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Hybrid simulation–optimization methods: A taxonomy and discussion

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ABSTRACT

The possibilities of combining simulation and optimization are vast and the appropriate design highly depends on the problem characteristics. Therefore, it is very important to have a good overview of the different approaches. The taxonomies and classifications proposed in the literature do not cover the complete range of methods and overlook some important criteria. We provide a taxonomy that aims at giving an overview of the full spectrum of current simulation–optimization approaches. Our study may guide researchers who want to use one of the existing methods, give insights into the cross-fertilization of the ideas applied in those methods and create a standard for a better communication in the scientific community. Future reviews can use the taxonomy here described to classify both general approaches and methods for specific application fields.

1. Introduction

Simulation and optimization were traditionally considered separate (or alternative) approaches in the operational research field. However, tremendous leaps in computational power promoted the appearance of methods that combined both. Simulation-based approaches started involving the optimization of the model inputs (also called controllable parameter settings). On the other hand, optimization-based approaches started using simulation for the computation of parameters (e.g. in queuing systems) or the sampling of scenarios for mathematical programming models. Nevertheless, this dichotomy is gradually vanishing, as other approaches are applying a balanced use of simulation and optimization (e.g. ROSA – see Section 2.3.2 – for a complete list of acronyms see Appendix A). The idea is to explore simultaneously the great detail provided by simulation and the ability of optimization techniques to find good or optimal solutions.

One of the main challenges hybrid simulation–optimization tries to answer is uncertainty. This aspect is addressed by a variety of (more conventional) approaches, such as stochastic programming, fuzzy programming and stochastic dynamic programming. The accuracy and detail of these models are however much lower when compared to simulation approaches. Furthermore, the difficulty in dealing with pure mathematical models leads in most cases towards the use of simulation for some computations. For instance, stochastic programming is most common in the form of scenarios (which may apply Monte Carlo simulation to perform the sampling), since the mathematical manipulation of probability distributions easily becomes intractable. Stochastic dynamic programming makes also use of simulation, when solving large complex models with the so-called reinforcement learning algorithms. A good overview of stochastic, fuzzy and stochastic dynamic programming is given by Sahinidis [1].

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Another major challenge is the consideration of nonlinear relationships, qualitative aspects or even processes hardly modelled by analytical expressions. The problem tackled in [2] is an example of a completely deterministic problem that requires simulation. Indeed, the core advantage of simulation is its ability to deal with complex processes, either deterministic or stochastic, with no mathematical sophistication.

Still, combining simulation and optimization typically results in highly demanding methods in terms of computational effort, even for today's standards. Hence, the design of a good interaction is crucial. For that reason, and because the possibilities of combining them are so vast, it is very important to have a good overview of the different approaches. There is thus the need for a taxonomy which covers the full spectrum of these hybrid approaches and launches the discussion on the different strategies (their advantages and limitations).

A number of taxonomies and classifications have been proposed in the literature using different criteria. Some distinguished simulation–optimization methods by the applied techniques (e.g. statistical procedures, gradient approaches, heuristics, etc.) or their properties of convergence, optimality and correct selection [3–5]. Other frameworks focused on the optimization problem, i.e. the solution space and objective function [6–9]. Shanthikumar and Sargent [10] suggested a classification schema, according to the hierarchical structure of both simulation and optimization models. The authors have further distinguished between "hybrid models" (which they classify) and "hybrid modelling" (previously classified in [11]). In the former both analytic and simulation models are combined into one single model, whereas in the latter each model is able to generate a complete solution, but the final solution results from information exchanges between their executions.

While helpful for understanding the extent of research and practice in the field, these classifications have focused only on particular streams of methods. The last two considered only the cases where an analytical model exists *a priori* (which does not happen in several simulation–optimization approaches, such as stochastic approximation). The remaining papers addressed only the optimization of simulation model inputs, commonly known as "simulation optimization" (SO). Here, we refer to "hybrid simulation–optimization" (or simply "simulation–optimization" – S–O) as any combination of these two major OR approaches.

Another aspect of those classifications that is subject to improvement is the possibility of combining different criteria. In fact, relating different dimensions and perspectives in a single classification can be critical when trying to grasp the essence of S–O methods and discover new opportunities for the cross-fertilization of ideas or the exploration of new approaches.

Finally, important criteria were overlooked. The first concerns the purpose of the simulation component in the overall design. This is the criterion that distinguishes the main streams of research in S–O. Fu [12] outlined this dimension in two main categories ("optimization for simulation" and "simulation for optimization"), but the author has not developed it further. Another key dimension is the search scheme with respect to the series of solutions and realizations considered for evaluation. We refer here to "realization" as a short sample path (or simulation run) or part of a long path. The search scheme not only separates methods that tackle deterministic problems from those that address stochastic settings, but also discriminates the different strategies for dealing with the latter.

Two other papers [13,14] sought to create taxonomies for simulation optimization problems and methods, in order to facilitate numerical comparisons and code reuse. Nevertheless, the interaction between simulation and optimization was not discussed and their studies were confined solely to SO methods.

In light of the above discussion, we propose a comprehensive taxonomy for S–O methods. Our classifying framework comprises four key dimensions: Simulation Purpose, Hierarchical Structure, Search Method and Search Scheme. The first two are related to the interaction between simulation and optimization, whereas the other two concern the search algorithm design. Considering these four dimensions (and their full spectrum), we are able to cover the complete range of S–O methods and distinguish virtually all of them in at least one dimension. The categories of each dimension had to be created from scratch, even for those already considered in the literature, since the confrontation of multiple criteria so required. The range of S–O methods includes: "simulation optimization" (already mentioned); "simulation for optimization", where simulation helps enhancing an analytical model; and "optimization-based simulation", where simulation generates the solution based on the optimization output (optimization does not need any simulation feedback).

One may question whether a so ambitious taxonomy is reasonable, or if it would make more sense studying and discussing those main streams of methods separately. The issue is that in many applications, even the choice of the main approach is not straightforward and consequently requires the consideration of methods that are entirely different in spirit. Moreover, some of these methods are more similar than it might appear at first sight.

This paper makes a clear distinction between the characteristics of the problem and those of the method and suggests connections between both. Our work has therefore a threefold contribution:

- give an overview of the full spectrum of simulation–optimization approaches, providing some guidance for researchers who want to use one of the existing techniques;
- explore the characteristics of these methods, giving insights into the cross-fertilization of their ideas and showing gaps that may result in new approaches;
- create a standard for a better communication in the scientific community, either when comparing existing S–O methods or when proposing a new one.

As opposed to other papers, we start by reviewing a variety of well-known methods (in Section 2) and only then propose our taxonomy (in Section 3). We do not intend to do an extensive review. Our aim is just to provide an overview of the main