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Some efficient approaches for multi-objective constrained optimization of computationally expensive black-box model problems

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ABSTRACT

Multi-objective constrained optimization problems which arise in many engineering fields often involve computationally expensive black-box model simulators of industrial processes which have to be solved with limited computational time budget, and hence limited number of simulator calls. This paper proposes two heuristic approaches aiming to build proxy problem models, solvable by computationally efficient optimization methods, in order to quickly provide a sufficiently accurate approximation of the Pareto front. The first approach builds a multi-objective mixed-integer linear programming (MO-MILP) surrogate model of the optimization problem relying on piece-wise linear approximations of objectives and constraints obtained through brute-force sensitivity computation. The second approach builds a multi-objective nonlinear programming (MO-NLP) surrogate model using curve fitting of objectives and constraints. In both approaches the desired number of approximated solutions of the Pareto front are generated by applying the ε-constraint method to the multi-objective surrogate problems. The proposed approaches are tested for the cost vs. life cycle assessment (LCA)-based environmental optimization of drinking water production plants. The results obtained with both approaches show that a good quality approximation of Pareto front can be obtained with a significantly smaller computational time than with a state-of-the-art metaheuristic algorithm.

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1. Introduction

A wealth of generic mature derivative-free meta-heuristic algorithms (e.g. genetic algorithms, particle swarm optimization, differential evolution, etc.) (Zhou et al., 2011; Deb, 2014) is available nowadays. They are suitable especially for black-box multi-objective optimization (MOO) under constraints, where well-established derivative-based mathematical programming methods cannot be applied due to the unavailability of the problem formulation in analytical form. Meta-heuristic algorithms are reliable, can explore very complex optimal trade-off Pareto fronts (e.g. discontinuous, non-convex, etc.) in a single run but suffer, among other issues, from the curse of dimensionality and slow convergence in the neighbourhood of the optimum.

These algorithms can be classified into two main categories:

- *Pareto dominance-based* e.g. Non-dominated Sorting Genetic Algorithm (NSGA-II) (Deb et al., 2002), Strength Pareto Evolutionary Algorithm (SPEA2) (Zitzler et al., 2002), adaptive evolutionary algorithm (Hadka and Reed, 2013), etc.
- *non-Pareto dominance-based* e.g. scalar objective function problem decomposition-based algorithm (Zhang and Li, 2007), or hybrid algorithms combining global and local search (Sindhya et al., 2013).

Many of these meta-heuristic algorithms have been developed aiming to accurately approximate very complex Pareto fronts, their performance being tested using computationally inexpensive (generally unconstrained) benchmark MOO problems from the literature. Most of these algorithms have been also successfully applied for various practical engineering problems in many fields. However, in some engineering fields the black-box model evaluation can be computationally expensive while the computational time budget may be limited. Under these stringent assumptions the above mentioned well-established generic

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algorithms may not complete and hence they may not provide a satisfactorily accurate and/or evenly distributed Pareto front. This class of computationally expensive MOO problems with limited number of black-box model evaluations opens the way to the development of new algorithms with different accuracy/speed trade-offs. The few existing approaches in this emerging research field rely on Gaussian stochastic process modelling (Jones et al., 1998; Knowles, 2006; Zhang et al., 2010; Zuluaga et al., 2013).

In this paper we propose two new approaches for black-box model expensive MOO problems. These approaches aim to build an approximate model of the black-box MOO problem, which can be efficiently solved, in order to generate potentially promising new solutions. The first approach builds a MO-MILP approximation of MOO problem relying on brute-force sensitivity computation, mimicking thereby first order derivative-based problem modelling. The second approach builds a MO-NLP surrogate model based on (objectives and constraints) functions curve fitting. These problem formulations take advantage of the maturity reached in fields of MILP and NLP, respectively.

The proposed approaches are illustrated, without loss of generality, for the bi-criteria (cost vs. environmental impact) optimization of drinking water production plants. In this work the environmental impact is modeled adopting a life cycle assessment (LCA) approach. LCA is a standardized methodology (ISO-14040, 2006) which analyzes the lifecycle (generally from raw material extraction until product end-of-life) environmental performance of any product chain but without intrinsically providing solutions for reducing the environmental impact.

The MOO of various industrial processes to additionally account for environmental constraints has been extensively investigated so far, e.g. Jacquemin et al. (2012) and Pieragostini et al. (2012). Most of the previous works assume that the process can be (approximately) modeled analytically allowing thereby resorting to mathematical programming-based methods such as: linear programming (Azapagic and Clift, 1999), NLP (Gebreslassie et al., 2009), MILP (You et al., 2012), mixed-integer nonlinear programming (Guillén-Gosálbez et al., 2008; Guillén-Gosálbez and Grossmann, 2010; Yue et al., 2013; Gong and You, 2014), etc. Most of these works rely on expert solvers for the given class of optimization problem, while some develop in-house approaches (e.g. Gong and You, 2014 combines a branch-and-refine algorithm based on successive piecewise linear approximations and an exact Newton's method-based parametric algorithm). However, the LCA optimization of drinking water production plants has received little attention so far, e.g. Wallace et al. (2014) uses the Nelder-Mead local search method for the single objective optimization of a given environmental impact, (Capitanescu et al., 2015) relies on global optimizers (e.g. SPEA2 and NSGA-II) for the cost vs. LCA-based environmental impact bi-criteria optimization, and (Ahmadi and Tiruta-Barna, 2015) proposes a hybrid algorithm combining global search algorithm NSGA-II and local search algorithm COBYLA for three-criteria optimization (cost vs. LCA-based environmental impact vs. water quality).

The remaining of the paper is organized as follows. Section 2 briefly describes the water production plant simulator, called EVALEAU, formulates conceptually the MOO problem and presents the MOO – process engineering – LCA tool. Section 3 describes the proposed general methodology and the two proposed approaches for the MOO. Section 4 provides optimization results with these approaches for a realistic model of a real-world drinking water production plant. Section 5 concludes and provides directions for future work.

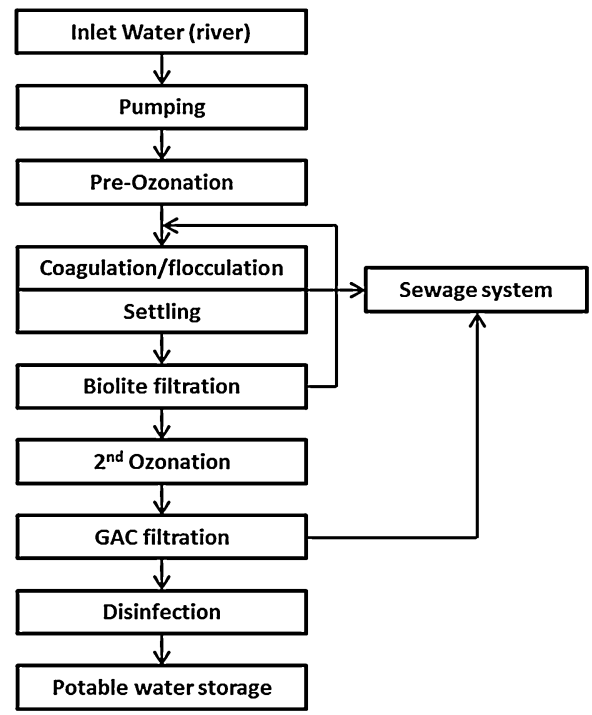

Fig. 1. Flowchart of the potable water production plant used in the case study.

2. LCA – process engineering – multi-objective optimization problem

2.1. EVALEAU simulator

The EVALEAU simulator is a state-of-the-art process modelling – LCA tool for prospective and retrospective simulation of potable water treatment chains (Méry et al., 2013). The simulator comprises a certain number of unit processes (UPs) for water treatment which can be combined to simulate a specific treatment chain (see Fig. 1). The simulator was developed in the LCA software Umberto®, relies on the software PHREEQC (Parkhurst and Appelo, 2013) for the model of chemical reactions in aqueous solutions, and is linked to the Ecoinvent® database (Weidema et al., 2013) for the life cycle inventory (LCI) of background processes.

"The UP modules are mathematical models consisting mainly of a set of equations defining energy and mass balances. They can represent the removal of pollutants via chemical reactions (precipitation, coagulation, and oxidation), separation (settling, filtration, etc.), elimination of microbiologic pathogens, and other treatments such as mineralization and softening to correct water quality. The modelling parameters for the different UPs include engineering design choices (i.e. device hydrodynamics, pipe diameter, efficiencies), technical issues (i.e. pumping height, backwashing schedule, filtering area, etc.), and legal restrictions (i.e. the disinfection requirement criteria)" (Ahmadi and Tiruta-Barna, 2015).

The input of EVALEAU is the inlet (river) water, which quality is described by a set of "more than hundred criteria including parameters such as temperature, pH, turbidity, UV absorbance, dissolved organic carbon, pathogenic microorganisms, inorganic compounds, micro-pollutants, and reaction products" (Ahmadi and Tiruta-Barna, 2015). The outputs of the simulator are (see Fig. 2): the outlet treated water, which quality is described by the same set of parameters as the inlet water, the operation cost of the plant, and the LCI.

EVALEAU-LCA considers the functioning stage of the plant life cycle and neglects the construction and decommissioning steps as

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