Variance in Steady-State Simulation Optimization: Key Challenges and Algorithms *

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Abstract. Simulation and optimization enable decision-makers to tackle complex, stochastic problems by modeling uncertainty and identifying effective solutions. While these methods help explore large solution spaces, simulation outputs often contain variance coming from two sources: simulation variability due to randomness in finite runs, and parameter variability from uncertainties in input values. However, this variance poses challenges for optimization, as fluctuating inputs can destabilize convergence, particularly if the variance is unknown. Therefore, this paper reviews techniques to estimate and manage simulation output variance, identifying the asymptotic normality theory for mathematical optimization, and bootstrapping and the two-point method for approximate algorithms as the best method. Although these methods improve reliability, they come with computational costs. Future research should focus on integrating variance quantification into optimization algorithms to enhance decision-making in uncertain environments.

Keywords: Simulation · Optimization · Algorithms · Complex decision-making · Heuristics · Metaheuristics · Stochasticity

1 Introduction

In many real-world systems, decision-makers rely on models to simulate the behavior of complex processes and tp optimize their performance. Fields such as manufacturing, logistics, and healthcare increasingly adopt simulation and optimization to do research on system behaviors in several situations and come up with optimal solutions for resource allocation, scheduling, and process improvements (40).

The integration of simulation and optimization methods makes it possible to analyze large solution spaces where traditional analytical methods fall short. This combination is especially useful in systems characterized by uncertainty and stochastic behavior, where simulation can model the randomness, and optimization algorithms can identify near-optimal solutions (7).

However, when simulation outputs exhibit significant variability due to underlying randomness, this can pose challenges in using the data as input for

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optimization algorithms, potentially leading to non-convergence or unreliable results. For example, in manufacturing systems where machine breakdowns occur at random intervals, simulations might generate stochastic outputs related to production times and system performance. An optimization algorithm designed for deterministic inputs may struggle to use this data effectively, leading to scheduling inefficiencies or flawed resource allocation strategies (13) (20).

Additionally, even when the simulation model reaches a steady state, it is often unclear what the variance of the simulated parameters is. This lack of clarity can complicate the interpretation of results, as uncertainties in variance can distort performance measures and lead to sub-optimal decisions or unreliable optimization outcomes (45).

1.1 Scope and objective

This paper focuses on examining the influence of stochasticity on simulation output variance, focusing on how the stochastic output from simulations can be appropriately handled as input for different optimization techniques. Methods for variance estimation, such as batch means and bootstrapping, which allow practitioners to quantify variability effectively, will be explored (9). At the same time, this paper explores which combinations of simulation and optimization methods are best suited for managing stochastic inputs and proposes strategies for dealing with variance issues to ensure more reliable decision-making in complex systems. The investigation includes case studies from diverse application domains to illustrate the challenges and solutions for variance control in simulation-based optimization.

By exploring variance estimation techniques and optimization strategies, this paper provides insights into improving the stability and reliability of simulation outputs. The discussion aims to contribute to the academic understanding of simulation optimization and offer practical recommendations for addressing the impact of stochasticity on variance in real-world applications.

1.2 Structure of the Review

The structure of the paper is as follows: section 2 outlines the research methodology, followed by section 3, which examines historically relevant milestones and solutions applicable to present-day contexts. section 4 addresses stochastic inputs in optimization models, while section 5 explores the stochastic nature of simulation outputs, detailing their generation process and non-standard distribution characteristics. The paper concludes with a comprehensive discussion and final remarks in section 6 and section 7, respectively.

2 Method

To investigate the variance of simulated parameters when the simulation is in steady state, a structured literature review was conducted. The process involved several key steps:

Reputable academic databases were selected, including *Google Scholar*, *IEEE Xplore*, *ScienceDirect*, and *SpringerLink*, which provide access to peer-reviewed journal articles, conference papers, and technical reports.

The search was conducted using a combination of specific keywords and phrases such as *steady-state simulation*, *variance estimation*, *batch means method*, *simulation optimization*, and *convergence in simulations*. This gave information on both simulation optimization methods and variance distribution(26).

Several studies were reviewed and grouped based on how they measured variance. There was a focus on techniques used to calculate this variance, such as "batch means," where results are divided into smaller sections for analysis, and "spectral analysis," a method for examining patterns in data over time. The main focus of this paper was on methods that can be applied when the simulation reaches a steady state (34).

When a paper or book turned out to be useful for this research, other literature from the reference lists was consulted. This is called backward snowballing. Forward snowballing on the other hand means that one checks where the book or paper was cited elsewhere. This method was used occasionally, to validate the information received from literature (18).

3 History

Simulation and optimization methods have developed over centuries. Among the many facets of simulation, the behavior of simulated parameters, particularly their variance in steady-state conditions, has been a pivotal area of research. This section highlights the evolution of simulation techniques, with an emphasis on methods that address the variance of parameters when simulations reach a steady state.

3.1 Early Developments of Simulation Methods

The concept of randomness in simulations can be traced back to the Monte Carlo method, one of the earliest and most influential simulation techniques. Originating from Buffon's needle experiment in 1777 (22) and later expanded by Laplace (41), Monte Carlo simulations allowed for the approximation of outcomes through random sampling. This method, based on the law of large numbers, was foundational in analyzing systems with inherent randomness, which set the stage for addressing questions of variance in simulated outcomes.

After the second world war the field of simulation grew, mainly because of two major developments. Firstly, the introduction of the general-purpose electronic computers (6) and secondly, the use of the Monte Carlo method on computers used to estimate the probability that the chain reaction needed for the atom bomb would work successfully (4). Later the Monte Carlo method was complemented with random number generators (23). The broader availability of computers, combined with more user-friendly programming languages, led to a rapid development of simulation techniques.

3.2 Addressing Steady-State Variance

By the late 1960s, the development of simulation methods reached a critical juncture when researchers recognized the challenges involved in quantifying the variance of parameters in steady-state conditions. Steady-state refers to the point in a simulation where initial conditions no longer influence the outcomes, and the system stabilizes around a long-term equilibrium.

However, three major issues emerged in simulation studies (16):

1. The start-up problem: How can we ensure the simulation has reached steady state?
2. **The variance of simulated parameters in steady state: How do we accurately measure the variability once steady state is achieved?**
3. Comparing different simulation configurations to identify the optimal setup.

The focus on steady-state variance became particularly important because variance is a key measure of a system's stability and reliability. High variance in steady-state parameters could indicate that a system is unstable or that the model needs refinement.

3.3 Conway's Contribution to Variance Measurement

In 1963, Richard Conway made significant contributions to addressing the second issue: measuring variance in steady-state simulations. His batch means method revolutionized simulation analysis. The idea was to divide the steady-state period into several "batches" and calculate the mean for each batch. By analyzing the variance between these means, one could estimate the variance of the steady-state parameters (11). This technique remains widely used today because of its simplicity and effectiveness in reducing noise from initial simulation conditions.

Conway's work laid the groundwork for further studies on simulation variance, particularly in long-term simulations where the challenge is not only achieving steady state but also ensuring that the variance of parameters remains within acceptable bounds.

3.4 Later Developments and Continuing Challenges

As simulation methods advanced in the 1980s and 1990s, particularly with the integration of simulation and optimization techniques, the question of steady-state variance continued to play a central role (43). Methods like simulated annealing and genetic algorithms, which relied on optimization within a simulated environment, further highlighted the importance of understanding parameter variance.

While these optimization techniques enabled better analysis of solution spaces, the computational cost of running these simulations, especially when accounting for variance, became a limiting factor. The challenge was to strike a balance between accuracy in measuring variance and the practical limitations of computational power. Many of these challenges remain subjects of ongoing research, particularly in areas like high-performance computing and large-scale system simulations (10).

3.5 Modern Approaches to Variance in Steady-State Simulations

Today, addressing variance in steady-state simulations involves a combination of classical methods like batch means and newer techniques designed for high-complexity systems. Techniques such as regenerative simulation and spectral analysis (43) have been developed to improve variance estimation in systems that exhibit periodic or cyclic behavior. These modern methods aim to provide more precise and reliable variance estimates, even in simulations with complex or stochastic dynamics.

Nevertheless, the variance of simulated parameters remains a critical metric in determining the reliability of any steady-state simulation. As simulations continue to be applied in fields as diverse as finance, engineering, and public policy, understanding and controlling this variance is key to producing accurate and actionable insights. Therefore, section 5 will highlight different options to better understand or control the variance. Prior to this, section 4 will focus on the stochasticity in different optimization model to highlight the importance of controlling the variance.

4 Stochasticity in Optimization Models

As the previous section highlighted, simulation models leave an output with stochastic characteristics. This section will focus on how this stochasticity affects optimization models, especially when combining optimization with simulation. Different optimization methods will be reviewed to highlight why combining them with simulations can be beneficial. With this, it will be discussed how the randomness in simulation impacts the optimization.

4.1 Introduction into Optimization Methods

There are different possibilities to classify optimization methods, with one being the distinction of mathematical optimization and approximate algorithms. Mathematical optimization is a combination of techniques and methods for finding the best possible solution to a problem within a set of constraints. Therefore, they are computationally intensive, but aim to provide accurate solutions. Exemplary research areas from the field of mathematical optimization are linear and non-linear optimization (35). Approximate algorithms are more flexible, using randomness to explore different solutions. These are especially useful when the problem is too complex or time-consuming for exact mathematical methods (36). There are two main types: heuristics and metaheuristics (44). Heuristics are problem-specific shortcuts that provide quick, but not always perfect, solutions. Metaheuristics, on the other hand, are general strategies guiding multiple heuristics that can be applied to many different problems.

4.2 Mathematical Optimization

As aforementioned mathematical optimization is characterized by aiming for optimal solutions under the consideration of constraints (35). For simpler problems, like those solved with linear optimization, one can use methods like the Simplex Method to get solutions efficiently. However, non-linear optimization (where relationships between variables are more complex) can be much harder and may require a lot more computing resources (19).

Non-linear programming, despite its capacity to model complex real-world problems through intricate variable relationships, often falls into the NP-hard complexity class, resulting in substantial computational demands. Moreover, algorithms like Gradient Descent cannot guarantee convergence to global minima in non-convex landscapes. Thus, even in the absence of stochastic considerations, numerical optimization models do not guarantee the discovery of global optima (8).

Simulation-based optimization offers approaches to address this complexity. Sensitivity analysis can elucidate the impact of parameter variations on optimization outcomes (37; 12). This approach can be extended to a broader exploration of the solution space, guiding the search process more effectively. For instance, in Gradient Descent, the identified optimum is heavily influenced by initial parameters. Strategic selection of starting points through comparison of simulation results can enhance the likelihood of finding an optimal solution (5). Additionally, simulation can serve to validate the obtained solutions (28).

However, the stochastic nature of simulations introduces challenges in interpreting results derived from numerical algorithms. The inherent variability in simulation outputs may lead to conclusions that diverge from those suggested by deterministic models (28). In sensitivity analysis, stochastic noise can obscure meaningful patterns. Similarly, solution space exploration becomes more complex, as high variability in simulation outputs complicates the identification of advantageous starting points. The validation of optimization results is also rendered more challenging, necessitating assessment through multiple stochastic simulation outcomes (29).

4.3 Approximate Algorithms

As already examined in subsection 4.1, heuristics and metaheuristics can be distinguished (44). While heuristics are often designed to find acceptable solutions for specific problems in a reasonable amount of time, metaheuristics allow a broader usage, by providing guidelines or strategies for developing heuristic optimization algorithms (25; 15). Because of their flexibility, they are also the choice for solving a lot of real-life problems including vehicle routing and nurse rostering (33; 32). Therefore, this subsection will concentrate on metaheuristics and their integration with simulations.

Three different classes of metaheuristics can be distinguished based on how solutions are further developed. These are local search metaheuristics, constructive metaheuristics, and population-based metaheuristics (15).

Local search, or iterative improvement, finds good solutions by iteratively making small changes to the current solution. One exemplary metaheuristic in this field is simulated annealing (15). Simulations can be utilized to evaluate the performance of these algorithms by generating multiple random instances of the problem and assessing how well the local search algorithms perform under different conditions (27).

Constructive metaheuristics do not improve complete solutions, but by adding elements to a partial solution. This is often done by the integration of greedy algorithms, which try to add the best possible element at each iteration (15). Simulations can assist in evaluating the effectiveness of different construction strategies by allowing for the testing of various heuristics in a controlled environment (39).

The last field of metaheuristics is population-based metaheuristics, which find their solution by iteratively selecting and combining existing solutions. Evolutionary algorithms like for example genetic algorithms can be classified as population-based metaheuristics (15). Simulations allow the evaluation of the fitness of each candidate solution within the population (14). Moreover, simulations can facilitate the exploration of the search space by enabling the population to adapt dynamically based on the performance of its members, thus improving the balance between exploration and exploitation (24).

While metaheuristics can handle stochasticity to some degree, the randomness from simulations can still cause issues. Since simulation results can change each time they run, the performance of these algorithms may vary. This makes it harder to measure how well an algorithm is truly working because some of its success could be due to random luck rather than the algorithm's actual strength (2).

To summarize, simulation can be helpful to improve the performance both in mathematical optimization and approximate algorithms. The possible uses can vary from finding better starting positions to validate final results. Nevertheless, the variance of simulation outputs undermines the benefit of simulation-based optimization. Therefore section 5 focuses on a distinction of the different types of stochasticity and on possible solutions to handle the variance. section 6 will then outline which solution can be combined with which optimization model.

5 Stochasticity in Simulation Outputs

This section focuses on how simulation outputs are generated and how stochasticity plays a role in this. Simulation models are built using input distributions, which are simulated using Monte Carlo techniques. These models have Monte Carlo errors, because a model has to have a finite-length simulation run (1; 45). A second way that errors slip into simulation models is due to the system modelling real-world situations. Real-world phenomena can be complex but have to be simulated using finite samples of real-world data, leading to error propagation (1). The two names for these phenomena are *simulation variability*, for errors due to finiteness of simulation output sample, and *parameter variability*, for errors due to uncertainty in the input model's parameters compared to the real world (9).

Calculating the confidence intervals of the output is a good way to figure out how well a simulation model is performing. This section will discuss some methods used in the field to calculate that interval where both simulation variability and parameter variability are taken into account.

5.1 Asymptotic Normality Theory

The asymptotic normality theory refers to a statistical concept where, as the sample size grows larger, the distribution of the sample mean tends to follow a normal (Gaussian) distribution, regardless of the original distribution of the data (31). This concept is useful in simulation because, after running a sufficient number of simulations, the outputs can be approximated as normally distributed. Using this normality, one can compute confidence intervals for simulation output. In practice, it allows to assume that simulation averages behave predictably, even when individual simulations may show a lot of variability due to randomness (17).

For large-scale simulations, this means that as more iterations are run, the effect of simulation variability diminishes, and more precise estimates about the true behavior of the system can be made. This method, however, requires that the simulation has run long enough to achieve steady-state behavior and that the distribution of the outputs converges. A potential drawback is that it might take a large number of runs to reach this steady-state condition, especially in systems with high stochasticity (9).

5.2 Bootstrapping

Bootstrapping is a resampling technique used to estimate the properties of a distribution, such as its variance or confidence intervals, without making strong assumptions about the underlying distribution (21). In the context of simulation, this method involves generating many different resampled datasets from the original simulation output by randomly drawing samples with replacement.

By repeatedly resampling the data, bootstrapping can provide a better estimate of the variability in the simulation's outputs, helping to account for both simulation and parameter variability. Bootstrapping is particularly useful when there are few simulation runs or when the output distribution is not known to follow a standard statistical distribution. (3) One advantage of bootstrapping is that it does not require a large number of assumptions about the data, but it can be computationally intensive as it involves many resampling iterations (1).

5.3 Direct Two-Point Method

The direct two-point method is a simple technique for estimating the variance of simulation outputs by running two different simulation configurations or runs (30). The idea is to perform two independent simulations, each with different seeds for random number generation, and then compare the difference in their outputs.

This method helps to isolate simulation variability by focusing on how the results vary when the stochastic elements of the simulation change while keeping all other factors constant. Although it is a straightforward approach, it may not be as robust as more advanced statistical techniques like batch means or bootstrapping, especially in complex models with high levels of parameter uncertainty (1; 45). However, it can still offer a quick and easy way to get a rough estimate of output variance, especially in early stages of model validation.

5.4 Other Solutions

Another way to minimise parameter variability is by allocating the simulation budget more efficiently. For instance, this was done for a Ranking and Selection problem, creating an algorithm for an efficient trade-off between collecting input data and running simulations (42). Making sure the simulation budget is being allocated efficiently is useful for every type of problem.

6 Discussion

This paper examined the impact of stochasticity on simulation and optimization, highlighting persistent challenges in measuring variance despite technological advancements. Two main sources of error in simulation models are simulation variability and parameter variability (9). To assess model performance, the paper discussed methods for calculating confidence intervals, including asymptotic normality theory, bootstrapping, and the direct two-point method. These techniques provide a framework for evaluating simulation reliability amid inherent randomness.

In optimization, the paper categorized techniques into mathematical optimization and approximate algorithms. Mathematical methods, while precise, can be computationally demanding, especially in non-linear scenarios. Simulations offer tools like sensitivity analysis to explore solution spaces more effectively. Approximate algorithms, particularly metaheuristics, provide flexible approaches to complex problems but face challenges from stochastic simulation outputs, which complicate performance evaluation.

The final question is now how to combine the optimization models with the possible solutions to handle the variance. Starting with mathematical optimization models, these algorithms rely on precise numerical values. Therefore, bootstrapping and the direct two-point method are not applicable, because these solutions focus on a better understanding of the distribution of simulation results instead of finding precise values.

This is the case when applying the asymptotic normality theory by running more iterations. The problem in this case is that the requirement of precise values lead to strong convergence criteria which result in even more iterations and computational time for the simulation. Consequently, the complexity of the optimization problems leads to high computational times for the mathematical optimization models and the asymptotic normality theory leads to high computational times due to the high number of simulation runs. Therefore, the benefit of the use of simulations for mathematical optimization models gets limited as of today because of the variance in simulation results.

For approximate algorithms, the use of the asymptotic normality theory is also not effective. Approximate algorithms focus on finding fast instead of optimal solutions. The increase of iterations would lead to a rise in computational time, which would undermine the benefit of heuristics and metaheuristics. For these algorithms, bootstrapping and the direct two-point method can be more applicable.

These alternative methods prioritize understanding the distribution of simulation results over precise estimations, aligning well with the goals of approximate algorithms. Local search metaheuristics exemplify a potential application. There, by having a better understanding of the distribution of simulation results, different instances of the problem can be compared (27).

Beyond traditional metrics like mean and standard deviation, this approach enables the use of risk-focused measures such as Value-at-Risk (VaR) and Conditional Value-at-Risk (CVaR). These metrics evaluate the lower end of the simulation result distribution, ensuring robust performance even in worst-case scenarios (38). By selecting instances that perform well under these criteria, the chosen solution is more likely to maintain effectiveness across a range of potential outcomes.

This example illustrates just one way bootstrapping and two-point methods can enhance the reliability of simulations in approximate algorithms. Their application demonstrates that simulation-based optimization is already proving beneficial when used in conjunction with metaheuristics or heuristics, offering a pragmatic balance between computational efficiency and solution robustness.

7 Conclusion

This paper has examined the complex interaction between stochasticity and optimization methods in simulation-based frameworks. When simulation models have a stochastic output, some optimization methods are unable to process this information as input. This paper has given several solution directions to overcome this problem.

For mathematical optimization the increase of the number of iterations based on the asymptotic normality theory can lead to precise values. The increase of computational time due to more simulation runs is in conflict with the initial goal of reducing computational time by taking simulation results into consideration.. Therefore, the variance of simulation outputs limits as of today the use of simulations in mathematical optimizations.

This is not the case for approximate algorithms. There, solutions like bootstrapping and the two-point method lead to a better understanding of the distribution of simulation results, which can then be implemented through different metrics like e.g. the Value-at-Risk to improve metaheuristics and heuristics.

Therefore, the stochasticity of the simulation results can be used for these types of algorithms.

By utilizing these combinations, decision-makers can optimize performance in systems that have randomness and uncertainty. The integration of these methods not only enables analyzing large solution spaces but also mitigates the challenges posed by variance in the parameters. Future research should further explore how variance quantification can be integrated with optimization algorithms. This way, simulation outputs can be more effectively used for reliable and optimal decision-making in complex systems.

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