EXPLOITING VARIANCE BEHAVIOR IN SIMULATION-BASED OPTIMIZATION

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ABSTRACT
The methodological contribution proposed herein arises from considering the integration of stand-alone optimization techniques in discrete-event simulation, in order to model dynamic logistic processes, under realistic conditions of uncertainty. A simulation-based optimization approach is investigated to optimize overall system performance measures. A special focus is laid on evaluating alternative system solutions when they are either known *a priori* or revealed at run-time. To this end, a variance-guided statistical technique for the ranking and selection of candidate solutions has been devised and integrated into a solution generating algorithm on which the search process for the best solution may be centered. The findings returned from this work have been coupled with a queuing network model developed and applied in container stacking/retrieval operations via *dts - direct transfer system* on the yard of a real maritime container terminal for pure transshipment.

Keywords: discrete-event simulation, optimization, simulation-based optimization, metaheuristics, logistics

1. INTRODUCTION
Many modern day systems providing products and services in popular fields such as logistics, manufacturing, transportation, network-centric computing, etc., are studied with the objective of carrying-out performance analysis and optimization. The greater the complexity of similar systems, the more the common approach to problem design and solution is based on decomposing the original problem into several smaller models. However, when dealing with dynamic and random-based activities, to deliver overall optimized system performance, a more satisfactory contribution could spring from the combination of stand-alone algorithms used for optimum-seeking with discrete-event simulation used for performance evaluation. This awareness has lead to the introduction of an integrated methodology which significantly aids decision-making under uncertainty: Simulation-based Optimization (SO).

In (Fu 2005), the author divides the types of SO techniques in the following main categories:

- statistical procedures (e.g. ranking & selection procedures and multiple comparison for the comparison of two or more alternative system configurations);
- metaheuristics (methods directly adopted from deterministic optimization search strategies such as simulated annealing);
- stochastic optimization (random search, stochastic optimization);
- other (including ordinal optimization and sample path optimization).

Here we focus on procedures, included in the first two categories, to generate and estimate the best among a set of alternative solutions, whether they are all known in advance or actually revealed during a simulation run. To select the best system, we devise a decisional mechanism based on variance estimation with the purpose of guiding the sampling activity required to perform the analysis of simulation output. We then integrate the SO models proposed into a computational framework and exploit this unifying structure with reference to the container stacking/retrieval process occurring in the container terminal of Gioia Tauro in Southern Italy. The final objective amounts to selecting the best among a set of different policies adopted by the operation manager to transfer yard cranes from one block of the container storage area to another.

2. SIMULATION-BASED OPTIMIZATION

2.1. The Methodology
Simulation-based optimization consists in searching for the settings of controllable decision variables that yield the maximum (minimum) expected performance of a stochastic system that is represented by a simulation model (Fu and Nelson 2003). Formally,

$$max\ (min)\ E[f(\theta)] \quad (1)$$

where θ is the vector of decision variables and $E[f(\theta)]$ the mathematical expectation of the performance measure of interest which should be estimated by statistics on random variates returned from simulation-generated sample paths.

As we will later see, the alternative systems to be simulated can either be a limited number and all known in advance or a great, but countable number and generated by a properly designed optimization procedure. Whatever the case, the simulation component of the SO solution effort calls for the following considerations.

Performance evaluation is based on observations that are random variates returned by a simulation process. Thus, one may or may not select the system solution which is truly representative of the best solution. To deal with this, we consider an indifference-zone (IZ) ranking and selection (R&S) procedure and give some background information for this approach.

In terms of notation, let

k	the number of alternative simulated system solutions ($i=1..k$),
n	the number of observations sampled from each system solution ($j=1..n$),
$\mu_1,\mu_2,\ldots,\mu_k$	the unknown k expected values of the performance measure of interest,
$\mu_{[k]}\geq\ldots\geq\mu_{[k]}$	the ordered unknown k expected values of the performance measure of interest,
$\overline{X}_k,\ldots,\overline{X}_1$	the sample means of the performance measure of interest for each system solution,
$P\{CS\}$	the probability of correct selection,
δ	the indifference zone chosen by the experimenter.

An IZ procedure is statistically indifferent to which system solution is chosen among the k competing alternatives when all these alternatives fall within a fixed distance δ from the best solution. In a maximization problem the probability of performing a correct selection with at least level of confidence P^* is

$$P\{CS\}\hat{=}P\{\mu_k>\mu_i\ \forall i\neq k \mid \mu_k-\mu_i\geq\delta\}\geq P^*. \qquad (2)$$

Under the hypothesis of normality of the statistics involved, this probability was first computed by Rinott in (Rinott 1978) starting from the following inequality

$$P\{CS\}\geq\int_{t=0}^{\infty}F_{T_{k-1}}(t+h)f_{T_k}(t)dt \qquad (3)$$

where

$$T_k\hat{=}\frac{\overline{X}_k-\mu_{[k]}}{\delta/h} \text{ and } T_{k-1}\hat{=}\frac{\overline{X}_{k-1}-\mu_{[k-1]}}{\delta/h} \qquad (4)$$

are distributed according to Student's law. The above integral is set equal to P^* and solved numerically for h, for different values of n. Numerical values for h, which is also known as Rinott's constant, are tabled in (Wilcox 1984).

In conclusion, when simulating k alternative system solutions, IZ procedures guarantee the selection of the "best" solution or a "near best" according to a pre-specified probability. From a practical point of view, considering a large number of simulation replications for each solution reduces sampling errors; on the other hand, the computational expense of even one single replication of any simulation model is likely to be cumbersome. Bearing in mind these conflictual objectives, pioneering two-stage indifference-zone ranking and selection (R&S) procedures (Rinott 1978, Dudewicz and Dalal 1975) have been followed by more recent and advanced procedures based on an n-stage logic, with $n>2$ (Kim and Nelson 2001, Chen and Kelton 2005). In our SO approach we also exploit an n-stage IZ R&S procedure where the idea of "efficient" sampling is pursued by basing the number of output observations to be taken from each system on the corresponding variance behavior (i.e. how variance changes as the sample from simulation output grows), given a fixed computing budget. Thus, for our enhancement, it is necessary to establish how such variance should be estimated.

If for system i ($i=i..k$) the n elementary output observations $X_i\hat{=}\{X_{ij}, j=1..n\}$ returned from a simulation run are independent and normally distributed, one may pursue variance estimation by simply using classical statistics and computing the sample mean

$$\overline{X}_i=\frac{1}{n}\sum_{j=1}^{n}X_{ij}, \qquad (5)$$

followed by the unbiased sample variance which is used as variance estimator

$$VAR[X_i]=S_i^2=\frac{1}{n-1}\sum_{j=1}^{n}\left(X_{ij}-\overline{X}_i\right)^2. \qquad (6)$$

Should this not be the case - as customary in a simulation-based study of practically any real-life system - then one must start from the output stochastic process, organize its data and compute the process variance.

For example, for system i let $\{X_1,\ldots,X_j,\ldots,X_n\}$ be a *weekly dependent* stationary output process with mean μ_X and variance σ_X^2. This process is said to be *weakly dependent* if the lag-j covariance

$$\gamma_j \hat{=} Cov\left[X_i, X_{i+j} \right], \quad j = 0, \pm 1, \pm 2, \ldots \tag{7}$$

satisfies $\gamma_j \to 0$ as $|j| \to \infty$ (Billingsley 1995).

If one chooses to organize this data in batches of size k, the sample mean for batch i is given by:

$$\overline{X}_i(k) \hat{=} \frac{1}{k} \sum_{j=i+1}^{i+k} X_j \tag{8}$$

and according to the Central Limit Theorem

$$\overline{X}_i(k) \overset{D}{\to} Z(\mu_X, \sigma^2(k)/k), \; k \to \infty \;\; \forall i \tag{9}$$

where

$$\sigma^2(k) = \sigma_X^2 + 2\sum_{j=1}^{k-1} \left(1 - \frac{j}{k}\right) \gamma_j . \tag{10}$$

Furthermore, the variables in the following set

$$\left\{ \overline{X}_1(k), \ldots, \overline{X}_i(k), \ldots, \overline{X}_n(k) \right\} \tag{11}$$

become independent as $k \to \infty$ and

$$\lim_{k\to\infty} \sigma^2(k) = \lim_{k\to\infty} k \, Var\left[\overline{X}_i(k) \right] = \sigma_X^2 \,, \; \forall i . \tag{12}$$

By (Hogg and Craig 1978)

$$\frac{S_{\overline{X}}^2(n,k)}{\sigma_X^2 / k} \approx \frac{\chi_{n-1}^2}{n-1} . \tag{13}$$

Applying the mathematical expectation to the above formula

$$E\left[\frac{S_{\overline{X}}^2(n,k)}{\sigma_X^2 / k} \right] = E\left[\frac{\chi_{n-1}^2}{n-1} \right] = 1 \tag{14}$$

and thus

$$E\left[k \cdot S_{\overline{X}}^2(n,k) \right] = \sigma_X^2 \tag{15}$$

where

$$S_{\overline{X}}^2(n,k) \hat{=} \frac{k}{n-1} \sum_{i=1}^{n} \left(\overline{X}_i(k) - \overline{\overline{X}}(n,k) \right)^2 \tag{16}$$

is the estimator of the (output) process variance.

This stated, our procedure uses a variance-weighted decisional mechanism based on the variance estimator described above to guide the sampling activity on the number of additional simulation output observations to be taken from each system. Practically speaking, when process variance decreases this multi-stage procedure is expected to terminate faster than classical two-stage R&S algorithms because of its auto-adaptive control. In every other case, the number of iterations during which the sample variance either remains constant (during the last x runs) or increases is controlled by an upper bound (UB) on the number of additional simulation runs to be carried-out which is given by the well-known formula based on Rinott's constant

$$\text{additional runs} = \left(h^2 S_i^2 / \delta^2 \right) \tag{17}$$

The following pseudo-code provides a high-level description of our approach when considering a maximization problem:

Table 1: Our IZ R&S Procedure

P^*, δ, n_0, h, x, UB $\leftarrow$ select procedure settings
for *i = 1* **to** k **do**
  for *j = 1* **to** n_0 **do**
    X_{ij} $\leftarrow$ take a random sample of n_0 from each of the k systems
  end for
  $\overline{X}_i$ $\leftarrow$ compute an estimate of the sample mean of the performance index of interest for system i
  update *stopping condition[n]*
end do
$N_i = \max\left(n_0, h^2 S_i^2 / \delta^2\right)$ $\leftarrow$ determine the sample size to take from each system
if $n_0 \geq \max_i N_i$ **then**
  $\max_i \overline{X}_i$ $\leftarrow$ select system with greatest sample mean as best and **stop**
Else
  For *i = 1* **to** k **do**
    while $N_i \leq UB$ **do**
      X_{ij} $\leftarrow$ take one additional random sample for system i
      $\overline{X}_i$ $\leftarrow$ compute an estimate of the sample mean of the performance index of interest for system i
      S_i^2 $\leftarrow$ compute a run-weighted estimate of the sample variance of the performance index of interest for system i
      $N_i = \max\left(n_0, h^2 S_i^2 / \delta^2\right)$ $\leftarrow$ determine the new sample size for system i
      if $N_i \leq n_0$ or $S_i^2 = \text{constant}$ in the last x runs then

stop sampling for system i
end while
End for
$\max_i \overline{X}_i \leftarrow$ select system with greatest sample mean as best

So doing, our approach avoids relying on too much information obtained in just one stage and, at the same time, allows to save on computing budget.

2.2. The Framework

The simulation-based optimization framework now proposed in Table 2 serves a double purpose. On one hand, it offers a common ground where to define and compare the different IZ R&S techniques that, in turn, are recalled throughout this work or in companion papers (Legato, Canonaco and Mazza 2009). On the other, it shows how a simulation engine inserted in an optimization algorithm is often the only practical solution method available when dealing with difficult-to-solve combinatorial problems, embedded in realistic dynamic logistic processes characterized by several elements of randomness.

Table 2: SO Framework for Solution Generation and Evaluation

1	k, $n=0$, *stopping condition[0]* $\leftarrow$ select procedure settings
2	$i^* = i$ $\leftarrow$ set best solution = initial solution
3	**while** *stopping condition[n] = false* **do**
4	$n = n + 1$
5	$i_1(n), i_2(n),..., i_k(n)$ $\leftarrow$ at iteration n take/generate k alternative solutions
6	$i^* = \text{best}\{i^*, [i_1(n), i_2(n),..., i_k(n)]\}$ $\leftarrow$ compare the k alternative solutions at iteration n with current best and, eventually, update the best
7	update *stopping condition[n]*
8	**end do**
9	i^* $\leftarrow$ return best solution

As one may observe, on line 5 solutions are either taken or generated. In the latter case, a metaheuristic approach based on a variant of the well-known Simulated Annealing (SA) algorithm (Alrefaei and Andradóttir 1999) has been adopted. Besides discarding the basic assumption according to which the temperature $Temp_k \to 0$ as $k \to \infty$ by assuming $Temp_k = Temp$ $\forall k$, this approach bears two possible ways of estimating the optimum solution. It either uses the most visited solution or selects the solution with the best average estimated value of the objective function. The effectiveness of this constant temperature approach is not yet consolidated for complex and large practical applications. (Mazza 2008) discusses this issue and introduces a guided-search refinement in the SA algorithm based on choosing the candidate solution j among m neighboring solutions $j_1, j_2,..., j_m$ of the current solution i.

As for solution comparison and selection, the procedure reported in Table 1 is inserted on line 6 of the above schema.

3. APPLICATIONS IN PORT LOGISTICS

Container terminal logistics have received great interest in the scientific literature from both the theoretical and practical standpoint (Stahlbock and Voß 2008). The reason for such concern is straightforward if one considers the number and random nature of operational activities carried-out in these facilities: vessel arrival and berthing, resource assignment and scheduling, container transfer and handling, emergency management (e.g. equipment failure, congestion phenomena, weather conditions) and so on. In a maritime container terminal many different company-based rules, regulations and practices can be the grounds of application for the simulation-based optimization framework previously described. Real case studies are given in companion papers (Legato, Mazza and Trunfio 2008; Legato, Mazza and Trunfio 2010). Here we consider the yard and some organizational and operational issues pertaining to its role within the terminal. We then propose to manage the yard activity with respect to policies and equipment employed for container stacking/retrieval by applying the SO approach.

3.1. Problem Description

The purpose of a stacking yard in a terminal is to provide storage space for containerized cargo during import, export or transshipment operations. Whether dedicated or shared among different shipping companies, suitably-sized lots of the yard are generally assigned to each company and equipped with technological means in order to enable the stacking/retrieval of container batches (i.e. a set of containers sharing some common properties).

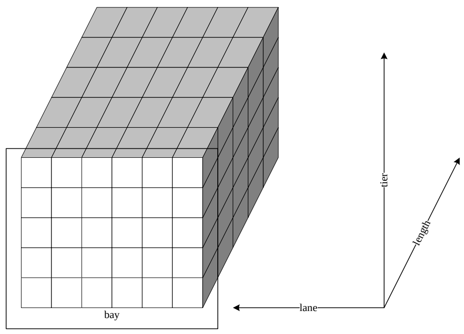

Figure 1: Definition of a Yard Block.

A yard is typically organized in *zones* that, in turn, are divided into *blocks*. As shown in Figure 1, the size of a block is defined by three dimensions: *i*) number of *lanes* or *rows* (e.g. 6 or 13, along with an extra lane if internal trucks are used to perform container transfer);

ii) number of container *tiers* or stack height for each lane (e.g. 5); *iii*) number of containers in length (e.g. 20). A vertical section of a block (e.g. 5 tiers * 6 lanes) is normally referred to as *bay*.

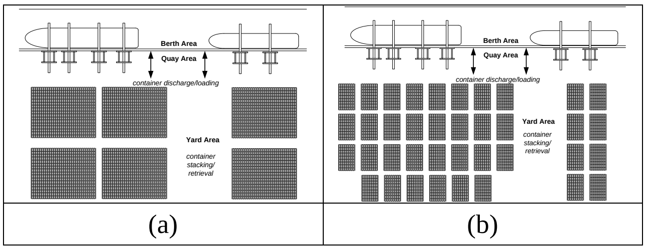

Figure 2: Two Alternative Yard Organizations.

It is worth observing that both the number and size of blocks in a yard affect the average travel time of shuttle vehicles cycling between the quay and the yard areas, as well as the container handling time on the yard. For instance, in the yard organization depicted by Figure 2.(a), the average distance to be covered in order to reach a container is greater than the average distance deriving from the solution portrayed in Figure 2.(b). On the other hand, more container handling equipment can be concentrated in a specific area in the former case, thus returning a smaller service time, whereas this possibility is prevented in the latter case due to potential interference between container movers meant to operate on adjacent yard bays

If container stacking/retrieval on the yard is performed by transfer cranes, such as rail-mounted gantry cranes (RMGCs) or rubber-tired gantry cranes (RTGCs), then a common operational issue actually consists in periodically deciding how many and which cranes are to be assigned to a block. This decision usually depends on the expected daily workload in each block and, therefore, on the total crane capacity (measured in time units) required to complete container stacking/retrieval operations.

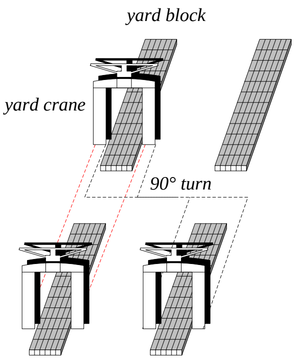

Figure 3: Possible Intra-block Crane Transfer.

To do so, cranes must be transferred from one block to another. If we consider RTGCs, these cranes can travel between adjacent yard blocks without any turning motion or by changing lanes. In the former case, crane transfer can take about 10 minutes; in the latter, about 5 additional minutes are required to perform 90 degree turns (see Figure 3). These movements are exclusively referred to inter-block (and not inter-zone) crane transfer.

In our study, we focus on the new operational scenarios generated by five alternative management policies - all known a priori - for assigning yard cranes to yard blocks and accounting for order, times and routes of the crane transfer. The objective is to select, by way of the SO framework, the policy which allows us to minimize the maximum average time to complete stacking/retrieval operations of suitable batches of containers in the yard.

3.2. Numerical Experiments

To perform the comparison of five alternative system solutions we consider the corresponding variance patterns with respect to a hypothetical operational scenario in which average container traffic in yard blocks is at a medium level (e.g. not many shipping lines stack/retrieve containers in that area) and average crane transfer times between blocks are high (e.g. in an extensive yard area). Figure 4 illustrates an example of how variance changes as the samples taken from system simulation under different policies grows. Observe that for the first three policies variance behavior is stable, meaning that are no significant changes in variance estimation as the sampling procedure progresses. Thus the algorithm continues adding single observations (or batches or simulation replications) as required by the "stable" variance estimate until the upper bound provided by Rinott's two-stage procedure is reached (Legato and Mazza 2008). When the variance pattern increases, as for policy n°4, the upper bound is still provided by Rinott's procedure.

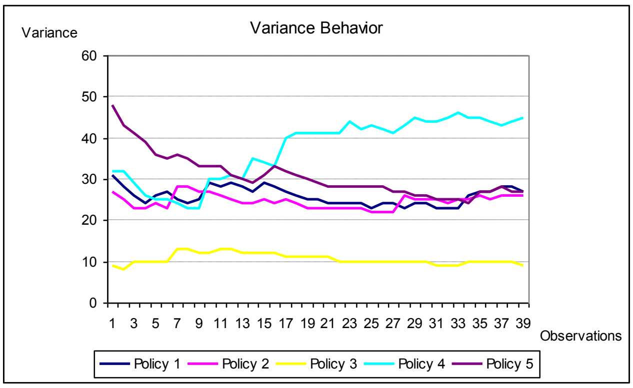

Figure 4. Sample Paths of Variance Behavior

Instead, in policy n°5 the variance estimate has a decreasing trend and, thus, the algorithm is expected to terminate faster. This expectation is justified by the auto-adaptive control of the procedure which can be monitored according to a step-by-step logic. In this sense, Table 3 provides a trace of the variance behavior for policy n°5. As one may observe, after setting $n_0 = 10$, $P^* = 0.90$, $\delta = 5$ and, thus, $h = 3.137$, according to Rinott's procedure the number of runs to consider for system i are

$$N_i = \max\left(n_0, h^2 S_i^2 / \delta^2\right)$$
$$= \max\left(10, 3.137^2 * 120.30/5^2\right) = 48 \qquad (18)$$

So, $N_i - n_0 = 38$ additional runs must be added to guarantee the predefined probability of correct selection $P^* = 0.90$. Alternatively, as shown in Table 3, our procedure after only one supplementary run at step 11, returns

$$N_i = \max\left(11, 3.137^2 * 108.30/5^2\right) = 43 \qquad (19)$$

meaning 32 additional runs (i.e. 43 – 11 previous runs). It, thus, realizes a gain of 6 runs after one single run.

Table 3: Step-by-step Trace of Variance Behavior for Policy n°5

Step	N° of observations for policy i=5		N_i
	Sample mean	**Sample variance**	
10	92.34	120.30	48
11	92.39	108.30	43
12	92.96	102.34	41
13	92.48	96.85	39
14	92.20	90.49	36
…	…	…	…

In numerical terms, given that both procedures choose policy n°3 as best, in the worst case our procedure returns the same results as Rinott's two-stage procedure (Δ =0%), while for decreasing variance behavior our procedure is more efficient by 31,25%, as illustrated in Table 4.

Table 4: Comparison of Observations Required by Rinott's Procedure (RP) and Our R&S procedure

Alternatives	N° of observations		Our Performance (Δ%)
	RP	**Ours**	
policy 1	31	31	0%
policy 2	27	27	0%
policy 3	9	9	0%
policy 4	32	32	0%
Policy 5	48	33	+31.25%

4. CONCLUSIONS

An n-stage indifference-zone based ranking and selection procedure has been proposed to "hopefully" deliver more efficient sampling than classical two-stage algorithms. Its performance has been tested by some numerical experiments. Rather than just using a classical sample mean, it appears that tracking the variance behavior reveals improvement margins when the variance pattern is decreasing. In the future, a further possibility may lie in investigating how to use an estimate of the skewness of the sample mean distribution, given that the normality assumption is approximately verified only after a large number of simulation runs - a condition one should avoid, due to the computational burden it is bound to bear.

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