

Optimization of Stochastic Discrete Event Simulation Models

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Abstract. This short note gives a brief overview of optimization approaches for stochastic discrete event simulation. In particular it shows how by the combination of different methods hybrid algorithms can be composed that allow a fairly efficient and reliable optimization of medium sized models.

Keywords. Stochastic discrete event simulation, optimization, hybrid algorithms.

1 Introduction

Many systems in logistics can be adequately modeled using stochastic discrete event simulation models. A large number of modeling paradigms are available for this purpose which are often related to software tools or environments to perform simulation experiments [1,2]. A stochastic model allows one to analyze the performance or reliability of the modeled system by performing simulation rather than physical experiments. However, often the goal is not only the analysis of some configurations, it is the improvement of configurations or the finding of an optimal or at least good configuration. This implies that some form of optimization has to be performed where the stochastic simulation model defines the goal function. At an abstract level, the problem can be interpreted as a stochastic optimization problem where the goal function can only be evaluated at specific points and the results are only observable with some additional noise.

Thus, the problem of *simulation optimization*, how it is sometimes named, is the finding of an optimal configuration for a stochastic function with an unknown structure. It is, of course, hopeless to search for a general purpose algorithm that is able to find a global optimum. Instead, in practice, often ad hoc heuristics are applied which means to improve some configuration instead of really performing optimization. Only recently methods have been developed that allow one to give some stochastic guarantees about the behavior of the algorithm. However, these algorithms still need to be integrated in optimization software and need to be applied to practical models.

In this short note, we first give a brief summary about optimization of discrete event simulation models. Afterwards a general framework for optimization algorithms is presented. The note ends with an outline of some open research problems in the area.

2 Simulation Based Optimization

Although simulation based optimization is already a topic in simulation textbooks and survey articles for many years [3,4], it is in general still a challenge since efficient and reliable methods are almost completely missing and probably do not exist due to the generality of the problem. Formally we have to find

$$\mu^* = \min_{\mathbf{x} \in \mathcal{W}} (f(\mathbf{x}))$$

where function $f(\cdot)$ is defined by a simulation model with parameter vector \mathbf{x} of length m . Vector \mathbf{x} will be denoted as the configuration. The output of the simulation model is usually a random variable Y and we are searching for the minimum of the expectation (i.e., $E[Y]$ which implies $f(\mathbf{x}) = E[g(\mathbf{x})]$ and $g(\mathbf{x})$ is the output of the simulation model) and use the notation response for this expectation. We use the notation $\mu_{\mathbf{x}}$ for the response of the model with parameter vector \mathbf{x} . The feasible set of parameters \mathcal{W} may be defined directly as a subset of \mathbf{N}^m or \mathbf{R}^m or by some constraints of the form $g_i(\mathbf{x}) \leq 0$ ($i = 1, \dots, k$). We assume here that \mathcal{W} can be characterized without running simulation experiments. We further assume that the response is a scalar and do not consider multiobjective optimization, although this is an important topic in practice. Since $f(\cdot)$ is defined by a stochastic simulation model, the response can only be observed via experiments. For a fixed sample path θ which is in computer simulation determined by a sequence of random numbers, the output of the simulation is deterministic. We denote by $f(\mathbf{x}, \theta)$ the output of the simulation for the sample path θ . Estimates for the mean and variance of the simulation output can then be computed as

$$\hat{\mu}_{\mathbf{x}} = \sum_{i=1}^n f(\mathbf{x}, \theta_i) \text{ and } \hat{s}_{\mathbf{x}}^2 = \frac{1}{n-1} \sum_{i=1}^n (f(\mathbf{x}, \theta_i) - \hat{\mu})^2$$

from n experiments independent sample paths θ_i . $\hat{\mu}_{\mathbf{x}}$ can be used as estimate for $\mu_{\mathbf{x}}$ and confidence intervals can be computed with standard means [4].

In this very general setting (meta)heuristics [5] and metamodel based approaches [6,7] can be applied for the optimization. The problem with these methods is that they give no guarantees for the quality of the solution and are not specifically tailored for stochastic simulation. Heuristics and metaheuristics usually require a large number of function evaluations and do not explicitly consider stochastic result measures. Thus, they assume fast evaluations of the goal functions whereas simulation models are costly to evaluate. This implies that these methods often require long optimization times and unreliable results without any stochastic guarantees when applied to stochastic simulation models. Some extensions have been proposed which integrate stochastic evaluation techniques with heuristic optimization methods like evolutionary algorithms [8,9] but these extensions only partially alleviate the mentioned problems. Metamodel based methods have originally been developed to optimize systems from physical experiments. The methods are based on a metamodel which is fitted at some

points known from experiments and on the finding of a promising search direction or a point with a possibly small response by evaluating the metamodel. Common metamodels are regression models resulting in the response surface method (RSM) [6] or correlation models often in form of so called Kriging models (KM) [7]. However, both approaches are not well suited to be applied with stochastic simulation since they are not defined for a complete tool integration without manual user support and they also do not exploit stochastic techniques for the evaluation of results. Extensions to integrate RSM [10,11] and KM [12] with stochastic simulation models are available but have not been applied to large and realistic models and will probably fail to optimize such models.

Ideally, one would have the following properties of an optimization approach:

1. If the algorithm runs infinitely long, then the probability of finding a point \mathbf{x} such that $|\mu^* - f(\mathbf{x})| < \epsilon$ should approach zero for any $\epsilon > 0$. This is the intuitive definition of so called *almost sure convergence* [13].
2. The algorithm should quickly find points with a small response.
3. If the algorithm determines point \mathbf{x} as the point with the smallest response, then a confidence interval for $|\mu^* - f(\mathbf{x})|$ should be computable, if \mathcal{W} is finite.

For general problems of the type considered here the first point cannot be achieved and the second one will be hardly achieved with available methods. Thus, usually the parameter space is restricted to $\mathcal{W} \subseteq \mathbf{N}^m$ such that \mathcal{W} becomes countable or even finite. This is from a practical point of view not a hard restriction since in real problems parameters are rarely continuous. Consequently, we consider only this case in the sequel.

However, even with this restriction, the mentioned optimization techniques do usually fulfill none of the three requirements. In particular, there is a conflict between methods observing 1 and those observing 2. To obtain almost sure convergence, one has to assure that all points in \mathcal{W} are visited infinitely often, if the number of experiments tends to infinite. To compute good solutions quickly, it is often better to improve after some global search the best solutions locally without considering the rest of the search space. This indicates that a combination of different methods or the decomposition of the optimization process in phases is the best way to optimize stochastic simulation models. In the next section the corresponding algorithms are briefly outlined.

3 Hybrid Approaches

To observe the points 1 and 2 above, an optimization algorithm usually has to contain two phases, namely an *exploration phase* where the search space is explored to find promising regions and an *exploitation phase* where the promising regions are further exploited by finding local minima in the regions [14,15] which in a final step have to be compared to find the global minimum. The final steps can be made by some ranking and selection procedure [16] which computes out of a set of configurations \mathcal{X} one configuration \mathbf{x} such that

$$Prob \left(\left(\min_{\mathbf{y} \in \mathcal{X}} (f(\mathbf{y})) - f(\mathbf{x}) \right) \leq \delta \right) \geq 1 - p^* \text{ for any predefined } \delta, p^* > 0 .$$

Ranking and selection methods can also be applied to fulfill the third condition above, if \mathcal{W} is finite. In this case, the whole set \mathcal{W} is used as set of configurations in a ranking and selection approach. However, since ranking and selection methods are usually very conservative, the effort for finding the *best* configuration can be very high and the resulting probability is often much higher than the bound $1 - p^*$.

Exploration and exploitation phase can be combined sequentially, iteratively or in an interleaved way, depending on the concrete realization of the algorithm [14,15,17]. Although the practical impact of the research in the area of simulation optimization is limited (see also the remarks in [14]), most available commercial software also use some combination of improved heuristics [18] which goes in a similar direction without proving convergence or computing confidence probabilities.

For the exploration and exploitation phase different methods may be used. The goal of the exploitation phase is to find regions that potentially contain the global optimum. To observe the first condition, the used algorithm has to be almost surely convergent to the global optimum. In [14] a niching genetic algorithm [19] is adapted which has shown to observe the convergence property. In [15] a random search approach is used which is also almost surely convergent. Alternatively, Kriging models may be used as global metamodels and the optimization step is performed using the results of the Kriging model [20,7]. However, Kriging models have originally been developed for deterministic functions, their use for stochastic functions still introduces some problems that are only partially solved yet [21,22] and almost sure convergence of the approach has not been proved yet. Nevertheless, the use of Kriging models to identify promising regions is interesting, in particular, if combined with some search heuristics since it uses some structure of the solution space. The corresponding algorithms have to the best of my knowledge not been fully developed yet.

For the exploitation phase one can use some local optimization algorithm. [23] presents a framework for locally convergent random search algorithm and an improved version of the COMPASS algorithm [24] for discrete optimization via simulation. In [25] pattern search is combined with ranking and selection procedures for the stochastic optimization. With both algorithms a configuration can be identified which contains with probability $1 - \epsilon_L$ a local optimum for any $\epsilon_L > 0$.

4 Conclusions and Open Research Questions

It seems that the gap between commercial optimization approaches and optimization algorithms developed in academia is slowly bridged by using newly developed hybrid algorithms which provide some stochastic guarantees and show for most models a performance comparable to commercially used approaches without any guarantees. However, to be really used in practice algorithms have to be further improved. It seems that the combination of different steps or phases in an algorithm results in a compromise between fast convergence towards a lo-

cally optimal solution and a probability of finding a configuration with a response that differs from the global optimum by less than $\epsilon > 0$ converges towards 1 when the runtime of the algorithms converges towards infinity. However, it is still unclear which are the best algorithms for each phase and how the phases have to be combined. Additionally, available algorithms have to be integrated in publicly available software tools which can be combined with different simulation engines. First prototype versions of those tools are available [26,27] but have to be improved to be really usable for practical problems.

References

1. Bause, F., Beilner, H., Fischer, M., Kemper, P., Völker, M.: The Proc/B toolset for the modeling and analysis of process chains. In Field, T., Harrison, P.G., Bradley, J., Harder, U., eds.: *Computer Performance Evaluation Modeling Techniques and Tools*, Springer LNCS 2324 (2002) 51–70
2. Kelton, W.D., Sadowski, R.P., Sadowski, D.A.: *Simulation with Arena*. 4 edn. McGraw-Hill (2007)
3. Fu, M.C.: Optimization for simulation - theory versus practice. *INFORMS Journal on Computing* **14** (2002) 192–215
4. Law, A.M., Kelton, W.D.: *Simulation modeling and analysis*. Wiley (2000)
5. Michalewicz, Z., Fogel, D.B.: *How to solve it: Modern Metaheuristics*. Springer (2000)
6. Myers, R.H., Montgomery, D.C.: *Response surface methodology*. Wiley (2002)
7. Santner, T.J., Williams, B.J., Notz, W.I.: *The design and analysis of computer experiments*. Springer (2003)
8. Boesel, J., Nelson, B.L.: Accounting for randomness in heuristic simulation optimization. In Zobel, R.N., Möller, D.P.F., eds.: *Proc. 12th European Simulation Multiconference, SCS Europe* (1998) 634–638
9. Buchholz, P., Thümmel, A.: Enhancing evolutionary algorithms with statistical selection procedures for simulation optimization. In: *Proc. 37th Winter Simulation Conference, ACM* (2005) 842–852
10. Buchholz, P., Müller, D., Thümmel, A.: Optimization of process chain models with the response surface methodology and the ProC/B-toolset. In Lünther, H.G., Mattfield, D., Sul, L., eds.: *Supply Chains Management and Logistik*, Physica Verlag (2005) 553–573
11. Neddermeijer, H.G., van Oortmarssen, G.J., Piersma, N., Dekker, R.: A framework for response surface methodology for simulation optimization. In: *Winter Simulation Conference*. (2000) 129–136
12. Kleijnen, J.P.C.: *Design and Analysis of Simulation Experiments*. Springer (2008)
13. Andradóttir, S.: Simulation optimization with countably infinite feasible regions: Efficiency and convergence. *ACM Trans. Model. Comput. Simul.* **16** (2006) 357–374
14. Xu, J., Hong, L.J., Nelson, B.L.: Industrial strength COMPASS: A comprehensive algorithm and software for optimization via simulation. *ACM Trans. Model. Comput. Simul.* (to appear)
15. Prudius, A.A., Andradóttir, S.: Simulation optimization using balanced explorative and exploitative search. In: *Winter Simulation Conference*. (2004) 545–549

16. Swisher, J.R., Jacobson, S.H., Yücesan, E.: Discrete-event simulation optimization using ranking, selection, and multiple comparison procedures: A survey. *ACM Trans. Model. Comput. Simul.* **13** (2003) 134–154
17. Lin, X., Lee, L.H.: A new approach to discrete stochastic optimization problems. *European Journal of Operational Research* **172** (2006) 761–782
18. Fu, M.C., Glover, F., April, J.: Simulation optimization: a review, new developments, and applications. In: *Winter Simulation Conference*. (2005) 83–95
19. Sareni, B., Krähenbühl, L.: Fitness sharing and niching methods revisited. *IEEE Trans. Evolutionary Computation* **2** (1998) 97–106
20. Jones, D.R., Schonlau, M., Welch, W.J.: Efficient global optimization of expensive black-box-functions. *Journal of Global Optimization* **13** (1998) 455–492
21. den Hertog, D., Kleijnen, J.P.C., Siem, A.Y.D.: The correct Kriging variance estimated by bootstrapping. *Journal of the Operational Research Society* **57** (2006) 400–409
22. Huang, D., Allen, T.T., Notz, W.I., Zheng, N.: Global optimization of stochastic black-box systems via sequential Kriging meta-models. *Journal of Global Optimization* **34** (2006) 441–466
23. Hong, L.J., Nelson, B.L.: A framework for locally convergent random-search algorithms for discrete optimization via simulation. *ACM Trans. Model. Comput. Simul.* **17** (2007)
24. Hong, L.J., Nelson, B.L.: Discrete optimization via simulation using COMPASS. *Operations Research* **54** (2006) 115–129
25. Sriver, T.A., Chrissis, J.W., Abramson, M.A.: Pattern search ranking and selection algorithms for mixed variable simulation-based optimization. *European Journal of Operational Research* **198** (2009) 878–890
26. Arns, M., Buchholz, P., Müller, D.: OPEDo: A tool for the optimization of performance and dependability models. *ACM Performance Evaluation Review* **36** (2009)
27. Boesel, J., Nelson, B.L., Ishii, N.: A framework for simulation-optimization software. *IIE Transactions* **35** (2003) 221–230