SELECTING THE OPTIMUM BY SEARCHING AND RANKING PROCEDURES IN SIMULATION-BASED OPTIMIZATION

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ABSTRACT

Given a set of competing system alternatives to be evaluated and compared via simulation, *Ranking and Selection* (R&S) procedures are commonly applied to select the best system with respect to a predefined performance measure. In this paper we focus on two major classes of R&S techniques usually referred to as the *subset selection* and *indifference-zone* formulations. In particular, we discuss the performance of primitive and combined procedures that, at every iteration, evaluate different system configurations by sampling multiple or single additional simulation output observations to deal with complex systems. Procedure application is presented for different test cases in which either a small number of system configurations are known *a priori* or a large number of configurations are actually generated during simulation run by means of simulation-based optimization algorithms. Preliminary numerical results are given with reference to performance measures within the sub-systems of a real-world complex logistic system.

Keywords: discrete-event simulation, combinatorial optimization, statistics, metaheuristics.

1. INTRODUCTION

In a wide variety of application fields, such as logistics, production engineering and plant layout, computer-communication systems organization and others, discrete-event simulation is well recognized as an effective planning and control tool. By commonly adopting a simple *what-if* approach, simulation is also used for supporting decisions in system management and performance evaluation of policies and rules for resource allocation. The main reason for such versatility of simulation lies in its capability of representing the process of interest in a realistic, dynamic framework subjected to several elements of uncertainty and randomly occurring events and activity durations.

On the other hand, operations research models based on integer programming formulations (Nehmauser and Wolsey 1988) of combinatorial optimization problems are well consolidated as stand-alone tools for supporting specific decisions of resource allocation and activity scheduling. This is especially successful whenever the idea of fixing the process of interest at any given instant, in which the modeller may identify a set of resources and a set of tasks in a static, deterministic operational framework, results as a cost-effective choice.

The ultimate effort to spark and steer strong interplay and even overlap between these neighbouring fields of operations research is known as simulation-based optimization (Andradóttir 1998). This methodology consists in optimizing an expected performance measure based on outputs from stochastic simulations of any given system/process, whose dynamic behaviour is partially defined by some decision variables and constraints that could be optimally determined by an IP model. To fix ideas, one may think of a queuing network model of a general job shop system where the performance measure is the expected value of the *makespan* or the system *throughput* and should be estimated by solving the queuing network model proposed via simulation (Laganà, Legato, Pisacane et al. 2006; Canonaco, Legato and Mazza 2007; Canonaco, Legato, Mazza et al. 2008). Assuming that the allocation of servers to different queuing stations, as well as the selection of the service discipline are, respectively, the major resources to be allocated and the major scheduling policies to be organized, then it should not be difficult to recognize that a possible formulation of the simulation-based optimization problem would require replacing the objective function of the formulated combinatorial optimization problem with the following: $\min E[f(\theta)]$. The "f" function also accounts for implicit additional process features and queuing phenomena when searching for the optimal vector of decision variables, θ (representing resource allocation and scheduling policies).

Practically speaking, simulation-based optimization methods feature a "comparison step" between alternative feasible solutions and policies which is always based on the use of statistics to estimate the expected performance measure of interest (throughput, makespan, and so on). The above statistics are computed on a certain number of observations. Since these observations are random variates returned from a

simulation process, at each comparison there are no guarantees of selecting the true best (optimal) solution, despite it being truly representative of the best system configuration. Therefore, at the comparison step of a simulation-based optimization algorithm one should carefully design a statistical procedure to perform a correct selection with at least a user-specified probability. To this end, we discuss some *Ranking and Selection* (R&S) procedures (Goldsman, Kim, Marshall et al. 2002) which are commonly applied to select the system with the "best" (i.e. greatest or smallest) expected value of the predefined performance index (Kim and Nelson 2003).

The paper is organized as follows. In Section 2 we discuss the two major R&S approaches when all alternative simulated system designs are known in advance. In Section 3 we propose the combination of R&S and simulation-based optimization procedures to deal with system designs that are revealed during simulation experiments. Numerical experiments are presented in Section 4 and conclusions are drawn in Section 5.

2. RANKING AND SELECTION

In literature, homogeneity tests (Milton and Arnold 1986) are conventionally applied to assess whether there are statistically significant differences in various populations with respect to some characteristics. However, they provide no information in the prospect of selecting the "best" of these populations. Bearing in mind this expectation, *Ranking and Selection* techniques are the next step to take when searching for a decision procedure that allows to perform a correct selection at a pre-assigned level of probability.

Most of the research work in R&S can be classified into the following general approaches:

- *subset selection* procedures, which aim at producing a subset of (small) random size that contains the best system, with a user-specified probability;
- *indifference-zone* procedures, where either the best or whatever solution evaluated within a fixed distance from the best can be selected, with a user-specified probability.

When operating a selection of the best system or a subset of the best among a set of simulated competing alternatives, using an R&S technique rather than another depends on which of the available procedures will most benefit a given objective or constraint set by the experimenter.

Whatever the objective, an "educated" choice of an R&S procedure also requires a good knowledge of the structure of the problem space in view of the fact that the said structure impacts on the performance of the procedures that can be used for problem solving.

Everything considered, the performance level of an R&S procedure is affected by:

- the probability of selecting the alternative which is truly representative of the best system configuration (PCS – probability of correct selection);
- the above probability returned within a given predetermined time budget;
- the existence of extreme configurations in which, for example, all solutions have an equal mean value or every solution is distant exactly delta units from the best (a.k.a. the *least favorable configuration*) or ordered solutions are equally spaced from one another;
- the difference between solutions which is assumed to be statistically insignificant;
- the structure of the problem space.

This stated, it is quite logical that different problems require different approaches. For example, in complex systems one of the following situations might occur: *i*) all the possible alternative system configurations are known before experimentation or *ii*) system configurations are revealed (meaning generated) during experimentation. Obviously, these cases also call for the use of specific (meaning different) procedures.

In this paper, we consider selecting the best system(s) according to a user-defined probability under a pre-assigned time budget, whenever the solutions are either all known *a priori* (see Bechhofer, Santner and Goldsman 1995 for a complete summary) or revealed during experimentation (Hong and Nelson 2007). For the former case, we examine two stand-alone R&S procedures that belong to the *subset-selection* and *indifference-zone* approaches; for the latter, we combine the above R&S procedures with a simulation-based optimization algorithm whose objective is to generate new alternative systems at run-time.

In both cases, as far as notation is concerned, we use k to call the number of alternative simulated system designs ($i = 1..k$); n the number of observations ($j = 1..n$) sampled from each system design; $\mu_1, \mu_2, ..., \mu_k$ the unknown k expected values of the performance measure of interest; $\mu_{[k]} \geq ... \geq \mu_{[1]}$ the ordered unknown k expected values of the performance measure of interest (i.e. the system design in position k is the greatest); $\overline{X}_k, ..., \overline{X}_1$ the sample means of the performance measure of interest for each system design; σ^2 the common unknown variance of the alternative system designs; $\overline{S}_k^2, ..., \overline{S}_1^2$ the sample variance of the performance measure of interest for each system design; $1-\alpha$ the confidence level (or user-specified probability P^*). In a maximization problem, we also use k to call the system with the best (meaning greatest) performance measure of interest.

It is worth observing that the basic underlying assumptions for all these R&S procedures, meaning independent and identically distributed normal data with common variance, usually depart from the realistic

settings involved when simulating real-world systems. However, some important statistical results allow to extend the application of simulation-based optimization methods to problems in which simulation output data is not independent, nor normally distributed. These issues range from performing the proper process initialization (Law and Kelton 2000) to finding a consistent estimator for the sample variance (Meketon, and Schmeiser 1984; Goldsman, Meketon and Schruben 1990; Damerdji 1994; Song and Schmeiser 1995; Glynn and Whitt 1997; Steiger and Wilson 2002).

2.1. Subset-selection Procedures

Rather than claiming that one population is the best, perhaps it is more convenient to claim that one is confident that the best population is contained in a subset I of the $\{1,2,...,k\}$ competing simulated systems. Subset selection procedures are based on this logic. These R&S procedures aim at producing a subset of (small) random size that contains the best system, with a user-specified probability.

This R&S approach was first introduced by Gupta (1965) with the purpose of obtaining a subset $I \subseteq \{1,2,...,k\}$ according to which

$$P\{k \in I\} \geq 1-\alpha. \tag{1}$$

Basically, Gupta's idea was to include in I all the systems k that fall in the following interval:

$$\left[\overline{X}_k(n) - h\sigma\sqrt{\frac{2}{n}}, \quad \overline{X}_k(n)\right] \tag{2}$$

where σ is the common, known standard deviation and $\overline{X}_k(n)$ is the maximum among the sample means. Obviously, the most favorable case would be $|I| = 1$.

In order to guarantee (1), the value of h in (2) is determined as follows:

$$P\{k \in I\} =$$

$$= P\left\{\overline{X}_k(n) \geq \overline{X}_i(n) - h\sigma\sqrt{\frac{2}{n}}, \quad \forall i \neq k\right\} \tag{3}$$

$$= P\left\{\frac{\overline{X}_i(n) - \overline{X}_k(n) - (\mu_i - \mu_k)}{\sigma\sqrt{2/n}} \leq h - \frac{(\mu_i - \mu_k)}{\sigma\sqrt{2/n}}, \forall i \neq k\right\}. \tag{4}$$

If μ_k is the unknown performance measure of the "best" system, then $-\frac{(\mu_i - \mu_k)}{\sigma\sqrt{2/n}}$ is a positive value, thus

$$P\{k \in I\} \geq P\left\{\frac{\overline{X}_i(n) - \overline{X}_k(n) - (\mu_i - \mu_k)}{\sigma\sqrt{2/n}} \leq h, \forall i \neq k\right\} \tag{5}$$

and finally

$$P\{k \in I\} \geq P\{Z_i \leq h, \quad i = 1,2,...,k-1\} = 1-\alpha \tag{6}$$

where $(Z_1, Z_2, ..., Z_{k-1})$ are distributed according to a multivariate normal distribution with means equal to 0, variances equal to 1 and common pair-wise correlation equal to $1/2$. In order to guarantee (1), h must be the $1-\alpha$ quantile of the maximum value of $(Z_1, Z_2, ..., Z_{k-1})$.

The following pseudo-code provides a high-level description of Gupta's approach:

0. *select 1-α, n and h;*
1. *take a random sample of n from each of the k systems;*
2. *compute an estimate of the performance index of interest for each of the k systems;*
3. *include a system in subset I if the system's sample mean falls in (2).*

In the above procedure, the choice of $1-\alpha$ is left to the experimenter. Practically, $1-\alpha$ should be greater than or equal to 0.5, since any system could be included in I by simply tossing a fair coin. At the same time, $1-\alpha$ should also be greater than or equal to $1/k$ which is the probability of randomly selecting a system for inclusion in the subset. A pure empirical rule (Gibbons, Olkin and Sobel 1979) recommends $1-\alpha \geq 0.5 + (0.5/k)$.

2.2. Indifference-zone Procedures

Similar to any other selection procedure dealing with random variates returned from a simulation process, the indifference-zone based approach may or may not select the simulated system configuration which is truly representative of the best solution (if it does, then a correct selection (CS) is said to have been made). The novelty lies in the fact that this selection approach is statistically indifferent to which system configuration is chosen among a set of competing alternatives when these alternatives all fall within a fixed distance from the best solution.

This stated, let $P\{CS\}$ be the probability of correct selection and δ the indifference-zone chosen by the experimenter. In a maximization problem the probability of performing a correct selection with at least probability P^* is

$$P\{CS\} \hat{=} P\{\mu_k > \mu_i \forall i \neq k \mid \mu_k - \mu_i \geq \delta\} \geq P^*. \tag{7}$$

The probability of correct selection (7) was first computed in Rinott (1978) by resorting to numerical integration under the hypothesis of normality of the statistics involved. If $P(CS)$ is the probability that $\overline{X}_k(n_k)$ is the true "best" sample mean, namely it corresponds to $\overline{X}_{[k]}(n_k)$, then

$$P(CS) =$$

$$= P\left[\overline{X}_k(n_k) = \overline{X}_{[k]}(n_k)\right] \quad (8)$$

$$= P\left[\overline{X}_k(n_k) > \overline{X}_{k-1}(n_{k-1})\right], \text{ for short } P\left[\overline{X}_k > \overline{X}_{k-1}\right] \quad (9)$$

$$= P\left[\frac{\overline{X}_k - \mu_k}{\delta/h} > \frac{\overline{X}_{k-1} - \mu_{[k-1]}}{\delta/h} + \frac{\mu_{[k-1]} - \mu_{[k]}}{\delta/h}\right]. \quad (10)$$

Since $\left[\frac{\overline{X}_k - \mu_{[k]}}{\delta/h}\right] \hat{=} T_k$ and $\left[\frac{\overline{X}_{k-1} - \mu_{[k-1]}}{\delta/h}\right] \hat{=} T_{k-1}$ are distributed according to Student's law with $n_k = n_{k-1} = \cdots = n_0$ degrees of freedom (Law and Kelton 2000) and since $\overline{X}_k$ and $\overline{X}_{k-1}$ are assumed to follow a Normal distribution, then

$$P(CS) =$$

$$= P\left[T_k - T_{k-1} > \frac{\mu_{[k-1]} - \mu_{[k]}}{\delta/h}\right] \quad (11)$$

$$= P\left[T_{k-1} < T_k + \frac{\mu_{[k]} - \mu_{[k-1]}}{\delta/h}\right]. \quad (12)$$

According to the total probability distribution conditioned on T_k,

$$P[T_{k-1} < T_k] =$$

$$= \int_{t=0}^{\infty} P\left[T_{k-1} \le t \mid t < T_k \le t + dt\right] * P\left[t < T_k \le t + dt\right] \quad (13)$$

$$= \int_{t=0}^{\infty} F_{T_{k-1}|T_k}(t) f_{T_k}^{(m)}(t) dt. \quad (14)$$

Because of independence between T_k and T_{k-1} then

$$= \int_{t=0}^{\infty} F_{T_{k-1}}(t) f_{T_k}(t) dt. \quad (15)$$

In the particular case (maximization) under examination

$$P\left[T_{k-1} < T_k + \frac{\mu_{[k]} - \mu_{[k-1]}}{\delta/h}\right] =$$

$$= \int_{t=0}^{\infty} F_{T_{k-1}}\left(t + \frac{\mu_{[k]} - \mu_{[k-1]}}{\delta/h}\right) f_{T_k}(t) dt. \quad (16)$$

Since $\mu_{[k]} - \mu_{[k-1]} \ge \delta$, the final result is

$$P(CS) \ge \int_{t=0}^{\infty} F_{T_{k-1}}(t+h) f_{T_k}(t) dt. \quad (17)$$

Note that equality is verified when $\mu_{[k]} - \mu_{[k-1]} = \delta$. If the integral is set equal to P^* and solved numerically for h, for different values of n (the number of observations taken from the system to compute the sample mean), the results can be tabled and read to obtain h, which is also known as Rinott's constant. Numerical values for h are tabled in Wilcox (1984).

The following pseudo-code provides a high-level description of a two-stage indifference-zone procedure:

Stage 1

0. *select 1-α,δ, n_0 and h;*
1. *take a random sample of n_0 from each system;*
2. *compute the sample variance S_i^2 of the performance index of interest for each system;*
3. *compute $N_i=max(n_0, h^2S_i^2/\delta^2)$;*

Stage 2

4. *if $n_0>=max_i\ N_i$ then select the system with the greatest sample mean otherwise take an additional sample of N_i-n_0 from each system i and then select the system with the greatest sample.*

As shown at step 3, the total number of samples to be taken from each system mostly depends on sample variance and, thus, also on how the sample mean is computed. In two-stage R&S approaches, different methods are used for this purpose. Rinott (1978) uses a classic sample mean, while Dudewicz and Dalal (1975) use a weighted sample mean during the second stage. In (Canonaco, Legato and Mazza 2009), we investigate a moving-average sample mean whose early results are very promising.

3. SEQUENTIALLY REVEALED CONFIGURATIONS

The R&S procedures examined in the previous section are based on the common assumption that a (small) number of system configurations are known *a priori*. In this particular case, the guarantee of selecting the best or near-best alternative when all solutions have already been sampled and retained appears to be both very appealing and practicable. However, at times, a combinatorial, unknown number of configurations need to be explored. When this occurs, k different systems

configurations (with $k \geq 1$) can be revealed sequentially during a simulation run by means of a so-called system generating algorithm (SGA). Under this hypothesis, should an exhaustive coverage of all the possible system combinations be not reasonable, nor affordable from a computational point of view, then metaheuristic-based approaches would have to be addressed. Examples of similar new, promising methodologies are *simulated annealing* (Ahmed and Alkhamis 2002; Andradóttir and Prudius 2005) and *adaptive balanced explorative and exploitative search* (Prudius and Andradóttir 2004; Prudius 2007). Although these algorithms are not used to perform an exhaustive coverage of the sample space, nor do they provide any sort of control running on which part of the feasible set is being explored, the solutions returned as final output are likely to belong to the set of optimal global solutions (Legato, Mazza and Trunfio 2008). This is a major issue in light of how demanding a statistical guarantee of correct selection in each iteration can be, especially when the number of candidate solutions visited by the optimization process is very large. As matter of fact, the new sequential selection procedures presented in (Hong and Nelson 2007) are applicable to small-scale optimization problems alone (with a number of systems ≤ 500), while extensions of these procedures to optimization problems with a very large number of alternatives is currently a subject of ongoing research efforts.

This stated, an overall scheme of the experimental framework, providing both system design generation and evaluation for selecting the best among these competing alternatives, can be summarized by the following pseudo-code.

0. set initial system design to be the best system design and set iteration equal to 0;
1. update iteration and generate k (k≥1) alternative system designs during the current iteration;
2. compare alternative system designs generated with current best system design and, eventually, update the best;
3. if stopping condition is met then exit, otherwise go to Step 1.

The R&S procedures examined in the previous section are used for system comparison in the above schema (Step 2), while the simulated annealing (SA) algorithm now described is used as SGA (Step 1).

0. set input parameters (initial Temperature, lower bound Temperature, time-budget) and best system design to be initial system design;
1. while elapsed time is less than time-budget and the Temperature is less than the lower bound value:
(a) generate a system design from the current system design;
(b) if the new design is "better", then set best system design to be new design; else accept new design as best with probability p=exp(Δ/Temperature), where Δ is the difference between the two designs.

In brief, the SA approach is aimed to generate feasible schedules, explore them in a more or less restricted amount without getting caught in local minima and, finally, stop at a satisfactory solution.

4. NUMERICAL EXPERIMENTS

In this section, we present our efforts in searching for "intelligent" sample allocation when solving well-structured problems with significant constraints, especially within large, real-sized contexts. From a practical point of view, avoiding over-sampling affects the termination of the selection procedures and, thus, results are obtained with the least amount of simulation (i.e. execution time) possible.

Let us first examine the empirical performance of a primitive *Gupta-like* subset-selection procedure to select the best yard crane assignment and transfer policy in a terminal container. In particular, the objective is to select the policy which allows to minimize the maximum average time to complete stacking/retrieval operations of suitable batches of containers (BCT) in the yard. The scenario proposed features medium container traffic intensity and high crane transfer time among yard blocks. All experiments are carried out by setting $P^* = 0.90$, $k = 5$ and $n = 10$, under the realistic assumption of unknown, but common variance for each system design. To this end, Bartlett's test (1937) has been used to verify the common variance assumption.

Table 1: Simulation Results for the Five Alternative Yard Policies

Policy *i*	N° of Observations			Average BCT (minutes)
	SSP	RP	OP	
Policy 1	10	31	10	97.369
Policy 2	10	27	17	91.043
Policy 3	**10**	**10**	**10**	**78.177**
Policy 4	10	32	26	100.052
Policy 5	10	48	17	92.343

According to the subset-selection procedure (SSP), the interval defined by (2) for this particular problem is $[78.117,\ 90.155]$, thus $I = \{3\}$. This result has also been compared with those returned by another two R&S procedures: Rinott's procedure (RP) (1978) and our procedure (OP) (Canonaco, Legato and Mazza 2009). As one may easily calculate from Table 1, a cumulative (over all policies) number of 148 and 80 observations are required by these two procedures, respectively, whereas the SSP accomplishes the same result with only 50 observations. The case study just presented is representative of a typical situation where system configurations are well-spaced from each other, with

respect to the performance metric adopted for comparison. Here one may recognize that the SSP allows to screen suitable configurations with a very limited number of observations.

We now present a second case which requires the combination of multi-stage R&S procedures with simulation-based optimization approaches since the alternative systems are revealed during the execution of the experiment.

In the combined procedure (CP) proposed herein, we pursue the idea of "efficient" sampling by basing the number of observations to be taken from each system on the convergence of process variance and whether this occurs within a certain number of simulation runs. In other words, at each iteration, this variance-weighted decisional mechanism decides to switch between adding a single (Chen and Kelton 2005) or multiple additional simulation output observations (Kim and Nelson 2003). With this multi-stage approach, the procedure is expected to terminate faster.

We use the above framework to deal with a complex scheduling problem that arises in a container terminal when multiple quay cranes must be assigned to holds of the same vessel to perform discharge (D) and loading (L) operations. In this problem (also referred to as the *quay crane scheduling problem* QCSP, (Legato, Mazza and Trunfio 2008)), the classical objective is to minimize the vessel's overall completion time (*makespan*), while taking into account precedence and non-simultaneity constraints between holds when they are operated by crane. According to our experience based on real data, D/L operation rates have been fixed to an average value of 26 containers/hour. For sake of sensitivity analysis, we have defined two D/L distributions for operation times: a realistic 8-order Erlang distribution and a basic exponential distribution.

Table 2: Comparison of Simulation Results Produced by Rinott's Procedure and Combined R&S Procedure

D/L Distribution	Solutions Evaluated	Average Makespan (hours)	
		RP	CP
Erlang	20	17.74	17.4
	135	14.05	14.45
	1379	12.93	12.67
Exponential	20	17.77	16.45
	135	14.15	14.24
	1379	13.04	13.21

Observe that the variance associated to the individual discharge/loading service times does not significantly affect the performance of the different procedures in terms of the average quality of solution returned by each of them (i.e. final, mean value of the makespan), as illustrated in Table 2. Rather, it has a clear impact on the average number of observations (simulation runs) required to achieve solutions, as one may recognize from results in Table 3 where the number of observations corresponding to the set of solutions in Table 2 are reported. In particular, the CP procedure seems to definitely outperform the classical, two-stage RP procedure by at least 20% whenever service times becomes less regular (exponential case).

Table 3: Comparison of Observations Required by Rinott's Procedure and Combined R&S Procedure

D/L Distribution	N° of observations		CP Performance (Δ%)
	RP	CP	
Erlang	212	209	+1.42%
	1421	1405	+1.13%
	14421	14283	+1%
Exponential	1100	791	+28.1%
	7035	5268	+25.12%
	71727	54029	+24.67%

5. CONCLUSIONS

We have discussed some recent issues on searching and ranking feasible solutions when using simulation-based approaches to optimization problems in logistics. This has been accomplished for the case in which candidate optimal solutions are all available at the initial step of the simulation-optimization procedure, as well as for the case in which they are revealed during the execution of the procedure. A subset-selection technique is shown to be effective for the problem of selecting the best yard crane assignment and transfer policy in a terminal container, due to the specific structure of the candidate policies. On the other hand, dealing with the quay crane scheduling problem, we obtained encouraging numerical evidence on the idea that changing the number of observations from a single one to multiple ones, according to the stability of the estimate of the process variance, may result as a practical key for speeding-up the simulation-based optimization procedure.

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