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# Surrogate-Assisted Multicriteria Optimization: Complexities, Prospective Solutions, and Business Case

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## ABSTRACT

Complexity in solving real-world multicriteria optimization problems often stems from the fact that complex, expensive and/or time-consuming simulation tools or physical experiments are used to evaluate solutions to a problem. In such settings it is common to use efficient computational models, often known as surrogates or meta-models, to approximate the outcome (objective or constraint function value) of a simulation or physical experiment. The presence of multiple objective functions poses an additional layer of complexity for surrogate-assisted optimization. For example, complexities may relate to the appropriate selection of metamodelling for the individual objective functions, extensive training time of surrogate models, or the optimal use of many-core computers to approximate efficiently multiple objectives simultaneously. Thinking out of the box, complexity can also be shifted from approximating the individual objective functions to approximating the entire Pareto-front. This leads to further complexities, namely how to validate statistically and apply the techniques developed to real-world problems. In this paper we discuss emerging complexity-related topics in surrogate-assisted multicriteria optimization that may not be prevalent in non-surrogate-assisted single-objective optimization. These complexities are motivated using several real-world problems in which the authors were involved. We then discuss several promising future research directions and prospective solutions to tackle emerging complexities in surrogate-assisted multicriteria optimization. Finally, we provide insights from an industrial point of view into how surrogate-assisted multicriteria optimization techniques can be developed and applied within a collaborative business environment to tackle real-world problems.

**KEY WORDS:** Evolutionary multicriteria optimization, multiple criteria decision making, surrogates, meta-models, expensive optimization problems, machine learning

## 1 Introduction

In real-world optimization it is very common to use either physical experimentation or simulators to evaluate candidate solutions to a problem (see e.g. Rechenberg (2000); Jakumeit and Emmerich (2004); Knowles (2009); Small et al. (2011); Allmendinger et al.

(2014)). Such evaluation procedures can be costly and time-consuming, and often there is only a limited budget of evaluations available. *Surrogate-assisted optimization* (Jin, 2011; Santana-Quintero et al., 2010; Tabatabaei et al., 2015), which is sometimes also referred to as *metamodel-assisted optimization*, is a popular computational technique for tackling such prob-

lems. The focus of this paper is on surrogate-assisted multicriteria optimization, which is concerned with the development and application of surrogate-assisted optimization to problems with multiple (conflicting) objectives.

The motivation for using surrogate-assisted optimization is to reduce the number of expensive evaluations by approximating some of the evaluation outcomes (i.e. objective or constraint function values). Examples of expensive evaluations include time-consuming simulations, such as computational fluid dynamics (CFD) simulations (Rezaveisi et al., 2014), or a real physical experiment, such as drug mixing experiment (Small et al., 2011), all of which may take between hours and several days.

Over the last decade, the research field around surrogate-assisted optimization has been reviewed from different angles. For example, Ong et al. (2005) reviews frameworks that employ surrogate models, Santana-Quintero et al. (2010) reviews different surrogate techniques used within multicriteria evolutionary computation as well as their real-world applications, while Jin (2011) provides an overview of recent developments in surrogate-assisted evolutionary computation and suggests future trends in this research domain. Arguably, the most recent review in this field is the one of Tabatabaei et al. (2015) providing an overview of existing surrogate-assisted multicriteria optimization algorithms. Rather than focusing on specific algorithms, this paper fills a gap in the area by reviewing emerging complexity-related topics specific to surrogate-assisted multicriteria optimization, and then discussing recently proposed solutions or prospective solution ideas on how to tackle some of these complexities. Finally, to facilitate the process of tackling real industrial problems, this paper discusses the building blocks and steps involved in developing and applying surrogate-assisted multicriteria optimization within a collaborative business environment.

The remainder of the paper is organized as follows. Section 2 provides an overview of the state-of-the-art in surrogate-assisted multicriteria optimization with a particular focus on the evolution of this research field, commonly-used techniques, and various aspects that need to be accounted for when dealing with surrogates. In Section 3 we will outline sev-

eral challenging real-world problems in which the authors of this paper were involved. They can be viewed as motivational examples, pointing out where complexities in surrogate-assisted multicriteria optimization arise. Section 4 will review these complexities in more detail. Several promising research directions and initial ideas for tackling some of the complexities in surrogate-assisted multicriteria optimization are discussed in Section 5. Section 6 makes the crucial transition from academia to business by giving insights into how surrogate-assisted multicriteria optimization techniques can be developed in collaboration between an algorithm designer and an industrial partner to tackle real-world problems. Finally, the paper concludes with a summary in Section 7.

## 2 State-of-the-art in surrogate-assisted multicriteria optimization

A large number of surrogate-assisted multicriteria optimization algorithms have been proposed over the past years. In the following, we briefly review the state-of-the-art according to four important questions that need to be answered in surrogate-assisted optimization algorithms: (i) which type of models is used as surrogate, (ii) what should the surrogate model approximate, (iii) where to use the surrogate model, and (iv) how to manage the surrogate model. A few other issues related to surrogate techniques are also discussed.

### 2.1 Which model to use?

The first question to answer in surrogate-assisted multicriteria optimization is to decide which type of models should be used as the surrogate. Available models range from polynomials, also known response surface methods, Gaussian processes, often known as Kriging models, or design and analysis of computer experiments (DACE), support vector machines, feed-forward neural networks, recurrent neural networks, radial-basis-function (RBF) networks, or fuzzy systems.

Although there is no simple rule for determining which type of models should be used as surrogates (Santana-Quintero et al., 2010), it is important to consider whether a global model or a local model is more beneficial, and whether a deterministic or probabilistic model is more desirable. In particular, Kriging models have become increasingly popular for surrogates, mainly due to the fact that they are able to provide information about the model uncertainty that is very useful for surrogate management. Optimization using Kriging models is usually termed efficient global optimization (EGO) (Jones et al., 1998; Schonlau et al., 1998; Torczon and Trosset, 1997) although the ideas date back to earlier research by Mockus and Zilinskas (Mockus et al., 1978) under different names.

While most work on surrogate-assisted optimization uses a single surrogate model, using multiple models, either a plethora of models of the same type, or a number of different models is in principle helpful. For example, a surrogate combining a polynomial model and an RBF network for objective prediction for multicriteria hydraulic turbine diffuser shape optimization was reported in (Marjavaara et al., 2007). In (Lim et al., 2010), two surrogates were used in local search, one global surrogate, a low-order polynomial model to approximate the rough landscape, and a local surrogate consisting of an ensemble of models for learning local details of the fitness function. In (Rosales-Perez et al., 2013), an ensemble of support vector machines has been adopted for predicting the objectives. Similar ideas have also been reported in (Arias-Montano et al., 2012), where multiple surrogates are generated, from which one will be chosen to be re-evaluated based on a Tchebycheff scalarizing function. The idea of maintaining multiple metamodels or ensemble of metamodels where the best metamodel can be adaptively selected during the optimization run was adopted also, for example, in (Gorissen et al., 2009; Jin, 2011; Le et al., 2013; Yang et al., 2002). In (Pilat and Neruda, 2012), a surrogate is used to approximate a distance metric for selection while a second surrogate is used to approximate the objectives separately for local search.

## 2.2 What to approximate?

In single-objective optimization, surrogates are usually trained to approximate the functional map between the decision variables and the objective function to be optimized, with very few exceptions where the surrogate is employed to predict the rank of the solutions (Loshchilov et al., 2010b). Research results have also been reported, where an ensemble of recurrent neural networks are used for predicting the converged results of computational fluid dynamics simulations (Smith et al., 2013).

By contrast, in surrogate-assisted multicriteria optimization, various targets can be chosen for surrogates to approximate. The most straightforward idea is to approximate the objectives (Ahmed and Qin, 2012; Brownlee et al., 2015; Chafekar et al., 2005; Di Nuovo et al., 2012; Gaspar-Cunha and Vieira, 2005; Georgopoulou and Giannakoglou, 2009; Isaacs et al., 2007; Karakasis and Giannakoglou, 2005; Singh et al., 2010; Zhang et al., 2010); a review of these approaches can be found in (Tabatabaei et al., 2015). A different idea is to construct a single model of a scalarized function of the objectives as done by e.g. ParEGO (Knowles, 2006). An alternative idea is to approximate the distance of the candidate solutions to the non-dominated front in the current archive (Pilat and Neruda, 2011, 2012, 2013). This task has also been achieved using a data envelope analysis, see e.g. (Yun et al., 2004, 2011)

In multicriteria optimization, the absolute objective values may become less important if the dominance relationship is known. Therefore, surrogates have been trained to distinguish non-dominated solutions from dominated ones in (Loshchilov et al., 2010a). A more recent paper (Bandaru et al., 2014) proposed to train a multi-class surrogate classifier that is able to determine the dominance relationship between two candidate solutions. In (Bhattacharjee and Ray, 2015), a support vector machine based surrogate is trained to learn the ranking of solutions for constrained multicriteria optimization problems. In (Zhang et al., 2015), a classifier based on a regression tree or a k-nearest-neighbour (KNN) is trained to distinguish good solutions from bad ones.

In addition to constructing surrogates mapping from the decision space to objective space, other simple

strategies for fitness estimation, in particular similarity based methods can also be helpful (Fonseca et al., 2010; Sun et al., 2013). Moreover, techniques for the approximation of the Pareto front (Binois et al., 2015; Calandra et al., 2014; Campigotto et al., 2014; Miranda and Zuben, 2015; Eskelinen et al., 2010; Haanpää, 2012; Hartikainen et al., 2012; Monz et al., 2008) in combination of an inverse model based evolutionary optimization algorithm (Cheng et al., 2015a) may also be of interest. Here, the input for training the surrogate is a (small) set of precomputed non-dominated solutions. The resulting surrogate can then be used for example for fast decision making with interactive multicriteria optimization methods (Haanpää, 2012; Hartikainen et al., 2012) or a posteriori generation of non-dominated solutions (Cheng et al., 2015b). Typically in multicriteria optimization the number of objective functions is smaller than the number of decision variables and, therefore, building a surrogate for the Pareto front in the objective space can be beneficial.

Finally, for performance-indicator based multicriteria evolutionary algorithms, surrogates have been trained to approximate the hypervolume contribution of a newly created individual in a steady-state multicriteria evolutionary algorithm using an artificial neural network (Azzouz et al., 2014a).

### 2.3 Where to use surrogates?

In multicriteria optimization, a surrogate model can be used in various components of the evolutionary algorithm. In most cases, the surrogate is used in assisting the selection process in dominance based, performance indicator based or decomposition based evolutionary algorithms.

A slightly different approach is to use the surrogate for pre-selection or pre-screening. Pre-selection is often used in reproduction, where many additional candidate solutions are generated using crossover or mutation or other genetic operators (W.Gong et al., 2015; Loshchilov et al., 2010c). These solutions are then evaluated using the surrogate and the better ones according to the surrogate are indeed used as offspring.

Finally, surrogate models can be used in local search embedded in a multicriteria evolutionary algo-

rihm (Lim et al., 2010; Martinez and Coello Coello, 2013; Pilat and Neruda, 2012).

### 2.4 How to manage the surrogates?

One important issue, again similar to surrogate-assisted single-objective optimization, is to determine which solutions should be re-evaluated and when should the surrogate be updated. This is often known as model management, or evolution control in surrogate-assisted evolutionary algorithms. Depending on where the surrogate is employed in the evolutionary algorithm, the following criteria have been proposed for selecting individuals to be re-evaluated and then updating the surrogate.

The simplest approach to managing surrogates is to fully rely on the surrogate once it is created. This is clearly a simplistic approach, and it works only in very special situations where, e.g., the decision space is of very low dimensionality and sufficient number of training samples have been collected to train the surrogate so that the surrogate is able to adequately approximate the original objective functions without introducing false optima (Jin, 2005, 2011).

In single-objective optimization, better solutions according to the surrogates are often chosen for re-evaluation using the original expensive objective function. This is known as the best strategy (Jin, 2005). Similarly, in multicriteria optimization, non-dominated solutions according to surrogate can be selected for re-evaluation (Arias-Montano et al., 2012; Bhattacharjee and Ray, 2015; Di Nuovo et al., 2012; Karakasis and Giannakoglou, 2005; Seah et al., 2012).

When the surrogates are used for pre-selection, it is typical that all chosen solutions (better ones according to dominance or some distance measure) will be re-evaluated using the original expensive objective functions (W.Gong et al., 2015; Loshchilov et al., 2010b; Pilat and Neruda, 2012; Zhang et al., 2015). On the other hand, in case the surrogate is employed in local search, the found optimum at the end of the local search will be re-evaluated (Lim et al., 2010; Martinez and Coello Coello, 2013; Pilat and Neruda, 2014).

A commonly-used metric for choosing individuals for re-evaluation in surrogate-assisted optimization has been developed in combination with the Kriging

model or Gaussian processes. An excellent summary of this group of methods can be found in (Wagner et al., 2010; Horn et al., 2015).

Ideas of taking advantage of the prediction uncertainty introduced by the Kriging model were presented in (Dennis and Torczon, 1997; Schonlau et al., 1998) for managing surrogates in using traditional optimization methods. Three related but different criteria have been suggested, namely, lower confidence bound (LCB), probability of improvement (PoI) and expected improvement (EI). These ideas were at first applied to evolutionary single-objective optimization (Jin, 2011), where two slightly different criteria, termed expected improvement (EI) and probability of improvement (PoI) have been adopted (Ulmer et al., 2003; Büche et al., 2005).

One issue remains to be discussed when these criteria originally developed for single-objective optimization is to be employed for multicriteria optimization. The key question is how to measure the improvement of multicriteria optimization in terms of a scalarized function. In the literature, various definitions have been proposed, including an augmented Tchebycheff aggregation (Knowles, 2006), an EI for each objective separately (Jeong and Obayashi, 2005; Zaefferer et al., 2013), maximum over different weighted Tchebycheff aggregation (Zhang et al., 2010), Euclidean distance to the nearest vector of the Pareto front (Keane, 2006) and hypervolume (Emmerich et al., 2006b). Among these different approaches, empirical studies (Horn et al., 2015; Wagner et al., 2010) indicate that the distance based method (Keane, 2006) does not work well, and a performance based approach, e.g., a hypervolume based EI is usually better. The next section provides further background knowledge to the powerful EI metric and its application in multicriteria optimization.

#### 2.4.1 Multicriteria Expected Improvement (EI)

The concept of EI has its origin in Bayesian global optimization (Mockus et al. (1978)), which was later popularized and further developed under the new name efficient global optimization (cf. Jones et al. (1998)). In general this criterion requires surrogate models that output a prediction with a prediction variance, such

as Kriging or Gaussian Processes. It rewards points with high expected values and at the same time points in under-explored parts in the search space where the variance is high.

The first proposal to use EI for multicriteria computation was to compute the expected improvement of the hypervolume indicator (Emmerich, 2005). The hypervolume indicator measures the size of the space dominated by the current approximation of the Pareto front and cut from above by a reference point (to make the measure finite). It uses the predictor of Kriging models represented as multivariate random distribution. It rewards points that are located in less explored regions and therefore have a relatively high prediction variance (Emmerich et al., 2011). For a graphical explanation, see Figure 1.

The EI criteria can be used in the selection of evolutionary algorithms (Giannakoglou, 2002; Emmerich et al., 2005, 2006a; Azzouz et al., 2014b) or as in-fill criterion in efficient global optimization (Knowles, 2006; Ponweiser et al., 2008; Shimoyama et al., 2012; Zaefferer et al., 2013). Efficient exact computation algorithms for the multivariate expected improvement are discussed in Couckuyt et al. (2014); Hupkens et al. (2015). While its complexity is growing exponentially with the number of objective functions, under  $NP \neq P$ , in low objective space dimensions it can be computed efficiently in  $\Theta(n \log n)$  time (Emmerich et al., 2016).

Another proposal to generalize EI for multicriteria optimization was used in the ParEGO algorithm (Knowles, 2006). It computes the expected improvement with respect to weighted Tchebycheff distances to an ideal point and this way decomposes the multicriteria optimization problem into a series of single objective optimization problems. Different ways to define expected improvement in stochastic and deterministic multicriteria optimization are reviewed in Wagner et al. (2010) and in Zilinskas (2014). In a recent work the expected improvement criterion was also compared to probability of improvement criteria (Zilinskas, 2014).

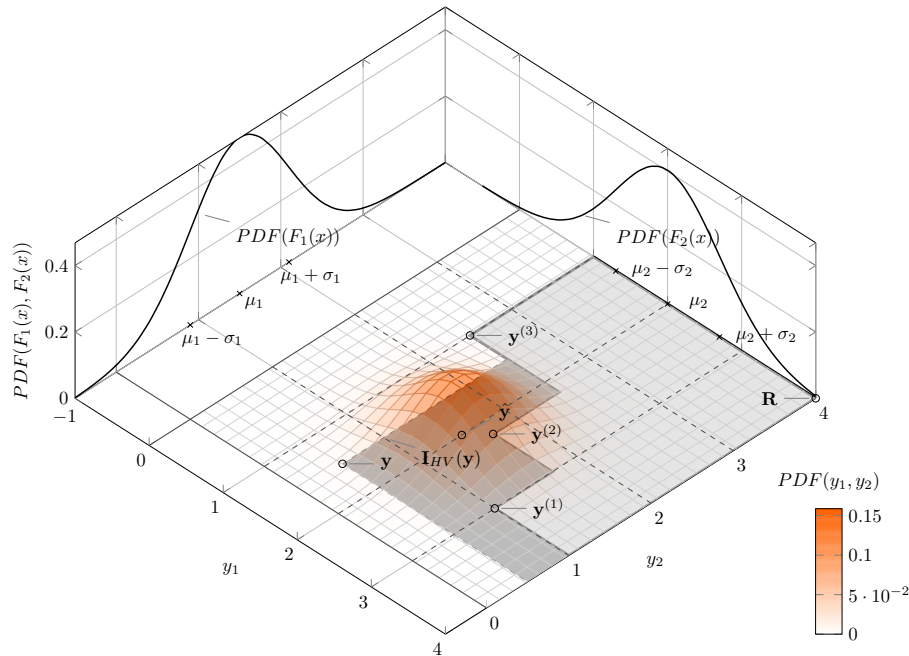


Figure 1: Schematic view of the expected hypervolume improvement for some bicriteria minimization problem. The horizontal axis span the objective space. A probability density function (PDF) defines the likelihood of different outcomes of the computer experiment at a design point  $x$ . The area of the light shaded is the hypervolume indicator of the current population ( $\mathbf{y}^{(1)}, \mathbf{y}^{(2)}, \mathbf{y}^{(3)}$ ). If the sample  $\mathbf{y}$  would be added to the population the hypervolume indicator would grow by the area of the dark shaded region ( $\mathbf{I}_{HV}(\mathbf{y})$ ). The mean value of the distribution is indicated with  $\hat{\mathbf{y}}$ . The expected gain in the hypervolume indicator  $\int_{-\infty}^{R_1} \int_{-\infty}^{R_2} dy_1 dy_2$  is the 2-D expected hypervolume improvement.

## 2.5 Other related ideas

A few important issues related to surrogate construction deserve some further discussions. First, it has empirically been demonstrated that using a design of experiments (DOE) method, e.g., the Latin Hypercube Sampling, for population initialization or even in reproduction is always beneficial. In addition, it might also be desirable to use certain resampling techniques in validating surrogates during optimization (Bischl et al., 2012).

Finally, surrogate-assisted combinatorial optimization (Brownlee and Wright, 2015; Zaefferer et al., 2014b), surrogate-assisted many-objective optimization (Pilat and Neruda, 2013), and surrogate-assisted

large-scale optimization are challenging research topics that need more research efforts. The next section will motivate some of these challenges using real-world applications in which the authors of this work were involved.

## 3 Applications of surrogate-assisted multicriteria optimization

Surrogate-assisted optimization has been applied to a variety of real-world multicriteria problems ranging from shape design problems and analytical instrument

setup problems over to manufacturing process optimization, evolutionary robotics, drug design, and protein folding. This sections describes some of these problems and highlights why surrogate-assisted optimization has been the preferred choice of approach.

### 3.1 Experimental optimization of chromatographic operating conditions

Purification is an essential step in the production of biopharmaceuticals aiming at separating the protein of interest from impurities and debris created further upstream in the production process. Chromatography (Scopes, 1994) is a commonly-used technique for purifying proteins but involves the tuning of several operating parameters (e.g. pH, salt and loading concentrations) to perform efficiently and cost-effective. Here, efficiency is commonly measured in terms of recovery yield and product purity (but additional objectives can be considered). A biopharmaceutical production process can consist of several chromatography steps (operated in sequence) resulting in 15 or more decision variables in total, which can be considered as a rather large search space in the context of surrogate-assisted optimization. Due to the limited knowledge in designing reliable and accurate simulation models for chromatography, the tuning of chromatographic operating conditions is primarily done via time-consuming and expensive physical experimentation. Figure 2 visualizes the experimental platform employed in (Allmendinger et al., 2014). To reduce costs and experimental time, an experiment (defined here as the evaluation of a sequence of chromatography steps) is often terminated prematurely as soon as a chromatography step (within a sequence of steps) with an unacceptable purity performance is evaluated, leading to missing objective function values. In (Allmendinger et al., 2014) this optimization scenario was simulated and a surrogate-assisted optimization algorithm was proposed to cope with missing objective function values.

### 3.2 Optimizing the energy performance of buildings

When designing buildings, so-called Building performance simulation tools can be used to simulate the en-

ergy flows in a building and relate it to energy performance indicators. In the design phase architects and engineers are working together. Typically there are some degrees of freedom that the design engineer can exploit to optimize energy performance, such as the positioning of the HVAC (climate control) and parameters of the windows. However, some material parameters and environmental parameters are typically unknown, and one design needs to be simulated under different settings in order to obtain a robust performance estimate. In the research by Hopfe et al. (2012), it was proposed to replace partially the simulator by a metamodel when it comes to robustness optimization. Note, that opposed to other approaches the uncertain parameters are not necessarily decision variables but uncontrollable (environmental) parameters. In the study by Hopfe et al. (2012) a worst case assumption was taken, that is a building should perform well in the criteria energy consumption and thermal comfort in the worst case over all tested parameter settings (cf. Figure3). The case study was done for a model of the Bouwhuis office building in Zoetermeer, The Netherlands.

### 3.3 Optimizing airfoil shapes

An area where surrogate-assisted multicriteria optimization has been studied already relatively early and intensely is the optimization of airfoils (Giotis et al., 2000; Giannakoglou, 2002; Jeong and Obayashi, 2006). The decision variables are typically Bezier control points that define the shape of the airfoil. The flow is then simulated by expensive computational fluid dynamics (CFD) solvers. Conflicting objective functions can be drag and lift at different flight conditions. Typically, radial basis function networks (Giotis et al., 2000; Giannakoglou, 2002) and Kriging methods (Jeong and Obayashi, 2006) have been used in this domain. A common scheme is to use the surrogate model as a pre-selection criterion in the selection operator of an evolutionary algorithm. In addition, also an estimate of the prediction uncertainty has been utilized in order to improve global optimization performance (see e.g. Emmerich et al. (2006a)).

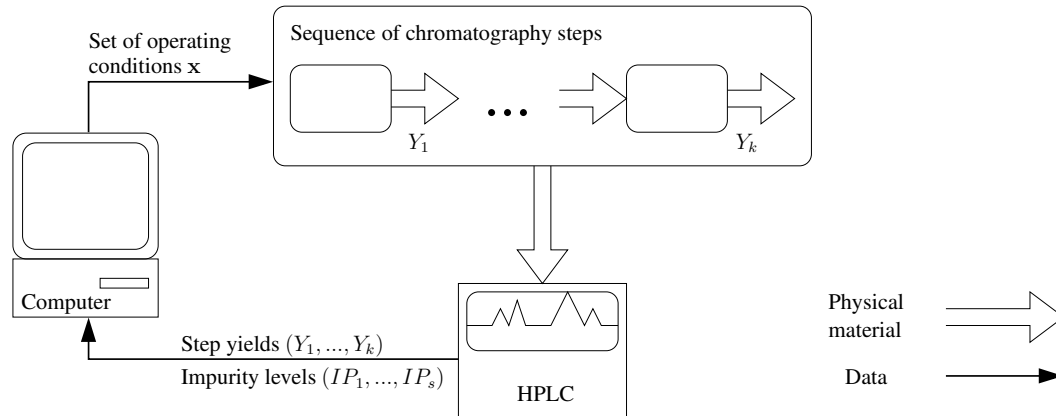


Figure 2: Schematic of a typical experimental setup for the optimization of chromatographic operating conditions. Following the set up of the operating conditions, defined by  $\mathbf{x}$ , the sample is passed through a sequence of chromatography steps  $i = 1, \dots, k$ . An HPLC device is used to obtain the step yields  $Y_i$  and the final levels of individual impurities  $IP_j, j = 1, \dots, s$ . Based on this quality measure, an optimizer running on the computer then selects the next set of operating conditions for testing.

### 3.4 Algorithm and controller configuration

There are various examples where surrogate-assisted search has been used in tuning or configuring the control parameters of algorithms and controllers. In Zafferrer et al. (2013) the parameters of an event controller for monitoring water quality are tuned by surrogate assisted multicriteria optimization, minimizing false positive rates and false negative rates. Due to a limited number of trials, efficient global optimization was used here that replaces the true objective function by a Gaussian process model that is used to identify additional points for precise evaluation. Similar ideas were studied for noisy objective functions (classification time, accuracy) in Koch et al. (2015). Here surrogate-assisted optimization of machine learning methods was performed, considering noise in the objective functions. Every run of the machine learning method on a randomized test set served as evaluation. This time consuming evaluation was then partially replaced by a surrogate model. The two objective functions that were considered were time (cost) of classification and the accuracy on the test data.

The next section will review the challenges arising

in problems that feature computationally expensive or costly evaluations, such as the ones outlined above, in more detail.

## 4 Challenges and sources of complexity in surrogate-assisted multicriteria optimization

The challenges present generally in multicriteria optimization like e.g. high number of objectives, constraints and decision variables are also relevant for surrogate-assisted multicriteria optimization. On the other hand, using surrogates to ease the computational complexity generates additional challenges that are not necessarily relevant for multicriteria optimization without surrogates. Examples of specific challenges arising from the use of surrogates are the role of the surrogate in multicriteria optimization, selection of specific metamodeling technique to be used and the training time required for obtaining accurate enough surrogate. A number of reviews related to surrogate-assisted multicriteria optimization have been published in recent years (see e.g. Knowles and

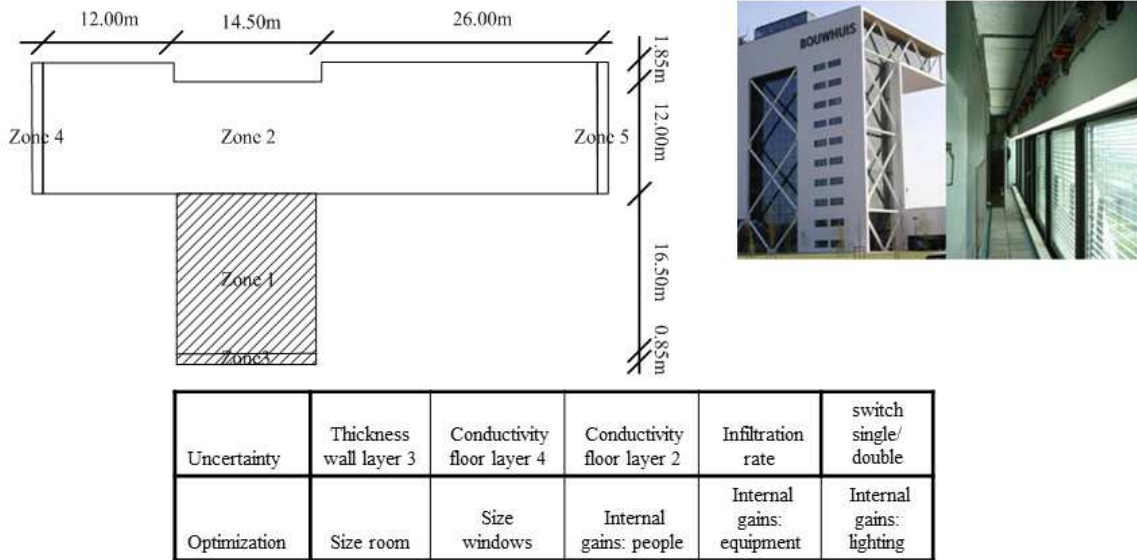


Figure 3: The simulation the building energy consumption and thermal comfort for a building over the period of a year takes several minutes. In order to test the sensitivity of the result several runs with different settings of the uncertain variables are required. In Hopfe et al. (2012) surrogate modeling was used to accelerate the sensitivity analysis of intermediate solutions in the optimization process which was carried out by a evolutionary multicriterion optimization algorithm (SMS-EMOA).

Nakayama (2008); Jin (2011); Santana-Quintero et al. (2010); Tabatabaei et al. (2015)) and some of the challenges related to computationally expensive multicriteria optimization problems have also been identified in a recent review on multicriteria evolutionary algorithms (Zhou et al., 2011). In what follows, the challenges identified in the above-mentioned reviews as well as challenges added by us are described in more detail in this section.

### 4.1 General challenges in multicriteria optimization relevant for surrogate-assisted optimization

Here the challenges present generally in multicriteria optimization are considered from the surrogate-assisted point of view.

#### 4.1.1 Large number of decision variables/constraints/objectives

Typical challenges in solving (multicriteria) optimization problems include a large number of decision variables as well as a large number of constraints (Coello Coello, 2002). When dealing with surrogate-assisted methods, a high dimensional decision space is challenging due to the frequent need of sampling in order to obtain accurate enough surrogates to be reliably used in optimization. The curse of dimensionality suggests that for many continuous function classes the number of samples that are required to achieve a certain model accuracy grows exponentially with the number of dimensions (Novak, 1988).

Handling high dimensional problems (decision variables/constraints/objectives) was identified as a challenge also in reviews (Knowles and Nakayama, 2008; Tabatabaei et al., 2015; Zhou et al., 2011).

Solving multicriteria optimization problems having a high number of objective functions is a challenging task. This has been especially relevant for evolutionary multicriteria optimization where approximating the whole Pareto front is not trivial for problems with more than 3-4 objectives, e.g., since most of the solutions become non-dominated in high dimensional spaces (Fleming et al., 2005; Ishibuchi et al., 2008). Recent methods like MOEA/D (Zhang and Li, 2007) and NSGA-III (Deb and Jain, 2014) have been able to overcome this challenge. However, these algorithms are not able to solve computationally expensive problems with a high number of objectives as such. One way to tackle this is to combine techniques of interactive multicriteria optimization (see e.g. Branke et al. (2008); Miettinen (1999)) and surrogates. Some examples of these are given in (Eskelinen et al., 2010; Haanpää, 2012; Hartikainen et al., 2012; Monz et al., 2008).

#### 4.1.2 Dynamic optimization / dynamically changing problem

Solving dynamic multicriteria optimization problems was identified as a challenge by Zhou et al. (2011), especially for surrogate-based methods (Jin, 2011). Recently, problems with dynamic resource constraints (termed by the authors as ephemeral resource constraints) (Allmendinger and Knowles, 2013b) and changing decision variables (Allmendinger and Knowles, 2010) arose, particularly in the experimental optimization community. Further, dynamically changing objective functions can increase the complexity further (Branke, 2001; Nguyen et al., 2012).

#### 4.1.3 Noise and uncertainty

Noise and uncertainty are byproducts that are common in simulation-based and experimental optimization, and appropriate methods are needed for solving such problems (Jin and Branke, 2005). Using surrogate-based multicriteria optimization methods for solving problems with noise and/or uncertainty remains a challenge as reported in Jin (2011); Tabatabaei et al. (2015) due to the fact that it is difficult to obtain accurate enough surrogates for such problems. Uncertainty can

exist both in the decision space and in the objective space. An example of noise is measurement errors typically present in experimental optimization (Small et al., 2011), whilst imprecise knowledge about the model used in simulation-based optimization would represent a classical example of uncertainty (Fleming et al., 2005).

#### 4.1.4 Optimal use of many-core computers

Recent problems in simulation-based (multicriteria) optimization may feature time consuming objective function evaluations (simulations). Those problems can be solved by using general optimization algorithms, but often, algorithms tailored for such problems are needed if, for example, there exist a time limitation (see Gong et al. (2015) for a recent review on distributed evolutionary algorithms). One approach could be to utilize parallelization of the algorithm or the function evaluations (Alba et al., 2013; Horn et al., 2015).

## 4.2 Challenges specific to surrogate-assisted optimization

In Section 2 we have reviewed the four main challenges that are specific to surrogate-assisted optimization including metamodel selection (Section 2.1), application (Section 2.2), usage (Section 2.3), and management (Section 2.4). In the following, we will point out several other challenges specific to surrogate-assisted optimization that may not be as prevalent or do not exist with standard optimization techniques.

### 4.2.1 Training time

An important aspect in surrogate-assisted optimization is the time needed to train the metamodels used. If training takes too long, then it can significantly reduce the time saved by metamodeling. For example, if the data used in training is large, then matrix inversion needed in some metamodels could be time consuming (Knowles, 2006). It is interesting to notice that in almost all publications of surrogate-assisted multicriteria optimization, the training time is not reported as pointed out in (Tabatabaei et al., 2015).

#### 4.2.2 Discrete and mixed-integer search spaces

While applications with both discrete and continuous decision variables feature a general challenge to optimization, their presence can become a serious issue for surrogate-assisted optimization (Jin, 2011; Knowles and Nakayama, 2008; Li et al., 2008). The reason is that surrogate models designed over continuous variables typically rely on the assumption of continuity meaning small changes in the variables will result also in small changes in the objective function values. This assumption may not be valid with discrete variables. For example, if a discrete variable represents different equipments in a manufacturing process optimization problem, then varying the variable and thus equipment may have a completely different impact on the objective function value (which e.g. could be process yield or costs). To cope with discrete variables, recent work looked, for example, at constructing surrogates based on alternative notions of distances between neighboring points in the search space. A popular approach here is to compute relative distances using radial-basis function networks (Li et al., 2008; Bajer and Holeňa, 2010; Moraglio and Kattan, 2011). Other research (Swiler et al., 2014) looked at special smoothing spline models, Gaussian processes with special correlation functions, and the treed Gaussian Process model (Gramacy, 2005). Recently, Hutter et al. suggested generalization of surrogate assisted optimization to combinatorial optimization (Hoos and Leyton-Brown, 2011).

#### 4.2.3 Multi-fidelity models

An approach to solve optimization problems with time consuming objective function evaluations is to use a collection of (meta)models that have different fidelity (Jin, 2011). In these approaches, one has to identify which (meta)model to use in which phase of the solution process. Controlling the model fidelity can be made dynamic by having an automated way of managing this at runtime (Lim et al., 2008).

#### 4.2.4 Heterogeneous objective functions

In multicriteria problems, heterogeneous objective functions (see e.g. Allmendinger and Knowles

(2013a); Allmendinger et al. (2015)) can provide additional challenges for both the algorithms and post-processing or decision making. Here, heterogeneity can mean, for example, that the evaluation time of different objective functions is in different scales or that the complexity of objective functions differs (e.g. linear vs. highly nonlinear). In the latter case, different types of metamodels could be needed for different objectives (Voutchkov and Keane, 2010).

#### 4.2.5 Additional measurements/outputs

Simulation-based and experimental optimization can produce a large amount of data although only a tiny fraction of it is utilized to compute the objective function values. It is an open question whether the remaining data can be utilized meaningfully to enhance search (Jakumeit and Emmerich, 2004). More precisely, the question arises, whether one should build metamodels for every single output and then aggregate the predictions to objective function values, or alternatively to build metamodels of the objective function values directly. The first strategy might for instance better capture dependencies between objective functions, while the latter requires less memory for storing historical values.

## 5 Prospective Solutions

The challenges discussed above can be tackled in different ways, of course. In the following we will elaborate on some interesting directions for prospective solutions.

### 5.1 Model learning for different objective and constraint functions

As outlined in the previous section, different objective and constraint functions can have different characteristics, such as computational effort, types of non-linearity, e.g. multimodality and discontinuities, and noise. In this context we would like to point to the fact that such heterogeneity in multicriteria optimization is an emerging research topic in itself but here we will

limit our discussion only to aspects relevant to surrogate models.

In (Rigoni and Turco, 2010) an automatic procedure for improving the accuracy of metamodels in an adaptive and iterative way is implemented. During the optimization process different modeling techniques are competing for modeling each single function. The performance assessment of metamodels is done independently for the different objective and constraint functions. Also, the evaluation takes place repeatedly during the run. In every iteration it is decided anew which model type is the best one to use for modeling a function. The last run's performance is decisive in this approach: Basically, the winning model on the data points evaluated in the last round will perform surrogate based optimization in the next round. Only, if one model becomes dominant in multiple runs it is taking over the task without further considering the other models (to save computation time).

This idea can be further elaborated by considering different online update schemes of the model-function assignment. An idea that seems to be straightforward in the machine learning context would be to use reinforcement learning (Sutton and Barto, 1998) here, in order to learn by reward and punishment gradually the frequency of models to be used. It is known that reinforcement is robust, but adapts the frequencies relatively slow. This is, why we render this strategy to be promising only if the budget of function evaluation is moderate (say  $\gg 100$ ) and not very small. A variation of the reinforcement paradigm that seems to lend itself well to online model selection is the multi-armed bandit paradigm (Drugan and Nowe, 2013), which has recently been used in operator selection for multi-criteria optimization. The reward function could take into account the achieved improvement (for instance in (hypervolume) set-performance indicators) or in average errors (model improvement). This kind of approach has been considered recently for single-objective optimization (Hess et al., 2013), and can serve as inspiration for the multiobjective optimization case.

More generally, in the context of constrained optimization, two promising research direction may be to learn the structure and location of the feasibility boundary as done e.g. in (Handoko et al., 2010), or extend the idea of cross-surrogate modelling (Le et al.,

2012) to constraint functions.

## 5.2 Handling of large of point sets

One of the main challenges specific to metamodeling is that the cost for training metamodels, in particular Gaussian processes (or Kriging) and to a smaller extend Radial Basis Function networks, becomes prohibitively high when the number of training instances (evaluated design points) becomes large.

Recall, that the computational cost of commonly used metamodels is related to the time required to invert the matrix of correlations based on the pairwise distances between design point. Therefore, the size of the matrix grows quadratically with the number of design points.

A solution to this problem that is often proposed is to use *fast approximate matrix inversion*. Although there are efficient algorithms for approximate matrix inversion available in the literature, they are to our knowledge not widely used in the surrogate-assisted optimization community. An interesting research topic would therefore be to compare these techniques in the context of surrogate-assisted optimization. As a first step in this direction we looked in the literature for some relevant techniques and overview papers.

The problem of approximate matrix inversion has been studied since the 1970's in applied mathematics (Flavell, 1977), and has received recently increased attention in the machine learning research community. A good survey paper for approximate techniques for matrix inversion in the context of Gaussian processes is (Quiñonero-Candela and Rasmussen, 2005). A state of the art method, that was implemented recently in mathematical packages is called Fully Independent Training Conditional (FITC), originally called Sparse Gaussian Processes using of Pseudo-Inputs (SGPP) (Snelson and Ghahramani, 2005). These methods make use of the positive definiteness of the correlation matrix. Moreover, they select a relevant subset of the training points and perform the matrix inversion only on the submatrix for these point, while the other points still contribute to the computation of the final result. However, the selection of a subset of points is still based on simple heuristic and it will be interesting to investigate this deeper.

Another technique that is already used in metamodel-assisted evolutionary computation is called *local metamodeling*, where, as stated in (Kampolis and Giannakoglou, 2008), 'models are trained separately for each new population member on its closest data among the previously evaluated solutions'. Here the term population members refers to new candidate design points. This method has the advantage of smaller training time, but also to provide metamodels that are more based on the regional characteristic of the response surface rather than on its global structure. This is of particular importance if there is non-stationarity and hyperparameters that lead to good performance in one region but do not perform well in other regions.

A problem that occurs in this context is that discontinuities arise, when the set of nearest neighbors changes, causing problems for gradient-based optimization methods that require smooth surfaces. Moreover, artifacts such as local optima might be created – although this has hardly been studied up to now. In addition to this, if only the nearest neighbors are considered, clustering of sets might lead to ill-conditioned matrices or introduce a bias (e.g. considering points in one direction only). An interesting technique could be to use an adaptive archiving technique, similar to those proposed in (Kruisselbrink et al., 2010) in the context of global robust optimization. The idea is to generate a design of experiments, for instance a Latin Hypercube Design (Box et al., 2005), around the new design point and collect a nearest neighbors for each design point from the database. If there is no near neighbor to one of the design points, then a new evaluation is scheduled at this point. This strategy is a variant of an *active learning* approach (Cohn et al., 1996), but more targeted towards the needs of optimization. In the context of multi-criteria optimization the amount of information and the radius of the design of experiments should be based on the characteristics of the function, which in first approximation can be derived from the hyperparameters of the model (for instance the estimated auto-correlation(s) and variances in Kriging/Gaussian process models). Already in the classical book on spatial statistics by Cressie (1993) some advise for the radius in which relevant training points can be found was given, albeit for rather low dimensional data sets (2

and 3 dimensions). Recent work in this direction include the active learning approach for multiobjective optimization proposed in (Zuluaga et al., 2013, 2016).

There are also some promising ideas for fast metamodels using hierarchical Kriging or Gaussian Process models, such as treed Gaussian Processes (Gramacy, 2005) or recent work on optimally weighted cluster Kriging (Stein et al., 2015).

### 5.3 Exploiting dependencies between objective and constraint functions

Nowadays, the common approach to use metamodels in multicriteria optimization is to train independent models for each objective and (implicit) constraint function. This makes computations simpler, for instance to compute multicriteria expected improvement (Couckuyt et al., 2014; Shimoyama et al., 2012; Wagner et al., 2010), but on the other hand these models cannot exploit the possible correlation between different response variables. Hence, there are two difficulties that arise when using dependence information and we will briefly describe which techniques look promising in order to meet them:

Firstly, the computation of metamodels needs to be adapted. In the statistical community, it was dealt with using a technique called multi-output nonparametric regression (Matías, 2005). More specifically, in the context of Kriging metamodels, it has been recently discussed under the term *multi-response metamodels* (Romero, 2008). The idea in both approaches is to exploit the covariance between output variables (which could be objective function values or constraint function values). Also the computation of metamodel indicators will become more difficult.

Secondly, in order to compute measures, such as expected improvement, based on multivariate response formula, exact computation schemes (Hupkens et al., 2015) need to be modified. The block decomposition schemes right now need to be adapted by computing truncated multivariate Gaussian distributions. Recently, a package on truncated multivariate Gaussian distributions became available (Wilhelm and de Matos, 2013), which could be a good starting point in this direction. However, it is worthwhile noticing that multivariate Kriging metamodels can also

have limitations over univariate Kriging metamodels as pointed out in (Kleijnen and Mehdad, 2014; Fricker et al., 2010; Svenson, 2011).

#### 5.4 Creating a virtual library for benchmarking multicriteria optimization methods

Since the 1980's a number of test problems, benchmark suites and schemes for creating test functions have been proposed by the multicriteria optimization community. Table 1 characterizes some of the most commonly-used synthetic problems. More detailed reviews of some of these problems have been published e.g. by Coello Coello (1996); Van Veldhuizen (1999); Huband et al. (2006). It can be seen clearly from the table that, in recent years, the community has put significant effort in creating problems that feature complex shapes of the Pareto-optimal front, and have a scalable number of objectives and decision variables. On the other hand, there seems to be a declining interest in the design of synthetic problems with constraints, a complexity that is commonly featured by real-world problems as can be observed from Table 2. Moreover, real-world problems come often with a discretized (pseudo-continuous) or mixed-integer search space as opposed to a purely continuous space (see e.g. Belegundu and Arora (1985a); Eschenauer et al. (1990); Rajeev and Krishnamoorthy (1992); Li et al. (2013)). While this complexity has been considered by the single-objective optimization community (see e.g. Li (2009)), it is absent in the multicriteria community.

An alternative approach to validate surrogate-assisted optimization algorithm is to link them with an interactive program that simulates and analyzes a real-world problem. Table 3 lists some freely-available simulation programs and their application domains. While this approach seems to be ideal to test surrogate-assisted optimization algorithms, it involves an initial phase of understanding the simulation program and linking it to the optimization model. Also, there is a lack of benchmark results against which a newly developed algorithm can be compared.

Finally, another approach to validate a surrogate-

assisted optimization algorithm is to fit a model to existing or published experimental data (i.e. data from real physical experiments), and then use this model as the fitness landscape to evaluate the objectives of a solution. This approach was used, for example, by Allmendinger and Knowles (2013b); Allmendinger et al. (2014). In particular, in (Allmendinger et al., 2014), a Kriging model was fit to two performance metrics, yield and purity, obtained experimentally from biochemical experiments, which in turn were reported in (GE Healthcare Life Sciences, 2012). Unfortunately, experimental data is often only published partly or in form of heatmaps (see e.g. GE Healthcare Life Sciences (2012)), requiring tedious mapping of experimental inputs to outputs.

To address these gaps in benchmarking multicriteria optimization techniques (designed for expensive problems), we aim to create an online library containing existing multicriteria test problems, problem simulators, and pre-processed experimental data, all of which accompanied by descriptions explaining what difficulties these problems / data pose to surrogate-assisted multicriteria optimization and multicriteria optimization in general. The recently released virtual single-objective test problem library of Surjanovic and Bingham (2015) shall serve as inspiration for this project.

#### 5.5 Metamodels for mixed-integer and combinatorial optimization

A first approach to use metamodels in mixed-integer and discrete parameter optimization is described in (Li et al., 2008). It uses a heterogeneous metric that was developed for radial-basis function neural networks (Wilson and Martinez, 1996). In the context of combinatorial optimization and permutations a comparison of distance measures was recently conducted by Zaeferrer et al. (2014a). Although using distances is an approach that works on more parametric problems, it could be interesting to look at machine learning approaches that can model discrete decision variables in a more problem specific way. Often the meaning and impact of a discrete decision variable can be estimated a-priori (e.g. switching on and off a process alternative in a flowsheet). In such cases modeling a problem specific graph metric could be a promising direction, e.g.

by defining a transition graph and computing path distances in it. Also, as opposed to neural networks, the theory of Gaussian processes is more heavily based on the assumption of learning continuous functions. In this case we suggest to instead consider Markov random field models or Gaussian Markov random fields, when it comes to combinatorial search spaces. These also model local correlations, but are more natural to the problem and by introducing edge weights (transition probabilities) a neighborhood in terms of design point similarity can be modeled in a more intuitive manner. An open question, to our knowledge, is however to generalize the theory of Gaussian processes to mixed-integer spaces and fundamental research needs to be done in this direction.

## 6 Surrogate-assisted multicriteria optimization in a collaborative business environment

In the previous sections we have neglected the procedure of solving practically a challenging optimization problem when the algorithm designer is not aware of all details of the problem and/or not an expert in the field of optimization. This can be the case when tackling real-world problems in an industrial setting. In such a setting, solving an optimization problem is a complex engineering process, where different actors need to collaborate for achieving a common goal: improving product performances and reducing costs and time to market. Apart from dedicated consultancies (both private and academic), industry can rely on different optimization software solutions: they can build their own in-house tools or they can make use of publicly available software products, both open-source or commercial. In this section we present the experience of ESTECO SpA - a private company developing different commercial optimization products - in interacting with diverse industrial customers. In particular we focus on how surrogate-assisted multicriteria optimization techniques can be developed and applied within a collaborative business environment.

Firstly we introduce separately the different challenges and background of industrial customers and

software vendors, and then we expose how they positively interact for finding a mutually agreed solution in a complex scenario, given the number of steps and actions involved in this process.

Industrial needs have been already outlined in Section 4, where they have been presented in terms of challenges posed to current surrogate-assisted multicriteria optimization techniques. Further specific issues and requests may arise from the organizational structure of the company undertaking the design optimization of a product. Big companies are often organized in multiple departments, characterized by different expertise. In fact complex engineering products include many components: in general each part is described by different physics, requiring different engineering analysis (fluid-dynamics, structural, thermal, etc.). So the performance assessment of each component is in charge of a single department, involving the experts in that specific field. This represents a complex design scenario, that requires a discrete effort in terms of coordination and decision making. All the players involved in the process need to effectively collaborate by sharing different kind of knowledge, information, and resources. A similar situation occurs when different organizations collaborate in a common project (as different partners in a consortium). The need for collaboration is even more evident in case that different departments or different organizations are geographically dispersed. The challenges raised by this kind of collaborative, multidisciplinary, design optimization are described e.g. in (Vercesi et al., 2013).

As regards the challenges faced by a software vendor developing optimization software, they clearly include the issues typical of software development (such as software usability, software maintenance, and quality assurance), but also comprise issues peculiar to the use of the software in the context of engineering design (such as industrial applicability of the proposed solutions and the provision of direct integration with third-party Computer-Aided Engineering software). Some important organizational challenges for a multi-product software company are represented on one side by the development of different software products in the context of agile/scrum methodologies (promoting collaboration between different teams), and on the other by the conciliation between research and devel-

opment activities. A key feature for promoting process interoperability and the reusability of software components is the adherence to open standards in formalizing the process model. In fact standards promote technology persistence, fostering software maintainability. Furthermore standards can facilitate the collaboration between scientists and industrial partners, providing a common language in scientific and industrial publications. In this sense in (Comin et al., 2013) a well defined standard from the area of business processes has been proposed for the formal representation of scientific workflows in the context of optimization processes.

The interaction of ESTECO SpA with its industrial customers in some cases consists in a direct collaboration. In many other cases this interaction is mediated by a worldwide network of competent software distributors (representing the experts of their local markets): apart from providing technical support to software users, they take charge of reporting the needs and requests of the customers. In this sense they play the role of the industrial customer towards the software vendor.

The industrial customer, the software vendor, and their mutual interaction cannot be regarded as an isolated system. On both sides there is a beneficial exchange with the scientific community and academy. The state-of-the-art present in scientific literature represents a reference that always drives the development of new algorithms for solving industrial problems. The industrial applications and the proposed solutions are then published or presented at conferences (with the limit of confidentiality issues), closing a virtuous cycle.

The general interaction scheme between the software vendor and the industrial customer is visually represented in Figure 4. The process is divided into multiple stages, contextualized in the frame of software development life cycle. Seven steps have been identified: analysis, planning, design, prototyping, implementation, deployment, and maintenance. For each step, the inputs and the outputs (from the point of view of the software vendor) are listed, along with the actions undertaken by the software vendor. For example, for the initial analysis stage, the input given by the industrial customer to the software vendor is represented

by a new feature request (outlined in blue in the figure). The actions undertaken by the software vendor (outlined in red) are: literature research, requirements analysis, market analysis. Finally, the output provided to the industrial customer (outlined in green) is the request for specifications.

Tight collaboration is needed in order to achieve an agreed solution, with a regular exchange of information and feedback between the two players. In this sense, the adoption of agile/scrum methodologies showed to be beneficial.

## 7 Summary

Complexity in different forms is inherently present in many real-world optimization problems starting from a need to consider multiple objectives which are often evaluated through computer simulations or physical experiments resulting in long evaluation times and possibly uncertain evaluations. In this paper, we have considered using surrogate-assisted multicriteria optimization for solving such problems. We have identified different sources of complexity arising from these problems and various challenges they propose for surrogate-assisted optimization methods. Through selected real-world case studies we have illustrated these challenges and we also described how surrogate-assisted multicriteria optimization is considered in a collaborative business environment. Finally, we have proposed some prospective solutions to overcome some of the challenges identified. Among these, a need for a virtual library for benchmarking multicriteria optimization methods was proposed that should include computationally expensive real-world multicriteria problems based on freely available simulation programs or datasets resulting from physical experiments. We feel that surrogate-assisted multicriteria optimization methods should be tested on these types of problems instead of synthetically generated test problems which has been extremely common in the multicriteria optimization field.

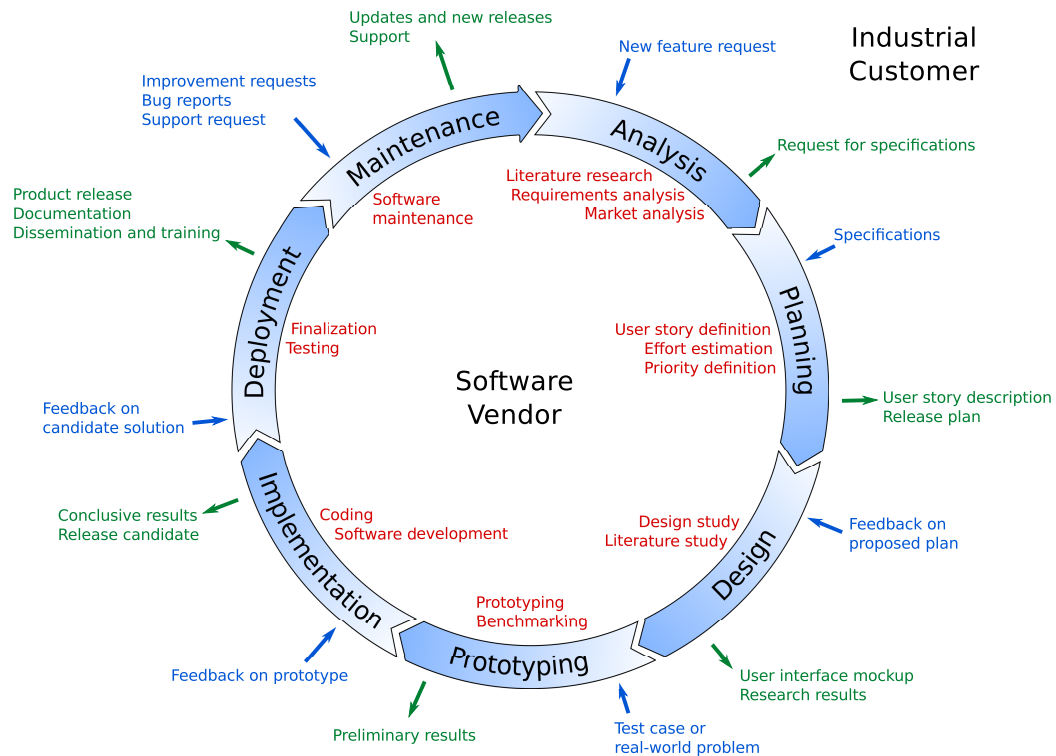


Figure 4: Interaction scheme between the software vendor and the industrial customer. The circle represents the software development life cycle, and it is divided in seven different stages. For each step, the inputs given by the industrial customer to the software vendor are outlined in blue, the actions undertaken by the software vendor are listed in red, the outputs provided to the industrial customer are drawn in green.

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Name	Reference	#Objectives	#Decision variables	Constraints	Shape of Pareto-optimal front
ZEL1-ZEL3	Zeleny (1982, 1986, 2005)	2 (ZEL1,ZEL3),	2 (ZEL1,ZEL3),	yes	linear
CH	Jiménez and Verdegay (1998)	3 (ZEL2)	3 (ZEL2)		
SCH1, SCH2	Chankong and Haimes (1983)	2	2	no	convex
	Schaffer (1985)	2	1	no	convex (SCH1), non-convex and disconnected (SCH2)
KUR	Kursawe (1990)	2	scalable	no	disconnected
BCSM	Belegundu et al. (1994)	2	2	yes	linear
SRN	Srinivas and Deb (1994)	2	2	yes	linear
FON1, FON2	Fonseca and Fleming (1995b,a)	2	3 (FON1), scalable (FON2)	no	concave
MUR	Murata and Ishibuchi (1995)	2	2	no	concave
OK1, OK2	Osyczka and Kundu (1995)	2	2 (OK1), 6 (OK2)	yes	convex (OK1), piecewise linear (OK2)
TMA1-TMA3	Tamaki et al. (1995)	2	2	yes	disconnected and concave (TMA1) convex (TMA2) concave (TMA3)
	Hiroyasu et al. (1999)				
TNK	Tanaka et al. (1995)	2	2	yes	disconnected
TKK	Tamaki et al. (1996)	3	3	yes	curved surface
VNT1-VNT4	Viennet et al. (1996)	3	2	no (VNT1-VNT3), yes (VNT4)	curved surface (VNT1, VNT4), disconnected (VNT2) curved line (VNT3)
BNH1-BNH3	Binh and Korn (1997a,b)	2 (BNH1, BNH3), 3 (BNH2)	2	yes (BNH1, BNH2) no (BNH3)	convex (BNH1, BNH3), concave (BNH2)
LIS	Lis and Eiben (1997)	2	2	no	concave
REN1, REN2	Valenzuela-Rendón and Uresti-Charre (1997)	2	2	no	convex
VQ	Vicini and Quagliarella (1997)	2	2	no	convex
LRS1, LRS2	Laumanns et al. (1998)	2	2	no	convex (LRS1), disconnected (LRS2)
OBA	Obayashi (1998)	2	2	yes	convex
QUA	Quagliarella and Vicini (1998)	2	16	no	convex
Test cases 6, 8 and 9	Binh (1999)	2	4 (Test case 6), 2 (Test case 8, 9)	no	convex (Test case 6), concave (Test case 8), disconnected (Test case 9)
Deb's problem toolkit	Deb (1999)	2	scalable	no	convex, non-convex, disconnected
POL	Poloni et al. (2000)	2	2	no	convex and disconnected
ZDT1-ZDT4, ZDT6	Zitzler et al. (2000)	2	scalable	no	convex (ZDT1, ZDT4), non-convex (ZDT2, ZDT6), disconnected (ZDT3)
CTP1-CTP7	Deb et al. (2001)	2	scalable	yes	discontinuous (CTP1), disconnected (CTP2-CTP5, CTP7), linear (CTP6)
DTLZ1-DTLZ7	Deb et al. (2002)	scalable	scalable	no	linear (DTLZ1), concave (DTLZ2-DTLZ4), convex and degenerated (DTLZ5), disconnected (DTLZ6), hyperplane (DTLZ7)
RETB1-RETB3	Tiwari et al. (2002)	2	12 (RETB1, RETB3) 3 (RETB2)	no (RETB1, RETB2), yes (RETB3)	convex (RETB1, RETB3) disconnected (RETB2)
OKA1, OKA2	Okabe et al. (2004)	2	2 (OKA1), 3(OKA2)	no	convex (OKA1), concave (OKA2)
WFG1-WFG9	Huband et al. (2005)	scalable	scalable	no	convex (WFG1), convex and disconnected (WFG2), linear and degenerate (WFG3), concave (WFG4-WFG9)
L <sub>1</sub> ,L <sub>2</sub> ,L <sub>3</sub> -ZDT and L <sub>2</sub> ,L <sub>3</sub> -DTLZ	Deb et al. (2006)	2 (L <sub>1</sub> ,L <sub>2</sub> ,L <sub>3</sub> -ZDT), scalable (L <sub>2</sub> ,L <sub>3</sub> -DTLZ)	scalable	no	same as for ZDT and DTLZ problems as problems extend ZDT and DTLZ problems with linkages among variables
KNO1	Knowles (2006)	2	2	no	convex
IHR1-IHR6	Igel et al. (2007)	2	scalable	no	same as for ZDT problems as problems are rotated version of ZDT problems
LZ1-LZ9	Li and Zhang (2009)	2 (F1-F5, F7-F9) or 3 (F6)	scalable	no	convex or concave (F9)
CEC2009	Zhang et al. (2009)	2 (UF4-UF7, CF1-CF7), 3 (UF9, UF10, CF8, CF9, CF10), scalable (UF11, UF12)	scalable	no (UF), yes (CF)	concave (UF4, UF10-UF12, CF8-CF10), linear (UF5, UF7, CF1), disconnected (UF6, UF9, CF2, CF3) piecewise linear (CF4, CF5) mixed (CF6, CF7)

Table 1: Overview of commonly used synthetic multicriteria optimization test problems. For all test problems, the search space is real-valued and bounded by box constraints.

Name	Reference	Application	#Objectives	#Decision variables	Type of variables	Constraints	Shape of Pareto-optimal front
GDDK	Ghiassi et al. (1984)	Machine operation planning	4	3	c	yes	unknown
OSY	Osyczka (1985)	I-beam design	2	4	c	yes	convex
BA1,BA2	Belegundu and Arora (1985b,a) Coello Coello (1996)	Plane truss design	3	20 (BA1), 29 (BA2)	d	yes	curved surface
KO	Armstrong et al. (1986); Koski and Osyczka (1990)	Robot arm design	4	4	c	no	unknown
EKO	Eschenauer et al. (1990)	Machine tool spindle design	2	4	c (2) and d (2)	yes	disconnected
RK1-RK3	Rajeev and Krishnamoorthy (1992) Coello Coello (1996)	Space truss design	3	10 (RK1), 8 (RK2), 12 (RK3)	d	yes	convex curve (RK2)
JV	Jiménez and Verdegay (1998)	Gasoline production	2	2	c	yes	linear

Table 2: Overview of real-world multicriteria test problems. In the column *Type of variables*, the characters *c* and *d* refer to continuous and discretized, respectively. Note, for all problems the search space is bounded by box constraints.

Name	Link	Application domain	Main user	Stable release
FoilSim	<a href="http://www.grc.nasa.gov/WWW/k-12/FoilSim/">http://www.grc.nasa.gov/WWW/k-12/FoilSim/</a> (A list of several other interactive NASA simulators can be found at <a href="http://www.grc.nasa.gov/WWW/k-12/airplane/">http://www.grc.nasa.gov/WWW/k-12/airplane/</a> )	Simulate and analyze flow of air past airfoils	Educational tool (NASA)	1996
Modelica Libraries	<a href="https://www.modelica.org/libraries">https://www.modelica.org/libraries</a>	Fluid systems, automotive applications, mechanical systems, energy systems, and many more	Automotive companies, power plant providers	1997
XFOIL	<a href="http://web.mit.edu/drela/Public/web/xfoil/">http://web.mit.edu/drela/Public/web/xfoil/</a>	Design and analysis of subsonic isolated airfoils	Aerospace companies	2001
PyKEP	<a href="http://esa.github.io/pykep/">http://esa.github.io/pykep/</a>	Global trajectory simulation and optimization	European Space Agency	2006
QBlade	<a href="http://www.q-blade.org/">http://www.q-blade.org/</a>	Wind turbine design and simulation	Aerospace companies	2013

Table 3: Overview of free interactive programs capable of simulating and analyzing real-world problems.