Why	Non-expert practitioner			X
Scalability	Time-complexity	Usual cases	$O(M^3q^3)$*	$O(l^3)$**
		The worst case	$O(M^6)$	$O(n\ l^2+l^2)$
	Sample-size support		Empirical	Theoretical and empirical

* M is the number of objectives and q is the number of clusters.
** l is the number of variables and objectives, and n is the number of data resamples.

The time complexity for usual cases and the worst-case estimates the overhead of the two procedures for the multidimensional data-driven structural learning when applied to MaOPs. The number of clusters in NL-MVU-PCA relates to the number of constraints to maintain the local isometry (Mq; in the worst case, q=M-1 and M^2) [9]. FS-OPA with usual resampling is $O(l^3)$ since $n \leqslant l$ (as in leave-one-out resampling) [24]. Moreover, l=M for a space analysis only uses objectives. Thus, the time complexities of FS-OPA and NL-MVU-PCA have a ratio of $(n+M)/M^4$ $(1/q^3)$ of running time for l=M in the worst case (in the usual case).

Another relevant factor for reliable results is the minimal amount of samples required. Usually, the sample size for PCA is empirically obtained. FS-OPA has a theoretical model to determine the minimal amount of samples to reach reliable results [24], which can also be empirically corroborated.

Figure 4 illustrates an FS-OPA output for DTLZ5(2,10), also used by Duro et al. [9] for explaining the capacity of the method of them to find redundant objectives (objectives f1, f2, f3, f4, f5, f6, f7, f8, and f9 are linearly correlated in DTLZ5(2,10)). A random population of size 31 with samples normalized and Euclidian distance was used to obtain a distance matrix. SS procedure in Figure 3 was not applied. The output of Figure 4 shows variables and objectives arranged into a phylogram with leaf nodes (the

objects under analysis) composing clusters (similarly to the end of the pipeline in Figure 1) - they are identified by the same colour.

Objective functions f1, …, f9 are partitioned into three neighbour clusters ({f1, f2}, {f3, f4, f5, f6} and {f7, f8, f9}) in the phylogram structure; while f10 is together with the leaf nodes corresponding to variables. The phylogram structure aggregates f1, …, and f9 into the same subtree, while f10 is isolated from the other objectives in the complementary subtree. The unique node with the label "100" (another type of result from a tree consensus) splits the phylogram into those two subtrees. Such a label ("100") means that the leaf nodes f10 and x1, .., x10, and f10 were in the same subtree (with the remaining leaf nodes in the complementary subtree) in 100% of all the constructed phylograms, independently on each subtree topology in a phylogram. Such an interpretation suggests a hypothesis: f10 is weakly correlated to the other objectives, which are significantly associated with themselves. Thus, f10 and one of the other objectives could compose an *essential objective set*; this result is consistent with the DTLZ5(2,10) problem structure. The FS-OPA also produces other outputs (useful for human comprehension of some classes of real-world problems), which are explored in Sections related to the extrusion problem.

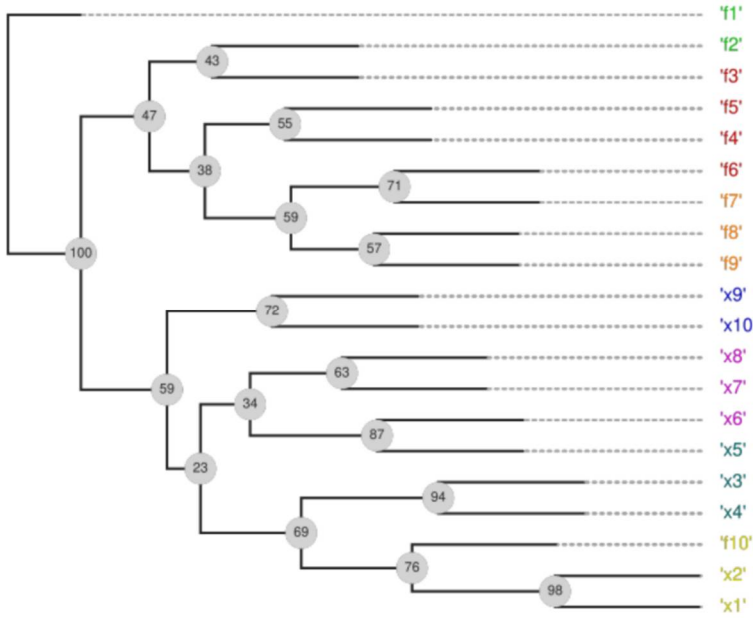


Fig. 4. Phylogram and clustering found for DTLZ5(2,10) with 10 variables in decision space.

4 Case Study

The methodology proposed will be applied to a real-world problem in polymer extrusion in which the complex thermomechanical environment involved is described in detail in Gaspar-Cunha and Covas [28, 29] encompassing the possibility of using inside

the same extruder alternately two different types of screws, a conventional and a Maillefer barrier screw. The complexity of the thermomechanical phenomena taking place, including the flow of solid pellets and melted polymer and the coexistence of both, is described in detail in reference [28], while in reference [29] the numerical model used was assessed experimentally. Table 2 shows the geometrical parameters involved in the description of both types of screws. Considering that only one screw can be used in the machine, an additional decision variable was added, case, to activate the decision variables correspondent to one of the types of screws, i.e., when case ranges in the interval [0.0,0.5] the decision variables of the conventional screw are used while when case ranges in the interval]0.5,1.0] the other screw is considered. Thus, the total number of decision variables is 15.

Table 2. Geometrical parameters of both conventional and Maillefer barrier screws.

Screw Type	**Decision Variables**								
Conventional screw	case	L1	L2	H1	H3	P	e		
Maillefer barrier screw		L1_	L2_	H1_	H3_	P_	e_	Hf	wf
Range of variation	[0,1]	[100,400]	[170.400]	[18,22]	[22,26]	[25,35]	[3,4]	[0.1,0.6]	[3,4]

In the extrusion system, the performance of the process depends on the polymer properties, machine operating conditions and geometry. In the present example, a Low Density Polyethylene (LDPE) is used and the operating conditions were fixed and include: screw rotational speed (N = 40 rpm) and barrel temperature profile in three zones (Tb1= 140ºC, Tb2= 150 ºC and Tb3=160ºC). The geometrical parameters are the decision variables defined randomly by the optimization methodology in the range identified in Table 2. The performance of the machine was quantified using six objectives, two to maximize (machine output, Q (kg/hr) and degree of mixing, WATS) and four to minimize (length of screw required to melt the polymer, L (m), melt temperature at the exit, T (ºC), mechanical power consumption required to rotate the screw, Power (W), and viscous dissipation quantified as the ratio between the melt temperature and the fixed barrel temperature, TTb). Due to a lack of space, more details about this process and all the decision variables and objectives involved the reader is referred to references [28, 29].

The optimizations were made using the SMS- EMOA algorithms. For comparison, and due to the stochastic nature, 11 independent runs with different random numbers were done. For all test runs the population size and the maximum number of generations were set to 50 and 100, respectively.

5 Results and Discussion

The following strategy for analyzing the potentiality of DAMICORE in reducing the number of objectives required for optimization will be pursued:

1. Perform 11 optimization runs using 6 objectives;
2. Apply DAMICORE to the initial population of one of the previous runs;
3. Obtain the phylogram and the distance tables;
4. Perform an analysis of the phylogram and tables and select the minimum number of objectives;
5. Perform 11 optimization runs using the minimum number of objectives;
6. Taking into account the distance between the objectives check if some other objectives can be added;
7. Perform 11 optimization runs using the number of objectives defined in 6;
8. Compare the optimization results using the hypervolume metric.

The application of DAMICORE to the random initial population of one of the optimization runs (steps 2 and 3 above) produces the results presented in Figure 5 and in Tables 2 and 3. Table 2 shows the distances between the decision variables and the objectives obtained from the phylogram of Figure 5. The average distance can quantify the degree of influence of each decision variable in the objectives.

Figure 5 shows the complex relations existent between the decision variables and the objectives, but also between the different objectives. The objectives, identified by black boxes, are assembled in different clusters and in pairs, having the minimum distance between themselves, specifically (Q, L), (Power, WATS) and (T, TTb). Simultaneously, it is possible to see that some decision variables are grouped together with these pairs of objectives, respectively (Q, L, L1, L2), (Power, WATS, L1_, L2_) and (T, TTb, Hf).

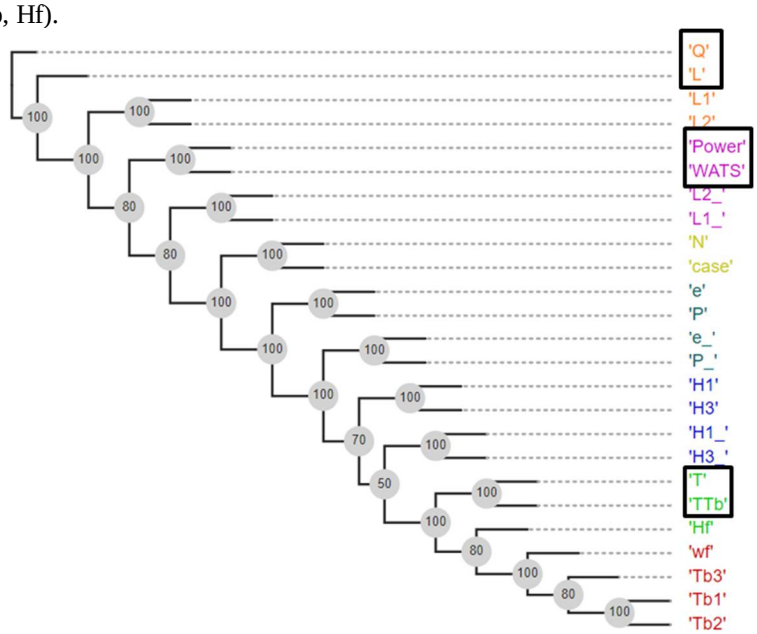


Fig. 5. Phylogram and clustering found for the extrusion problem – initial optimization of the optimization run (the cluster are identified by different colours).

Taking into account the knowledge about the process those relations are not easy to explain. In fact, if only the conventional screw is considered, Q and L depend mainly on the value of H3. Therefore, the application of DAMICORE constitutes, in this apparently simple example, a methodology that is able to capture some other information when the Maillefer barrier screw is also considered. This is, the technique applied is able to capture the indirect influence of the H3 on Q and L through the value of L1 and L2 because these variables (and also L1_ and L2_ for Power and WATS) determine the length of the barrier (since it finishes after L1+L2) and as consequence, the location of the screw were H3 acts.

Table 2. Distances between the decision variables and the objectives for the phylogram of Figure 5.

	'Q'	**'L'**	**'T'**	**'Power'**	**'WATS'**	**'TTb'**	**Average**
'L2'	0.20	0.20	0.73	0.27	0.27	0.73	**0.40**
'L2_'	0.33	0.33	0.60	0.27	0.27	0.60	**0.40**
'L1_'	0.33	0.33	0.60	0.27	0.27	0.60	**0.40**
'L1'	0.20	0.20	0.73	0.27	0.27	0.73	**0.40**
'case'	0.40	0.40	0.53	0.33	0.33	0.53	**0.42**
'N'	0.40	0.40	0.53	0.33	0.33	0.53	**0.42**
'e'	0.47	0.47	0.47	0.40	0.40	0.47	**0.44**
'P'	0.47	0.47	0.47	0.40	0.40	0.47	**0.44**
'e_'	0.53	0.53	0.40	0.47	0.47	0.4	**0.46**
'P_'	0.53	0.53	0.40	0.47	0.47	0.4	**0.46**
'H3_'	0.60	0.60	0.33	0.53	0.53	0.33	**0.48**
'H1_'	0.60	0.60	0.33	0.53	0.53	0.33	**0.48**
'H3'	0.67	0.67	0.27	0.60	0.60	0.27	**0.51**
'H1'	0.67	0.67	0.27	0.60	0.60	0.27	**0.51**
'Hf'	0.73	0.73	0.20	0.67	0.67	0.20	**0.53**
'wf'	0.80	0.8	0.27	0.73	0.73	0.27	**0.60**
'Tb3'	0.87	0.87	0.33	0.80	0.80	0.33	**0.66**
'Tb1'	0.93	0.93	0.40	0.87	0.87	0.40	**0.73**
'Tb2'	1.00	1.00	0.47	0.93	0.93	0.47	**0.80**
Average	**0.5647**	**0.5647**	**0.4384**	**0.5126**	**0.5126**	**0.4384**	

Some other relations can be explained, for example, the cluster (T, TTb, Hf) exists because the melt temperature (T) value is controlled by the viscous dissipation generated in the gap with size Hf.

A conclusion from the simultaneous analysis of Figure 5 and Table 3 is that, instead of using the 6 objectives, can be possible to use during the optimization only one objective of each pair (steps 4 and 5 above), for example, Q, WATS and T, given that the objectives belonging to the same cluster are strongly related.

Finally, an analysis of Table 3 (steps 6 and 7 above) shows that the minimum distance between objectives is 0.325 for Power and WATS. This clearly means that these two objectives (and also Q and L, since their distance is also low, 0.345) have a strong connection with all the others, i.e., they aggregate more information of all objectives and, as a consequence, of the decision variables. The idea is to include one of these objectives in the optimization process. In the end, instead of having 6 objectives, the optimization can be performed with three of four objectives.

Therefore, the following cases were selected to perform 11 optimization runs using SMS-EMO to compare the corresponding performance using the hypervolume metric:

Case 1- 6 objectives, Q, L, Power, WATS, T and TTb;

Case 2- 4 objectives: Q, L, WATS and T;

Case 3- 4 objectives: Q, Power, WATS and T;

Case 4: 3 objectives: Q, WATS and T.

The idea is to conclude what information is lost when the number of objectives is reduced taking into account the methodology proposed here.

Table 3. Distances between the objectives for the phylogram of Figure 5.

	'Q'	**'L'**	**'T'**	**'Power'**	**'WATS'**	**'TTb'**	**Average**
'Q'	0.00	0.07	0.73	0.27	0.27	0.73	**0.345**
'L'	0.07	0.00	0.73	0.27	0.27	0.73	**0.345**
'T'	0.73	0.73	0.00	0.67	0.67	0.07	**0.478**
'Power'	0.27	0.27	0.67	0.00	0.07	0.67	**0.325**
'WATS'	0.27	0.27	0.67	0.07	0.00	0.67	**0.325**
'TTb'	0.73	0.73	0.07	0.67	0.67	0.00	**0.478**

6 Conclusions

A methodology based on machine learning was presented and applied in the reduction of the number of objectives for multiobjective optimization using MOEAs. This approach has some important characteristics that are an important improvement concerning similar state-of-the-art methodologies, namely: it allows analysis of the relations variable-variable and variable-objectives (and not only objective-objective), does not need kernel function choice and parameters optimization, allows to interpret of the results to help the decision maker, its time complexity is low and supports theoretical and empirical sample-size.

The application of the methodology to the well-known DTZL5(2,10) benchmark problem showed its potential to reduce the number of objectives by capturing the complex relations between the different objectives, with an additional possibility that is to capture the relations objectives-variables.

The resolution of a difficult real-world problem using the approach proposed has proven that almost automatically it is possible to reduce the number of objectives by losing only less than ten per cent of the Pareto-optimal frontier obtained. Additionally, the intervention of the decision maker during the process, e.g., when selecting the objectives to be considered in the optimization, can be very useful because the person interested is able to see how the process works and to interpret the results obtained. Finally, an important characteristic of the method proposed is the capacity to explain the results obtained.

As a future work, the methodology will be compared with other approaches in the literature.

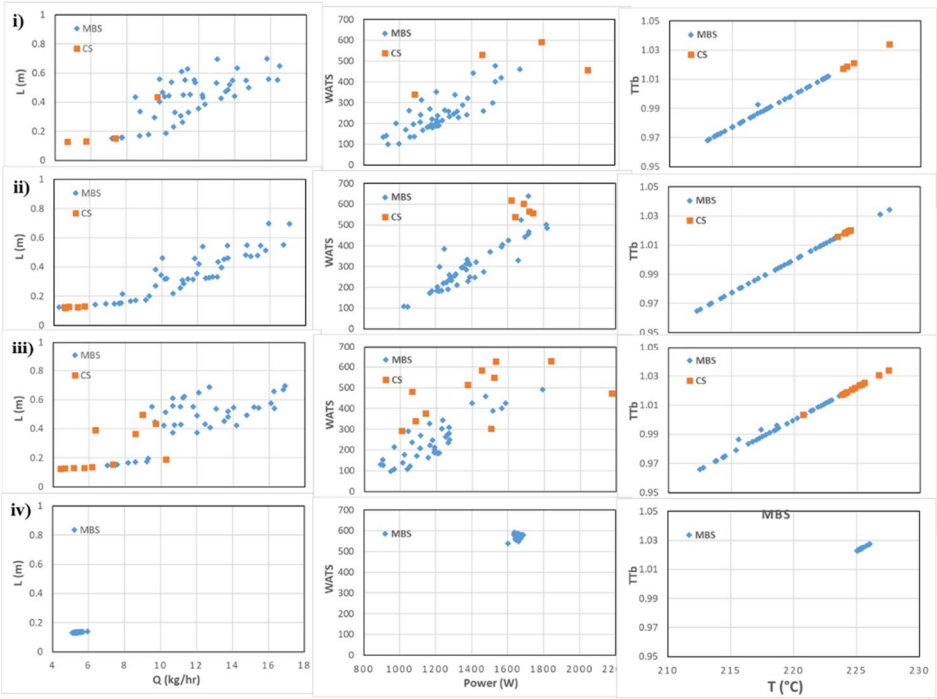


Fig. 6. Pareto-optimal fronts for the 4 cases studies: i) 6 objectives; ii) 4 objectives (Q, L, WATS, T), iii) 4 objectives (Q, Power, WATS, T); iv) 3 objectives (Q, WATS, T).

Table 4. Hypervolume for the 4 cases studied and relative loss percentage.

6 Objectives	4 Objectives (Q, L, WATS, T)	4 Objectives (Q, Power, WATS, T)	3 Objectives (Q, WATS, T)
0.24636	0.22754	0.22215	0.02117
----	7.6%	9.8%	91.4%

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