SIMULATION-BASED OPTIMIZATION IN TRANSPORTATION AND LOGISTICS: COMPARING SAMPLE AVERAGE APPROXIMATION WITH SIMHEURISTICS

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ABSTRACT

Simulation-based optimization (SBO) refers to a series of simulation-optimization methods that are employed to solve complex optimization problems with stochastic components. This paper reviews some recent applications of SBO in the area of Transportation and Logistics. This paper presents the stochastic variants for the team orienteering problem to show the application of the SBO solving methods. Similarly, we make a comparison of two of the most popular ones: the sample average approximation method and the simheuristic algorithms. Finally, the paper concludes by considering the value of the aforementioned approach and outlining further research needs.

1 INTRODUCTION

Simulation-based optimization (SBO) is a powerful modeling tool for analyzing complex systems that are usually non-linear and large-dimensional problems which require simplifying assumptions to solve the problem. This approach is frequently used to solve problems related to transportation and logistics (T&L), supply chain management, or smart cities. Generally, a stochastic simulation optimization problem consists of finding a configuration of resources aimed at an objective function, where the resources comprise the uncertainty in the system. As a consequence, the performance of any feasible solution needs to be estimated via simulation. Some system constraints are implicitly involved in the simulation process. However, there are problems where both performance and constraints must be evaluated with simulation. As a result, this approach allows us to estimate the expected performance through different system configurations or scenarios. In this sense, the assumptions contribute to make the problem easier to solve, but at the cost of not considering the real-life uncertainty that characterizes these systems. With the increasing advances in computing hardware and software, simulation has become a 'first-resource' method for analyzing complex systems under uncertainty (Lucas et al. 2015). However, traditional simulation approaches are not by themselves able to generate optimal or near-optimal distribution plans in scenarios with many possible

configurations. Hence, it makes sense to consider hybrid simulation-optimization methods that combine the best of both worlds (Faulin and Juan 2008). Reviews and tutorials on simulation-optimization can be found in Fu et al. (2005), Chau et al. (2014), and Jian and Henderson (2015).

In some cases, it is possible to differentiate between approaches that are more optimization-driven and those that are more simulation-driven. In SBO, the optimization algorithm plays the role of a 'driving' agent and simulation acts as an 'auxiliary' agent, being called whenever appropriate by the optimization agent. In optimization-based simulation, simulation acts as the driving agent to reproduce the behavior of a random system and then optimization is called from time-to-time in order to find optimal (or near-optimal) values of some simulation parameters.

This paper focuses on two popular SBO methodologies: the Sample Average Approximation (SAA) method and simheuristic algorithms. The SAA is a well-known method that provides a solution based on sampling of the random variables (Kleywegt et al. 2002). Considering this random sampling, the expected value of the stochastic objective function is approximated by a deterministic objective function and then solved using an optimization method, typically an exact method (Shapiro 1996). However, real-life optimization problems are often NP-hard and large-scale in nature, which makes traditional exact methods inefficient to solve them in reasonable computing times. Thus, the use of heuristic algorithms to obtain a variety of high-quality solutions in low computing times is required (Faulin et al. 2008; Juan et al. 2009). Simheuristic algorithms integrate simulation methods inside a metaheuristic optimization framework to deal with large-scale and NP-hard stochastic optimization problems (Juan et al. 2018). Hybridization of simulation techniques with metaheuristics allows us to consider stochastic variables in the objective function of the optimization problem, as well as probabilistic constraints in its mathematical formulation (Fu 2002). As pointed out by Glover et al. (1999) the combination of simulation with metaheuristics is a promising approach for solving stochastic optimization problems that are frequently encountered by decision makers in many industrial sectors. In this sense, a simheuristic algorithm extends a metaheuristic one by integrating simulation into it. In Grasas et al. (2016), the authors discuss how to extend an iterated local search framework into a simheuristic. Likewise, in Ferone et al. (2019) the authors explain how to extend a GRASP framework into a simheuristic. A simheuristic algorithm is typically composed of two different components: an optimization component which searches for promising solutions - and a simulation component – which assesses the promising solutions in a stochastic environment and provides feedback to the optimization component.

This paper illustrates the relative performance of both the SAA and simheuristic approaches by employing a case study based on the stochastic team orienteering problem (TOP). As depicted in Figure 1, in its deterministic version the main goal of the TOP is to find the vehicle-routing plan that maximizes the rewards obtained by visiting a subset of potential customers (Chao et al. 1996). Usually, a time- or distance-based threshold is imposed on each route. In the stochastic TOP, it is usual to consider either random rewards or random travel / servicing times. Several variants of the TOP have been employed in a number of applications related to different areas, such as city logistics, humanitarian logistics, and military logistics. Nevertheless, the literature related to stochastic versions of the TOP is still scarce, and most of the solution approaches rely on exact methods (Gunawan et al. 2018).

The remainder of this paper is structured as follows: Recent publications on simulation-based optimization and simheuristics are reviewed in Section 2; more details on the case study used for the methodology comparison are provided in Section 3; Sections 4 and 5 outline the SAA and simheuristic approaches for dealing with the case study; in Sections 6 and 7, some computational experiments are described and their results analyzed; finally, Section 8 highlights the main contributions of this work.

2 RELATED WORK

This section reviews recent works, in the area of transportation and logistics, related to the different solution concepts described in this paper: the general simulation-optimization methodology – including the SAA method – and the simheuristic algorithms.

Juan, Reyes-Rubiano, de la Torre, Panadero, Faulin, and Latorre



Figure 1: An illustrative example of the stochastic team orienteering problem.

2.1 Recent Work on Simulation-based Optimization

In the field of urban transportation, it is usual the utilization of traffic simulation models to evaluate the impact of changes in network design or network operations. This dynamic optimization problems, with time dependent decision variables, have been addressed through the use of analytical dynamic traffic models (mostly deterministic). Such models are based on an aggregate, low-resolution, description of traffic dynamics. Although, computationally efficient to evaluate, these models lack a detailed description of heterogeneous aspects, such as: traveler behavior, vehicle-infrastructure interactions, and traffic dynamics observed in urban areas. A detailed description of these dynamics is provided by a high-resolution simulation based traffic models. But, these simulators are computationally inefficient to evaluate, and the choice of which simulation model to rely on, a part from how to combine their use, is complex. A larger-scale model may, for instance, capture more accurately the local-global interactions; however, it would mean a higher computational cost. Hence, their use to address optimization problems has been limited to the evaluation of performance in small, set of predetermined alternatives (for instance, traffic management strategies).

In this regard, in Osorio and Selvam (2017) an optimization framework that enables multiple simulation models to be jointly and efficiently is proposed. This is achieved through the combined use of multiple stochastic traffic simulators. This permits to exchange the high computational costs of running accurate large-scale simulators for those less accurate in a smaller scale. The proposed methodology is illustrated with a signal control problem on both a small network example and on a city-scale network, and can identify signal plans with good performance at a significantly lower computational cost than when systematically running the accurate larger scale simulators. The methodology can enable the use of inefficient simulators for real-time traffic control. Moreover, it constitute a first step toward the objective of combining different types of simulation models to solve transportation optimization problems in a holistic manner.

In the same line in the urban transportation field, in Chong and Osorio (2017) a novel metamodel method that addresses large-scale SBO problems with time-dependent decision variables (evening peak period demand) is proposed. The model permits to enhance other algorithmic steps, such as sampling strategies, and ranking and selection strategies to statistically compare the performance of multiple points. Problems with simulation-based (i.e., stochastic) constraints require evaluating the feasibility of a point via simulation. However, it cannot be guaranteed. Instead of, it can be tested statistically but at the computational cost of obtaining an accurate estimate of the simulation-based constraints. Thus, this paper only considers constraints that are available in analytical, rather than simulation-based form. In transportation, examples of stochastic constraints would be, for instance, bounds on link or network performance metrics (e.g., travel times, emissions, energy consumption). According to the authors, efficient algorithms for such problems

are needed. So, the metamodel ideas of this paper could be used to formulate computationally efficient algorithms for SBO problems with stochastic constraints.

For the last decades, multimodal freight transportation has become a key factor for the success of service firms. Consequently, it is very common to combine multiple transportation modes such as railway, roadway and waterway in order to improve the efficiency in containerized freight delivery. Hence, and according to Wang and Wallas (2016), determining this optimal service schedule has become a fundamental tactical planning problem. In this regard, Layeb et al. (2018) have presented a new simulation-based optimization model for solving a deterministic optimization problem in a real-world case study. Although within a higher computationally cost, the model provides the optimal freight service schedule found with the analytical formulation. After that, the model was applied to solve complex stochastic network design problem, by integrating demand and travel times stochasticity with the corresponding realistic continuous distributions. Typical distribution shapes, commonly used in the transportation research field, such as skewness and multimodality are also considered.

Feng et al. (2018) develop a multi-objective network layout optimisation model solved by an improved Simulated Annealing Algorithm (SAAlg). The main objective is to coordinate inconsistent objectives in transport network design (i.e., the minimization of the travel time of the passengers, as well as the costs for construction and operations). The control variables work in cooperation in order to restart the optimum search from the latest temporary optimal solution if the search is made excessively in any searching direction, and are able to expand the searching area for the globally optimal network layout with the minimum operation cost. The genetic algorithm is embedded into the reversible SAAlg to iteratively provide a network configuration with the minimum operational cost, with the minimum total time expense of all the transport modes. According to the authors, the proposed method can be used to optimize configurations not only in urban transit lines for passenger mobility, but in logistics transportation routes for manufacturing production management.

2.2 Recent Work on Simheuristics

In recent years, the work on simheuristic algorithms has focused on achieving a deeper integration between the simulation and the heuristic components, as well as in enhancing the computing performance of the integrated approach –which otherwise can be extremely demanding in terms of computing times. Hence, the simulation component is not only employed after the optimization component with the goal of evaluating the quality of the solution, but it is also used to provide feedback to the optimization process itself (typically by using a stochastically-driven base solution from which new solutions are generated). Also, both methodologies are combined to provide a risk or reliability analysis on a set of 'elite' solutions.

Thus, the uncapacitated facility-location problem with stochastic service costs is analyzed in De Armas et al. (2017). First, the authors propose an extremely fast savings-based heuristic, which generates real-time solutions for the deterministic version of the problem. This can be extremely useful in telecommunication applications, where 'good' solutions are needed in just a few milliseconds for large-scale networks. The heuristic is then integrated into an iterated local-search framework, which allows us to compare it against state-of-the-art algorithms for the deterministic version. Finally, the metaheuristic is extended into a simheuristic and employed to solve the stochastic variant. As pointed out by the authors, the simulation layer is not only used to assess the stochastic value of the solutions generated by the iterated local search component, but the feedback from the simulation is also used to better guide the search process. In particular, the base solution inside the iterated local search is chosen according to the stochastic value provided by the simulation. These authors also introduce a procedure that 'filters out' non-promising deterministic solutions, so they are never sent to the simulation component to avoid an inefficient use of computing time. Additionally, that paper also discusses the convenience of considering complementary goals to the minimization of expected costs, e.g., solutions that minimize a given percentile, and solutions with different trade-off levels of expected cost and variability.

Juan, Reyes-Rubiano, de la Torre, Panadero, Faulin, and Latorre

Similarly, Gruler et al. (2017b) discuss the need for optimizing urban waste collection in modern smart cities and formulate the problem as an extension of the vehicle-routing problem. The authors first develop a competitive metaheuristic, based on a variable neighborhood-search framework, to solve the deterministic variant. Then, they extend their approach into a simheuristic to cope with unexpected waste levels inside the containers. Their algorithm is tested using a large-scaled benchmark set for the waste-collection problem with several realistic constraints. Their results include a risk analysis considering the variance of the waste level and vehicle safety capacities. An extension of the previous waste-collection problem to a multi-depot version is discussed in Gruler et al. (2017a), where horizontal cooperation strategies are employed to enhance the quality of the solution in clustered urban areas and large cities. The authors employ an iterated local-search metaheuristic to deal with the underlying multi-depot vehicle-routing problem. According to their computational experiments, the use of horizontal cooperation among vehicles belonging to different city districts (or even to different metropolitan areas) shows to be an effective strategy when dealing with uncertainty in waste levels.

Gonzalez-Martin et al. (2018) propose a simheuristic algorithm for solving the arc-routing problem with stochastic demands. Here, the authors use Monte Carlo simulation to extend the RandSHARP heuristic (Gonzalez-Martin et al. 2012), which was originally designed to solve the deterministic version of the problem. During the design of the routing plan, they make use of safety stocks, which allow vehicles to deal with unexpectedly high demands during the actual distribution process. These authors also introduce a reliability index to measure the 'robustness' of each solution with respect to possible route failures caused by random demands. By ensuring solutions with high reliability levels, they reduce the the overall cost of corrective actions associated with route failures.

Pages-Bernaus et al. (2019) consider a stochastic version of the capacitated facility-location problem, proposing two facility-location models representing alternative distribution policies in e-commerce (outsourcing vs. in-house distribution). The models consider stochastic demands as well as more than one regular supplier per customer. Then, two different methodologies are proposed to solve these models. While the first one is a classical two-stage stochastic-programming approach (which employs an exact solver), the second one is a simheuristic algorithm based on an iterated local-search framework. Computational experiments show that the former can be used to tackle only small-sized instances, while the latter allows dealing with large-scale instances in reasonably short computing times. The multi-period inventory-routing problem with stochastic customer demands is analyzed by Gruler et al. (2020). A variable neighborhood search is extended into a simheuristic algorithm to consider variations in the forecasted demands. With the aim of finding optimal refill policies for each customer and period combination, the authors take into account that the quantity serviced at the beginning of one period will affect the inventory levels at the end of that period. These inventory levels will also be affected by the random demand associated with each customer in that period. The total cost to be minimized will be the aggregation of both inventory and routing costs. Notice that the interdependences between consecutive periods, due to the existence of random demands, introduce additional complexities in the underlying optimization problem that can be conveniently addressed by simulation.

3 ADDITIONAL DETAILS OF THE CONSIDERED PROBLEM

The TOP with stochastic travel times and maximum travel time per route is an extension of the deterministic TOP, which is a *NP-hard* problem (Chao et al. 1996). Let us consider a directed graph G = (N,A), where: $(i) N = \{0, 1, ..., n+1\}$ is a set of n+2 nodes including *n* customers as well as an origin depot (node 0) and a destination depot (node n+1); and $(ii) A = \{(i, j)/i, j \in N, i \neq j\}$ is the set of arcs connecting the nodes. A fleet of *m* homogeneous vehicles travels through the graph *G* visiting some of its nodes, starting from the origin depot and finishing in the destination one. The first time a customer *i* is visited, a reward $u_i \ge 0$ is obtained ($\forall i = 1, 2, ..., n$). Thus, visiting a customer more than once will not pay off, since no additional reward is gathered. The origin and destination depots have no associated rewards, i.e.: $u_0 = u_{n+1} = 0$. In our stochastic version, each arc $(i, j) \in A$ is associated with a random travel time, $T_{ij} = T_{ji}$, which is

assumed to follow a best-fit probability distribution. The total time employed in completing any route is limited by a threshold value, t_{max} (e.g., the maximum duration of the batteries in case of electric vehicles or the maximum number of hours a driver can work per day). Hence, the main goal is to find the *m* visiting routes that maximize the expected aggregated reward. Since travel times are random, whenever a vehicle cannot complete the designed route on or before the deadline, the reward collected so far in that route is considered to be lost, i.e., we are assuming here that partial rewards obtained during a route are only consolidated if the vehicle reaches the destination depot.

Based on the TOP formulation introduced by Poggi et al. (2010), a formal description of the objective function and the hard constraints for the deterministic and stochastic versions of the problem is presented. According to that, for each arc $(i, j) \in A$ and each vehicle $d \in \{1, 2, ..., m\}$, let us consider the binary variable x_{ij}^d , which takes the value 1 if vehicle *d* covers arc (i, j) and the value 0 otherwise. Likewise, let us consider the binary variable y_j , which takes the value 1 if customer *j* is visited (i.e., $\sum_{d=1}^m \sum_{i \neq j} x_{ij}^d \ge 1$), and 0 otherwise. Notice that the actual reward collected from each node *j* is also a random variable named $U_j = U_j(x_{ij}^d, T_{ij})$, which depends on whether *j* is visited by a vehicle *d* or not; and, if so, on whether the route covered by vehicle *d* is completed before t_{max} or not. If the previous assumptions are not given, then $U_j = 0$. Thus, Equation (1) denotes the objective function to be maximized, where $E[U_j]$ represents the expected value of the U_j random variable, and constraint (2) ensures the continuity of the routes.

$$\max \sum_{\substack{(i,j)\in A\\i\neq j}} \sum_{d=1}^{m} E[U_j(x_{ij}^d, T_{ij})].$$
(1)

$$\sum_{i=0}^{n} x_{i,o,d} = \sum_{j=1}^{n+1} x_{o,j,d} \qquad 1 \le o \le n, 1 \le d \le m.$$
(2)

Moreover, constraints (3) impose that the expected time in traversing any route does not exceed the threshold (in the deterministic variant, this is a hard constraint, while in the stochastic one it becomes a soft one that can be violated at the cost of losing the rewards in the associated route):

$$\sum_{(i,j)\in A} x_{ij}^d \cdot E[T_{ij}] \le t_{max} \qquad 1 \le d \le m.$$
(3)

4 THE SAMPLE AVERAGE APPROXIMATION METHOD

As described in Verweij et al. (2003) and Kim et al. (2015), the SAA is a method that makes use of Monte Carlo simulation for solving stochastic optimization problems. Thus, for instance, when optimizing the expected value of a stochastic objective function, this objective function is approximated by a sample average estimate which allows to solve the problem as a deterministic one. The process is repeated with different samples to obtain candidate solutions along with statistical estimates of their optimality gaps.

In our case, the objective function represented in Equation (1) could be approximated by Equation (4):

$$\max \frac{1}{w} \sum_{j=1}^{n} \sum_{l=1}^{w} u_j(x_{ij}^d, t_{ij}^l), \tag{4}$$

where w > 0 and $(t_{ij}^1, t_{ij}^2, \dots, t_{ij}^w)$ represents a random sample of the random variable T_{ij} , to generate an equivalent random sample for U_j .

Hence, while the optimization problem displayed in Equation (1) was stochastic, the approximately equivalent one shown in Equation (4) is a deterministic optimization problem that can be solved using classical optimization methods. In this paper, the commercial solver CPLEX (https://www.ibm.com/analytics/cplex-optimizer) has been used to solve the deterministic optimization problem. Of course, the quality of the approximation increases as the size of the random sample grows. Also, variance-reduction

techniques can be employed here in order to reduce the sample size needed to achieve a specific level of approximation quality (Anderson et al. 2006).

5 A BIASED-RANDOMIZED SIMHEURISTIC APPROACH

Simheuristics combine heuristics with simulation techniques that allows using the feedback from the simulation to refine the setup of the heuristics. Apart from combining a metaheuristic framework with Monte Carlo simulation (Juan et al. 2015), our simheuristic algorithm also employs biased-randomization (BR) techniques (Grasas et al. 2017) in order to introduce a 'slight' random effect in the otherwise greedy behavior of the base heuristic employed to construct routing plans. BR techniques have been successfully applied in solving several optimization problems (Martin et al. 2016; Dominguez et al. 2016). The main steps of our simheuristic algorithm are described next and summarized in Figure 2:

- Firstly, an initial 'dummy' solution is built by constructing a route connecting each customer with the origin and destination nodes. In order to merge some of these routes, so that a single vehicle can visit more than one customer, a concept of 'preference' level is used: the time-based savings generated by merging any two routes is given by the savings in time associated with completing the merged route instead of the two original ones. This concept is extended to the concept of preference level, which is a linear combination of time-based savings and accumulated reward. This concept of preference level is used to generate a sorted list of potential merges, and these are completed following the corresponding order, from higher to lower preference level. Also, a merge can be completed only if the total expected time after the operation does not exceed the maximum time allowed for any route.
- Secondly, we employ BR techniques to transform the previously described heuristic into a probabilistic algorithm. Accordingly, an initial base solution is constructed by the BR algorithm. As described in Juan et al. (2015), the expected reward provided by the base solution is estimated using a Monte Carlo simulation simulation. Subsequently, the solution is enhanced employing local search process. This process includes a destruction-reconstruction procedure as well as the most commonly used neighborhood in the literature 2-opt local search. In the next step, each new solution is compared against the current base and best solutions to update them if appropriate. The search is interrupted after meeting the stopping criteria. This loop generates a set of 'elite' solutions that show high expected rewards for the stochastic version of the TOP.
- Finally, a more intensive simulation (one with a larger number of runs) is carried out over the elite solutions in order to obtain more accurate estimates on their expected reward. The simulation module relies on the following steps to assess the stochastic performance (travel time) of a given solution: (*i*) using random sampling from the assigned probability distributions, it is possible to run different executions of the routing plan in order to obtain random observations of the travel time; (*ii*) from these random observations, different statistic measurements can be computed for each routing plan, e.g.: average profit and variability of these profits.

6 COMPUTATIONAL EXPERIMENTS

The simheuristic algorithm was implemented in Java. The SAA method was compiled using the CPLEX 12.6 library. Both approaches were run on a computer with 64 GB of RAM and an Intel Xeon at 3.7 GHz. A total of 1,000 scenarios were considered for the SAA method. In the case of the simheuristic, 200 runs were employed for each of the fast simulations, while this value was increased to 1,000 runs for the more intensive ones. Both the SAA method and the simheuristic algorithm are used to solve the stochastic version of the TOP. With that purpose, we modified and extended the deterministic data sets proposed by Chao et al. (1996), which include the small-size sets p.1, p.2, and p.3 (less than 35 nodes each) as well as medium-and large-sized sets p.4 to p.7 (ranging from 60 to over 100 nodes each). These sets were extended by considering deterministic travel times as the expected values of random travel times following a Log-Normal

Juan, Reyes-Rubiano, de la Torre, Panadero, Faulin, and Latorre

probability distribution, which constitutes a 'natural' choice for modeling non-negative random variables. Hence, $\forall (i, j) \in A$ we assume that $T_{ij} \sim LogNormal(\mu_{ij}, \sigma_{ij})$ with $E[T_{ij}] = t_{ij}$ and $Var[T_{ij}] = c \cdot t_{ij}$, being c > 0 a design parameter that allows to consider different levels of uncertainty. In our case, we considered three variance levels: low (c = 0.05), medium (c = 0.25), and high (c = 0.75). It is expected that as c converges to zero, the results from the stochastic version converge to those obtained in the deterministic scenario. Equations (5) define the Log-Normal behavior for a random variable T_{ij} :

$$\mu_{ij} = \ln\left(E[T_{ij}]\right) - \frac{1}{2}\ln\left(1 + \frac{Var[T_{ij}]}{E[T_{ij}]^2}\right),$$

$$\sigma_{ij} = \left|\sqrt{\ln\left(1 + \frac{Var[T_{ij}]}{E[T_{ij}]^2}\right)}\right|.$$
(5)



Figure 2: Visual overview of our simheuristic approach.



Figure 3: A comparison of gaps w.r.t. the deterministic best-known solution.

7 ANALYSIS OF RESULTS

In our experiments, we consider the objective function value (the expected reward) and computational time of a solution as the performance metrics for the SAA and the simheuristic algorithm. We observed that after 100,000 seconds the SAA method using CPLEX was only able to find solutions for the small-sized instances (up to 35 nodes). On the contrary, the simheuristic algorithm was always able to find 'good' solutions in reasonably low computing times, regardless of the instance size. This constitutes an important difference between both methodologies that needs to be considered by the decision maker whenever he needs to design distribution plans for medium- and large-scale logistics networks. As shown in Figure 3, the simheuristic algorithm provides better solutions (solutions with a lower expected time and a lower variability) than the SAA approach.

According to Figure 4, it is clear that the simheuristic solutions are achieved in much lower computing times than the ones associated with the SAA approach. This reinforces the idea that simheuristic algorithms are not only able to solve large-sized instances in reasonable computing times, but that they do so in an efficient way, i.e., providing highly-competitive results.

8 CONCLUSIONS

Simulation-optimization methods are powerful tools for solving stochastic optimization problems. Consequently, there is a large number of studies that focus their interest on modeling and tuning approximated methods to solve such problems. So far, however, few papers have compared the sample average approximation (SAA) method with simheuristics. The team orienteering problem (TOP) with stochastic travel times and a maximum duration per route has been used as a case study for such a comparison. The stochastic version of the TOP has been addressed both using the sample average approximation (SAA) method as well as a simheuristic algorithm. For numerical purposes, the Log-Normal probability distribution has been employed to model the random travel times, but any other best-fit distribution could be used instead.



Figure 4: A comparison of computing times.

Our results suggest that stochastic programming methods like the SAA can efficiently solve small-scale instances. However, they find severe difficulties as the instance size grows. On the contrary, simheuristics can efficiently solve large-scale stochastic instances in low computing times. As a promising research line for the future, we are interested in hybridizing concepts from both the SAA method and the simheuristics problems related to transportation and logistics.

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