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AN INTEGRATED FRAME - WORK FOR EXPERIMENTAL INVESTIGATION BY SIMULATION MODELS

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Table of Contents

AN INTEGRATED FRAME-WORK FOR EXPERIMENTAL INVESTIGATION BY SIMULATION MODELS

By

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This paper is addressed mainly to researcher who wishs to conduct simulation experiments on models representing management and economic systems. Our main ambition is to show him how can controled experiments be achieved through discrete event simulation and to make him aware of the important statistical aspects of this technique.

Once a particular model is build and its computer program is prepared, the main task will be to manipulate computer runs in a way to get the desired information about the behavior of the simulated system. In the present research, we develop an integrated, framework for investigating simulation models and analyze the following three main strategic and tactic problems;

i - How each of test runs is to be executed and how to estimate simulation run length?

ii - How to design an experiment in order to explore the underlying mechanism governing the behavior of the simulated system?

iii - How to select an experimental plan in order to find the optimum operating conditions of the simulated system.

1. Introduction

The use of computer simulation technique to conduct artificial experiments on numerical models of complex systems, is an increasingly important tool in many desciplines today. Computer simulation offers many features that make it an attractive experimental method for studying management and economic systems.

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Some examples of such features are, the ability to test and evaluate new systems in advance, the ability to identify and control the source of variation in the experiment, etc. [16,29].

These advantages have encouraged operations researchers and statisticiens to improve its practice through the use of different statistical techniques to design and analyze simulation experiments [16,18,21, 28,29,30,34]. The results of these studies demonstrate the need to consider two problems. First, the special circumstances of simulation that lead to misinterpretation of results and then misunderstanding the simulated systems. Second; the difficulty to achieve the assumptions of the statistical theory, as indepe-ndence and homogeneity of variances. So either we manipulate simulation runs to match these assumptions, or we hope that the selected techniques are not affected by their violation.

The purpose of this paper is to develop an integrated framework for investigating, management systems by simulation technique and to find satisfactory solutions to problems that we might face when experimenting simulation models.

We suppose that simulation experiment is conducted in order to achieve two objectives; i) Investigating the relatiohship of simular response to input

specifications in order to determine the underlying mechanism governing the simulated process; ii) Finding the levels of input specifications at which simular response is optimized.

As any statistical investigations, we begin by selecting a sampling plan which specify, how each of test runs is to be executed, and how to determine simulation run length. The second phase, is to design an experiment that will yield the desired information. Finally, a data analysis technique is to be choosen in order to reach some conclusion about the simulated system.

In section 2, the mathematical base of simulation experiment is presented, the simular response function is defined, and different experimental desigs are formulated. A detailed discussion of the steps needed for investigating simulation models, apears in the remaining sections.

2. The Mathematical Model

In many simulation models the process of interest appears as a stochastic process[1], $\{Y(t), -\infty \leq t \leq \infty\}$. Considering discrete event digital simulations, we assume that during an interval Δt the process shows

(1) We will consider only the stochastic simulation models as most management or economic systems inevitably appear random to some degree in nature.

little, if any, change so that observing $Y(t)$ at periodic interval Δt result in no loss of information. For convenience, let Δt be unity, then

$$(1) \qquad Y_t \equiv Y(t)$$

so that the sequence $\{Y_t;\ t=0,1,2,\ldots,\infty\}$ corresponds to the Process $\{Y(t)\}$ at all integer values of the index t.(1)

In order to study several processes of interest, generated by different environmental conditions or input specifications, we would like to aquire a quantitative characterization of each of them. The mean of the process serves generally as the mathematical discriptor. Let $\{Y_t;\ t\varepsilon n\}$ be a time series of length n observed during the simulation run, the mean of the process "u" can be estimated by:

$$(2) \qquad \bar{Y} = n^{-1} \sum_{t=1}^{n} Y_t$$

where $\bar{Y}$ is called "<u>simular response</u>".

Since the stochastic features are spawned in the simulation model by incorporating the random number seed as an integral part of input specifications, the response $\bar{Y}$ becomes a random variable, because it is a transformation not only of the environmental conditions "$x_1, x_2, \ldots, x_p$",but also of the randomly selected seed "r".

(1) The index may be the time, for example Y_t may define the number of jobs in a production system. It may simply denote order; for example Y_t may represent the waiting time for the t^{th} job to receive service.

This relation is defined as:

$$(3) \quad \bar{Y} = \phi(x_1, x_2, \ldots, x_p; r) = \phi(\vec{x}, r).$$

Then for each permissible specification of environmental conditions $\vec{x}$, the set of all possible responses, (which arise from the selection of different random number seeds), might form a probability density function for simular response $\bar{Y}$.(1)

Consequently, the aim of the experimenter will be to estimate the moments of this distribution. Specifically, expected simular response "u" and variance of simular response var($\bar{Y}$), can help him in explaining the particular nature of the simular density function.

Then, regardless of the experimental objectives, we should define a procedure for estimating the mean and the variance of simular response; i.e to select a sampling plan. Once a method for their estimation is selected, we can proceed to the study of $\bar{Y}$ as a function of the p environmental conditions.

The environmental conditions or experimental factors are categorized as qualitatives and quantitatives.(2) Although the random number seed "r" consists of real numbers, it could not be classified as

(1) A detailed discussion of this point can be found in Mihram [34] pp 261-267.

(2) Examples of qualitative factors are policy specification, or discrete environmental conditions. Quantitative factors are examplified by input parameters that can usually be thought as continious variates.

quantitative factor because $\bar{Y}$ will probably not be continious function of it. The random number seed is then unique among quantitative factors, and relation (3) can be written:

$$(4) \qquad \bar{Y} = \phi(x_1, x_2, \ldots, x_p) + \varepsilon(r)$$

where $\varepsilon(r)$ is a random effect dependent upon the random number seed r. Further, if we assume that $\varepsilon(r)$ is independent of the factors $(x_1, x_2, \ldots, x_p)$ and that $E\{\varepsilon(r)\}=0$, the expected simular response can be defined:

$$(5) \qquad E(\bar{Y}) = \phi(x_1, x_2, \ldots, x_p) = \phi(\vec{x}).$$

It is the nature of the unknown function $\phi(\vec{x})$, termed simular response function, that we try to investigate by simulation experiment.

In practical simulation situations, any attempt to develop the exact form of $\phi(\vec{x})$ could not be justified from economical point of view. In addition, for many experimental purposes, it is unnecessary to consider the form of the true function, a flexiable graduating function, for example a polynomial, will often be satisfactory to express the relationship between $E(\bar{Y})$ and the "p" factors. Further more, many experimental strategies proceed by dividing the whole operability region of factors space, into a number of smaller

regions of immediate interest. Withen these regions of interest, the experimenter may feel it is reasonable to represent the response function by a known functional form, although he may know that such representation would be quite inadequate over the whole operability region.

As a result of the previous discussion, the simular response function may be approximated by

$$(6) \quad E(\bar{Y}) \simeq f(x_1, x_2, \ldots, x_p; \theta_1, \theta_2, \ldots, \theta_\ell) = f(\vec{x}, \vec{\theta})$$

where f is a known functional form indexed by some unknown vector $\vec{\theta}$.

The way by which we investigate the function $f(\vec{x}, \vec{\theta})$, in order to yield information about simulated system, depends on the experimental objectives. Accordingly we destinguish between two types of experiments, exploratory and optimization.

2.1. Exploratory Experiments

If the experimenter wish to study the relative importance of the factors $\vec{x}$ as they affect the expected simular response, he may select one of the following experimental designs.(1)

(1) In most designs, the constraint of experimental budget is considered either by fixing the number of experimental points or by selecting the plan that reduce this number as possible.

i) Screening designs

At the begining of investigation, specially with complicated simulation models, the experimenter may face the problem of so many factors. It may happen that not all the p factors are important but only a few, say p' factors. Therefore we may screen for these factors.

ii) Designs for Estimating Parameters

When experimenter has a prior knowledge about the simulated system due to theoritical backgrund or from previous investigations. He may assume that a particular functional form $f(\vec{x},\vec{\theta})$ is a good approximation to the true response function $\phi(\vec{x})$ in such a way that bias due to inadequacy of $f(\vec{x},\vec{\theta})$ to represent $\phi(\vec{x})$ can be neglected. In such case, his goal will be to select an experimental plan to estimate the unknown parameters $\vec{\theta}$ so that the variances of the estimators are minimized.

iii) Designs for Exploring Response Surface.(1)

When knowledge about simulated system is limited, the object is to approximate, withen a given region of the factors space, the function $\phi(\vec{x})$ by some graduating function $f(\vec{x},\vec{\theta})$ which most closely represent the true simular response function. The criteria of closeness is measured by the variance error caused by sampling

(1) These designs treat only the case of quantitative factors.

variation and bias error resulting from inadequacy of $f(\vec{x},\vec{\theta})$ to exactly represent $\phi(\vec{x})$.

2.2. Optimization Experiments

The purpose of this type of experiments is to find the combination of factor levels at which the simular response function $\phi(\vec{x})$ is optimized. Researchers of management science face frequently this experiment, The maximization of profit or the minimization of cost is a common objective in management studies.
To conclude, any attempt to develop an experimental method for investigating management systems by simulation, necessitate the choice of a sampling plan which defines an efficient procedure for estimating the variance of simular response. The estimated variance measures the accuracy of results and then can be used to determine the appropriate run length. Having accomplished this task, an experimental strategy may be defined for investigating the inter-dependence between the simular response and the experimental factors.

The rest of this paper will be devoted to the detailed discussion of the previous statistical aspects of simulation experiment.

3. The Stochastic Sequence generated by Simulation

At the begining of investigation, the study of the stochastic sequence, $\{Y_t, t=1,2,...\}$, generated by simulation, is important for the understanding of the process under study, and the reduction of the experimental effort needed in the next steps. The following three characteristics may provide the required information.

Stationarity. A sequence is said to be strictly stationary if every series, $\{Y_s, Y_{s+1}, ..., Y_{s+n}\}$, for $s=1,2,...,\infty$; will have the same probability density function. A wide sense stationary sequence, which is less restrective, will have the mean:

$$E(Y_t) = \mu < \infty \qquad (7)$$

and the autocovariance function

$$R_s = E\left[(Y_t-\mu)(Y_{t+s}-\mu)\right] \quad , \quad s=0,1,2,... \qquad (8)$$

The importance that the sequence, generated by simulation, be a stationary one is explained by the fact that its autocovariance function R_s depends only on one variable. Moreover, the spectral density function can be represented as the fourier transformation of the autocorrelation function [16]. These two facts are of immense assistance to facilitating the analysis of the sequence.

The existence of a trend in the generated squence will cause non-stationarity. In case of simulation, we can eliminate such trend, either by using an elimination technique [34], or simply by the clever choice of simular response. If we cannot avoid non-stationarity, replicating simulation runs will be recommended in order to generate uncorrelated observations and then to avoid the problems associated with the estimation of R_s.

Autocovariance Function. This function gives the experimenter an initial guess about the independence between events and then the degree of congestion of the simulated system. Since high congested systems need longer run lengths to liberate results from the imposed initial conditions, the choice of a starting policy(1), and the determination of sample size benefit from knowledge about autocovariance function. This function is also used in estimating the precision of simular response $\bar{Y}$ in case of autocorrelated observations.

Spectral density function. This function represents another measure of dependence between observations in the stochastic sequence. It is defined as:

$$(9) \qquad A_\omega = \pi^{-1} R_0^{-1} \sum_{\tau=-\infty}^{\infty} R_s \cos \omega s; \quad \omega \varepsilon \{0, \pi\}$$

(1) See section 5.1.

The estimate of A_w reveals the prominent periodicities in the generated time series. In simulation experiment the periodic components may apear as a consequence of building in the experiment rules that contribute an element of regularity recurring behavior to the sequence of interest. The existence of periodicity is un desired because it adds unnecessary variation to the sequence and create statistical problem when estimating R_s [16]. The formulas for estimating R_s, A_w can be found in references [16,34]. For their theoritical development see [22,36].

4. Termination rules in simulation

When conducting simulation experiments on models representing real systems, two situations can be faced:

i) Simulation run can be prolonged indifinitely. In that case we can increase sample size either by continuing the run or by replicating it. In either cases a stopping rule is needed to end simulation experiment. This situation is designated "non-terminating systems". Many simulation models behave as non terminating systems, for example, Jobshop, inventory or queueing models.

ii)- Simulation run ends with the occurance of a particular event. In that case the only way to increase sample size is replicating simulation runs. This situation is designated "terminating systems". It can take one of the following forms [30]:

- Phisically terminating system. For example, the simulation of equipment failure where run ends when equipment breaks down.
- Phisically non-terminating systems which behave exactly like terminating systems. For example, a bank that closes down at the end of the day, serves the remaining customers, and starts the next day in the empty state.
- Phisically non-terminating systems but experimenter is interested in transient behavior as a function of the initial conditions. Then as soon as the system reachs the steady state, the simulation run ends.

The classification of simulation model as terminating or non-terminating one will have an important impact on the selection of a sampling procedure (see next section).

5. Sampling Plan

This section addresses two central problems in simulation methodology. The estimation of simulation output accuracy and the determination of computer run length. We begin by explaining the initialization of simulation run and its impacton the obtained results. Then a particular attention will be devoted to variance and sample size estimation.

5.1 Start up Policy:

In the begining of simulation run, the experimenter should specify the initial state of the system entites.(1) If run length is not sufficiently large, the obtained results will be biased by these imposed conditions. The magnitude of this bias depends on the selection of the initial conditions, the length of simulation run, and the degree of autocorrelation between events.

To reduce the effect of this bias, we can delete "d" observations from simulation output and choose the appropriate initial conditions "I". The choice of "I" and "d" defines a start up policy [43,44]. The problem is that the deletion of observations affects not only the bias of simular response but also its variance. The effecton variance is to increase it. Consequently, the trade off between bias reduction and variance increase has to be considered in selecting a start up policy.

In mathematical term, for a generated sequence $\{Y_t, t=1,2,...\}$, the truncated mean is defined as:

$$(10) \qquad \bar{Y}_{n,d} = (n-d)^{-1} \sum_{t=d+1}^{n} Y_t$$

and the problem is to select I and d to minimize:

(1) For example, in queueing simulations, the investigator sets, the number of jobs in system, status of each job, status of each, server, etc.

$$MSE = Var(\bar{Y}_{n,d}/I) + [E(\bar{Y}_{n,d}/I) - \mu]^2$$

where the first term of the objective function is the conditional variance. The second term defines the bias.

In order to find the optimal solution, it is necessary to postulate a mathematical model representing the process $\{Y_t\}$, which is difficult to realise with complicated simulation models. Any how, general hypotheses can be advanced about the nature of this solution:

i) When the bias term $[E(Y_{n,d}/I)-u]$ decreases relative to variance term, as the case of systems with low degree of congestion, a policy of many short runs with small number of deleted observations d is advantageous. The application of Wilson's evaluation procedure [43] to a finite state markovian systems indicated that judicious selection of I appears to be more effective than truncation, and he recommended the steady state mode as the best initial condition.

ii) When the variance term $[Var(\bar{Y}_{n,d}/I)]$ decreases relative to bias term, as the case of more compilcated models where the degree of autocorrelation between observations is high, and then the influence of initial conditions decays very slowly. A policy of fewer runs, with more deleted observations d and longer run lengths is advantageous. In such case, we recommend the

utilisation of the "empty and idle" state[1] as initial condition since it reduces the programming effort. Then we can use one of the proposed heuristic rules [44] to take a decision about the number of observations to be deleted.

5.2 Variance Estimation

Being able to estimate, accurately, the variance of simular response is a major step towards determining the precision of simulation output. It remains to postulate the sampling distribution of $\bar{Y}$ in order to derive a confidence interval for the population mean "μ".

In simulation literature, there are five methods for estimating the variance; independent replications, subrun or batch mean method [12,18], independent cycles [20], autocorrelation method [16], and autoregression analysis [19].

The first three methods manipulate simulation runs to get independent observations. The last two methods use a single simulation run with autocorrelated observations.

Except the case of terminating systems, where we are forced to use independent replications[2],

(1) An empty and idle state "means that in the beginning of simulation the system is empty of temporary entities. For example, we begin with no customers in queueing systems or no Jobs in Production System".

(2) By definition, in terminating systems, simulation run ends with the occurance of a particular event and replication is then the only way to estimate the variance.

(see section 4), there must be some criteria for evaluating these methods. We considered the following criterias as the basis of our choice:-

- The precision of the obtained estimate
- The effect of increasing the complexity of the system on the behavior of the method.
- The simplicity and ease of calculation
- The possibility of incorporating the method in the main simulation program.

First, we selected the methods generating <u>independent observations</u> for the following reasons:

i) The results of the empirical comparison of Hauser [21] showed that the method of subruns take half the time needed for the autocorrelation method.

ii) Fishman and other authors [16,18,12] concluded that autocorrelation method is excessively costly in practice and requires a deep knowledge of time series analysis.

iii) The confidence interval estimation based on the central limit theorem, is more accurate when using independent observations

iv) Independent observations permit the use of the robust statistical techniques of the theory of experimental design.

Second, our choice of the <u>independent subruns</u> as the best alternative is explained by the fact that, with complicated simulated systems, the independent

replications method will be costly, as it requires adjustment for inital conditions and truncation point on each run. On the other hand, subruns method can be easily incorporated in the main simualtion program so that output accuracy can be measured sequentially. Finally, we did not consider independent cycles since its generalization to most simulation situations is discussable.

In subruns method, the generated simulation sequence $\{Y_t, t=1,2,\ldots\}$ is divided into k subruns, each contains "m" observations such that the autocorrelation between subrun means is approximately zero.

Considering the subrun means:-

$$(11) \qquad Y_{j,m} = m^{-1} \sum_{i=1}^{m} Y_{m(j-1)+i} \quad ; \quad j=1,2,\ldots,k$$

and the grand mean:

$$(12) \qquad \bar{Y} = k^{-1} \sum_{j=1}^{k} Y_{j,m}$$

then the variance of $\bar{Y}$ can be estimated by:

$$(13) \qquad \hat{Var}(\bar{Y}) = S^2/k$$

where

$$(14) \qquad S^2 = (k-1)^{-1} \sum_{j=1}^{k} (Y_{j,m} - \bar{Y})^2$$

As m increases, we get more accurate results because the following relation holds with negligible error:

$$\text{Cor}(Y_{j,m}, Y_{j+1,m}) \simeq 0 \qquad (15)$$

on the other hand k must be sufficiently large in order to obtain a more precise estimate of the variance and then an accurate wedth of confidence interval. Since we can simply prolong simulation run in order to achieve the most suitable k, the major problem is to find the smallest m, say m^*, such that (15) holds.

In some simulation experiments a prior information or the use of the estimated autocovariance function (see section 3), can provide an approximate estimate of m^*. Two more explicit proposals are presented by Mechanic and Mckay [33] and Fishman [18]. Mechanic and Mckay developed an iterative algorithm which was tested by Law [32] and the results were encouraging. The main disadvantage of this method is the need for a large sample size. Alternatively, Fishman proposed a method, that relies on the Von Neuman ratio, for testing the hypothesis of independence in a time series. The method has many attractive features such as, simplicity, the possiblity of incorporation in the simulation program, and the ability to deal with small samples.

Once the variance of simular response is estimated, we can calculate an approximated $(1-\alpha)$ confidence interval using results of the central limit theorem-

$$(16) \qquad \bar{Y} \pm t(\alpha)_{k-1} \cdot \left[\mathrm{Var}(\bar{Y})\right]^{\frac{1}{2}}$$

where α is the level of significance; $t(\alpha)_{k-1}$ is the $1-\frac{\alpha}{2}$ point of t distribution with k-1 degrees of freedom; and $\hat{\mathrm{Var}}(\bar{Y})$ is defined by (13)

5.3. Simulation Sample Size

In statistical literature three sampling procedures are proposed, fixed sample size, two stages sampling and sequential sampling.

In simulation experiments, fixed sample means that we select the number of subruns k before experimentation. Two stage sampling could be achieved by begining with an initial number of subruns k_0, then we test during simulation run if we need additional observations or not. With sequential sampling algorithm we estimate successively the variance or confidence interval and terminate simulation run when the desired accuracy is attained.

Each of the previous sampling procedures has its disadvantages when used with simulation. Fixed sampling assumes the knowledge of variance before conducting simulation runs. It is also designed to match exploratary experiments and is more adapted to case of qualitative factors. The efficiency of the two stages

procedure is affected by the choice of k_0. Large k_0 may cause additional unnecessary observations, inversly too small k_0 may lead to inexact variance estimator, (the number of degrees of freedom (k_0-1) will be small). The sequential sampling may result in excessive calculation effort as a consequence of successive variance estimation during simulation run.

So a compromise between the three previous sampling procedures is needed in order to increase the accuracy of simulation experiment and to reduce calculation effort.

We propose the following iterative algorithm that can be incorporated in the simulation program:

1. Use one of the methods estimating fixed sample size to calculate an initial guess of the number of observations, "say k_0"
2. Put $k \leftarrow k_0$; $n \leftarrow mk$, $i \leftarrow 0$
3. Generate n observations by simulation
4. Compute $\left[Y_{j,m};\ j=i+1,i+2,\ldots,i+k\right]$ using (11)
5. compute S^2 using (12) and (14).
6. Calculate $k^* = (t_{k-1}(\alpha)/c)^2 . S^2$
   where c is the desired wedth of confidence interval and is specified by the experimenter.
7. If $k^* \leq k$ end simulation, and appropriate sample size will be "k".

8. Otherwize set $i \leftarrow k$, $n \leftarrow \gamma(k^*-k).m$; $k \leftarrow \gamma k^* + (1-\gamma)k$ where $0 < \gamma \leq a$.

9. Go to 3.

Notice that in step 1, an initial guess of k_0 is estimated using fixed sample size formula [41,45]. This reduces the total number of iterations and avoid the risk of too small or too large initial sample size.(1) Furthermore, in step 8 we generate $\gamma(k^*-k)$ instead of (k^*-k) additional observations. This scaling increases the number of iterations, but more important decreases the probability of collecting unnecessary observations [19]. This algorithm is extensively tested by author and proved to be more efficient than the three previously stated sampling procedures, if appropriate "γ" is selected. (see Khorshid [28] pp 69-80).

6. Experimental Design Problem

At this point of discussion, it is necessary to define the experimental design problem and the basis for comparing different designs in order to facilitate the presentation of the experimental plans in the forthcoming sections.

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(1) In general k_0 is selected to be less than the calculated value since it is just an initial guess which will be augmented to get the approximate sample size.

6.1. Definition of an Experimental Plan

Consider the approximated simular response function. $\bar{Y} \simeq f(\vec{x},\vec{\theta}) + \varepsilon(r)$ where

$\vec{x} = (x_1, x_2, \ldots, x_p)'$ is a vector of p variables, (experimental factors) the setting of which determine a simulation run.

$\vec{\theta} = (\theta_1, \theta_2, \ldots, \theta_\ell)'$ is a vector of unknown parameters

and $\varepsilon(r)$ is a random effect dependent on the random number seed r.

Regardless of the selected function from $f(\vec{x},\vec{\theta})$, the experimenter generates by the simulation program N observations $\{\bar{Y}_1, \bar{Y}_2, \ldots, \bar{Y}_N\}$ corresponding to N different combinations of factor levels $\{\vec{x}_1, \vec{x}_2, \ldots, \vec{x}_N\}$, which are called "the experimental points".

If we grouped the N experimental points in an (Nxp) matrix we obtain the Design Matrix

$$(17) \qquad D = \begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1p} \\ x_{21} & x_{22} & \cdots & x_{2p} \\ \vdots & & & \vdots \\ x_{i1} & x_{i2} & \cdots & x_{ip} \\ \vdots & & & \vdots \\ x_{N1} & x_{N2} & \cdots & x_{Np} \end{bmatrix} = \begin{bmatrix} \vec{x}_1' \\ \vec{x}_2' \\ \vdots \\ \vec{x}_i' \\ \vdots \\ \vec{x}_N' \end{bmatrix}$$

The specification of the elements of D and the form of $f(\vec{x},\vec{\theta})$ determine an experimental plan. Once this task is a chieved, we can estimate the unknown parameters $\vec{\theta}$ using the model,

$$\bar{Y}_i = f(\vec{x}_i,\vec{\theta}) + \varepsilon(r_i) \quad ; \; i=1,2,\ldots,N$$

which can be defined in a matrix notation by

$$\vec{Y} = X\vec{\theta} + \vec{\varepsilon} \tag{18}$$

where

$\vec{Y} = (\bar{Y}_1\ \bar{Y}_2 \ldots \bar{Y}_N)'$ is a vector of N observations (simular responses).

$\vec{\varepsilon} = (\varepsilon(r_1)\ \varepsilon(r_2) \ldots \varepsilon(r_N))'$ is a vector of N random effects.

X is (Nxℓ) matrix which is defined by:

$$X = \{\frac{\partial f(\vec{x}_i,\vec{\theta})}{\partial\theta_j}\}_{\vec{\theta}=\vec{\theta}_0} \quad ; \quad i=1,2,\ldots,N; \; j=1,2,\ldots,\ell$$

Note that in case of non-linearity of parameters the X matrix contains some of the unknown parameters. It is therefore necessary to use an initial guess $\vec{\theta}_0$ in-order to find estimates of $\vec{\theta}$ [4].

6.2. Basis for Comparing Designs:

An experimental design should be judged partly by the precision of the estimated parameters and partly by the magnitude of the possible bias resulting from the inadequecy of $f(\vec{x},\vec{\theta})$ to exactly represent $\phi(\vec{x})$.

The parameters can be estimated using least squares formula:

$$\hat{\vec{\theta}} = (X'X)^{-1} X'\vec{Y} \tag{19}$$

and its variance-covariance matrix is defined by:

$$\mathrm{Var}(\hat{\vec{\theta}}) = (X'X)^{-1} \sigma^2 \tag{20}$$

where $(X'X)^{-1}$ is called the precision matrix and σ^2 is the error variance.

The formulas (19), (20) assume that

$$E(\vec{\varepsilon}) = 0$$

$$E(\vec{\varepsilon}\ \vec{\varepsilon}') = I\sigma^2$$

which means independence and homogeneity of variances. In case of simulation we can manipulate runs to obtain uncorrelated observations (see section 5), but the variances are generally non-homogeneous. Then the error variance-covariance matrix is defined by:

$$E(\vec{\varepsilon}\ \vec{\varepsilon}') = \begin{bmatrix} \sigma_1^2 & & & 0 \\ & \sigma_2^2 & & \\ & & \ddots & \\ 0 & & & \sigma_N^2 \end{bmatrix}$$

dividing $E(\vec{\varepsilon}\ \vec{\varepsilon}')$ by a common denominator, say σ^2, weget.

$$E(\vec{\varepsilon}\ \vec{\varepsilon}') = V\sigma^2$$

where
$$V = \begin{bmatrix} \sigma_1^2/\sigma^2 & & & 0 \\ & \sigma_2^2/\sigma^2 & & \\ & & \ddots & \\ 0 & & & \sigma_N^2/\sigma^2 \end{bmatrix}$$

and the generalized least squares formulas will be:

$$(21) \qquad \hat{\vec{\theta}} = (X'\ V^{-1}\ X)^{-1}\ X'\ V^{-1}\ \vec{Y}$$

$$(22) \qquad Var(\hat{\vec{\theta}}) = (X'\ V^{-1}\ X)^{-1}\ \sigma^2$$

since it is a general practice to replicate simulation run or to devide it into uncorrelated subruns, an estimate of the elements of $E(\vec{\varepsilon}\ \vec{\varepsilon}')$ can be obtained by

$$\hat{\sigma}_i^2 = \hat{Var}(\bar{Y}_i) \qquad ; \quad i=1,2,\ldots,N.$$

Then the precision of the estimated parameters depends on $(X'X)^{-1}$ or $(X'\ V^{-1}\ X)^{-1}$ which in turn depends on the arrangement of the experimental points. These matrices supply therefore an objective basis for comparing designs.

From bias view point suppose that the postulated model is:

$$\vec{Y} = X\vec{\theta} + \vec{\varepsilon}$$

but the true model could be

$$\vec{Y} = X\vec{\theta} + X_1\ \vec{\theta}_1 + \vec{\varepsilon}$$

where X_1 is (Nxs) matrix and $\vec{\theta}_1$ is (sx1) vector represe-nting the parameters which are not considered by the experimenter.

If we used the formula (19) to estimate the parameters $\vec{\theta}$ the expected value of $\hat{\vec{\theta}}$ will be [5,7,8,9]

$$E(\hat{\vec{\theta}}) = \vec{\theta} + A\,\vec{\theta}_1 \tag{23}$$

where the alias matrix A is defined by:

$$A = (X'X)^{-1}\,X'\,X_1 \tag{24}$$

since the bias depends partly on A and then on the arrangement of experimental points, the matrix A can be used to compare designs.(1)

7. Exploratory Experiments

When experimenter specifys how each test run is to be executed and how to determine sample size, he may turn toward the choice of an experimental strategy in order to explore the underlying mechanism governing the simulated process. As we indicated in an earlier section, the statistical theory offers three main types of exploratory experiments:

- Screening designs
- Designs for estimating parameters
- Designs for exploring response surface.

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(1) Note that estimating A requires some guess about the probable form of the true model. For example. In building a first order response surface design, we suppose that postulated model is first order polynomial, while the true model might contains second order terms. The selected plan is the judged by both A and $(X'X)^{-1}$.

7.1 Screening Designs:

If simulation experiment contains so many factors, we may wish to conduct a pilot investigations with the smallest number of runs in order to detect the most important factors. These designs could be helpful to simulation user in two circumstances. When he has no theoritical back ground about the simulated system (as the case of new or hypothetical systems), or when he is interested in a small subset of factors, but he do not know the relative importance of this subset when considering all factors.

In statistical literature many designs are developed. Fractional factorial designs [6], Random designs [40], super saturated designs [3], and group screening designs [37]. The investigator can select the design which fit his particular experimental situation.

The use of fractional factorial designs in screening experiments is reported by Box and Hunter [6]. These designs are simple to construct, easy to compute, (as $(X'X)^{-1}$ is diagonal), and provide minimum variance estimates due to the orthogonality of the design matrix D. Nevertheless, the number of experimental points N, of these designs, is a function of the number of factors p. So; if p is very lage, too many observations will be needed. Also, this type of designs exist only for N multiple of 4.

In random designs, all or some of the elements of the design matrix D is selected randomly. The attractive feature of these designs is that the number of observations N is independent of the number of factors p. So, N may be chosen even smaller than p. Unfortunately, these designs do not provide minimum variance estimates since we cannot guarantee the orthogonality of the columns of the design matrix.(1)

Super saturated designs are developed by booth and Cox [3] they proposed a number of designs, with N smaller than p. What N<p, not all the p columns of the design matrix D can be orthogonals, and then designs do not guarantee minimum variance. Nevertheless, we can increase the precision of the design by minimizing the maximum value of the inner product of columns of the D matrix.

$$(25) \qquad \min_{D} \max_{j' \neq j \in p} \left| \sum_{i=1}^{N} X_{ij} X_{ij'} \right|$$

Booth and Cox used a computerized algorithm to generate these designs for each combination (N,P). They showed also that these designs are more accurate than random designs.

In group screening designs, the p factors are combined into a number of homogeneous groups. Each

(1) Several authors [5,6,8] proved that orthogonality is a sufficient condition for minimum variance in case of linear models.

group is considered as a single factor. The group factors are then examined by a fractional factorial design. The non-significant group factors can be dropped from further investigation and the remaining factors are split into smaller groups, and so on.

To conclude, with very large number of factors or when experimental budget does not permit a number of runs N>p, the super saturated designs are recommended since we can use a computer algorithm to generate designs for any combination (N,p), with small variance. Since Booth and Cox concluded that their algorithm is time consuming, the author proposed a more efficient algorithm that provides approximately the same variances (see [28] pp 100-103). If, on the other hand, we can conduct experiments with N>p fractional factorial designs may be applied since they provide minimum variance estimates, can be augmented for further investigations, and permit the study of confounding structure of effects.

7.2 Designs for Estimating Parameters

As we mentioned in section 2, these designs can be used in simulation studies, either when prior knowledge and previous experimentation permit a satisfactory approximation of response function, or when bias

error is small compared to variance error. This may be a consequence of restricting the factors space to a small region of immediat interest.

Two basic approaches for designing experiments can be used in case of simulation.

i) To use a simple factorial or fractional factorial designs

ii) To selected a design based on a variance criteria, as D-optimal designs.

In Factorial designs the total number of experimental points N is the product of the number of levels of each factor. Then for p factors with S levels each $N=S^p$ points. If we considered, in addition, the run length or number of replications per point, the amount of computer time will be unmanageable.(1) Fractional factorial designs enable simulation user to estimate model parameters with small number of points. The price we pay is the possible bias in estimator. For example, designs of resolution III [6], comprise no more than N=p+1 points, but main effects will be biased by interaction effects. The most attractive features of these designs are simplicity, ease of computation due to orthogonality, and the possibility of augmenting design to match more complicated mathematical models,

(1) For example, if p=7 and S=3, then N=2187. So assuming that each run needs 2 minutes, then total computer time will be 72 hours.

(See Box and Hunter [6]). Unfortunately these designs are efficient only for estimating parameters of linear models, (the variance of the quadratic effect is not minimum [11]). In addition the design is restricted to specific numbers of factors "p" and factor levels "S".

The second approach is the use of an iterative algorithm, based on a variance criteria, for selecting an experimental plan. The msot attractive criteria is the maximization of "det{X'X}" and the developed design is called D-optimal design(1).

The basic elements of the theory of optimal design are developed by Kiefer [24,25] and Kiefer and Wolfowitz [27]. Further contributions and proposed algorithms are presented by Federov [15], Wynn [46], and Atwood [1].

Iterative algorithms are available for generating, absolute optimal designs, optimal designs corresponding to a fixed number of experimental points, and designs for estimating a subset of model parameters.

The author thinks that D-optimal designs can play an important role in simulation exploratory experiments, and it is preferable to fractional factorial

(1) For the advantages of the criteria "Max.det{X'X}", see Box and Draper [4] and Khorshid.M [28] pp 120-121.

designs for the following reasons;

i) The design procedure is not affected by any changes in the postulated model.

ii) There is no restriction on the number of experimental points N, the number of factors p, and factor levels. This is not the case with fractional factorial designs.

iii) The D-optimal algorithms can handle diverse design situations. For example, augmenting a planed experiment or estimating a subset of model parameters.

iv) Sequential design of experiments is easily handled, since resulting design of first stage can be used as an initial solution for the second stage.

v) The D-criteria is easily adjusted if the problem constraints are changed. For example, if independence and common variance conditions are not achieved, we can maximize "$\det\{X' V^{-1} X\}$", where V is the matrix of variances-covariances of errors or its estimate.

vi) When finding absolute optimum design presents difficult computing problem, the evaluation of $\det\{X'X\}$ at specific points in the factors space enable a better, if not the best design. The approach of evaluating only a number of candidate points, facilitates the programming of the search routine, permits the exclusion of undesired points, and finally enables the handling of qualitative factors.

vii) Some fractional factorial designs are generated by D-optimal algorithms, if the model is correctly identified and the experimental region is restricted to the cubic region [4].

The author proposed a number of modifications to the existing algorithms and conducted a detailed comparative study in order to obtain more accurate designs with less computational time,([28] pp 127-144).
Finally, it should be noted that statistical literature offers many other design types, for example, latin squares, Randomized block, etc. But we think that they are less adapted to simulation circumstances.

7.3 Designs for Exploring Response Surface:

If nothing is known in advance about the orientation of the simular respone surface $\phi(\vec{X})$, our objective will be to find the function $f(\vec{x},\vec{\theta})$, in a subregion of immediate interest, that most closely represents the true function. The following requirement have to be considered in constructing a design of this type:

i) The design should lend itself to be fitted into a sequential program of experimentation, so that designs of higher order can be formed with minimum loss of information.

ii) The design should consider not only the variance of estimates but also the inadequacy of the postulated model (bias error).

iii) The design should allow a check to be made on the representational accurcy of the postulated model.

Four authors have contributed to the developement of the basic response suface designs. Box and Wilson [7] proposed the central composite design, Box and Hunter [5] presented the concept of rotability, and Box and Draper [8,9] defined the optimality criteria of a design.

The author conducted a detailed Monte Carlo studies in order to reveal the bias and variance characteristics of the response surface designs and to select the most appropriate subset of them for simulation experiments (see KHORSHID [28] pp 173-186).

These designs are important not only for exploratory purposes, but also for finding an optimal solution using an experimental search procedure.

8. Optimization Experiments

The purpose of these experiments is to find the combination of factor levels at which simular response function $\phi(\vec{X})$ is optimum. In this case, the choice of an experimental strategy depends on the type of factors in the simulation model. When all factors are quantitatives, an optimum seeking routine can be used. But the existence of some qualitative factors,

as policy specifications or operating rules; limit the search procedure to the choice between a number of alternatives.

8.1 The search for an Optimum Combination of factor Levels:

When all factors are quantitatives, the investigator will wish to find in the smallest number of simulation runs, the point $(x_1^o, x_2^o, \ldots, x_p^o)$, within the factors space, at which $\phi(\vec{X})$ is a minimum or a maximum.

Since simular response function is not known in advance and is subjected to random variation, we think that the most reasonable strategy will be to fit a sequential program of investigation consisting of the following steps:-

i) Divide the whole region of interest into a number of small subregions, so that we can explore adequately a small subregion with a moderate number of simulation runs.

ii) Use the results obtained in one subregion to move to a second one in which simular response $\overline{Y}$ is better.

iii) Repeate the previous steps until the attainment of a near stationary region where no improvement in the simular response can be achieved.

iv) In this limited region, conduct a more detailed experiment in order to determine the local nature of the function $\phi(\vec{X})$.

In the following sections we discuss briefly the two main elements of this sequential program, seeking a near stationary region and exploring it.

8.1.1. Seeking a near Stationary Region

When the starting conditions of simulation are fairly remoted from the stationary point, an optimum seeking technique will be needed to move rapidly through the factors space to a near stationary region.

Brooks [10] compared four optimum seeking methods, steepest ascent, univariate, factorial, and random search. He concluded that, when sequential investigation is possible, steepest ascent seems to be superior to the others, except in case of large number of factors, where random search is more effecient.(1) Recently, Smith [42] showed that random search should not necessarily be the search technique selected in practical simulations even in case of so many factors and he recommended the use of the steepest ascent method.

Since the steepest ascent method is explained in detail in Box and Wilson [7] and Davies [13], we just mention, here, some remarks that should be considered when applying the method to simulation experiments.

(1) This is explained by the fact that, in random search algorithm, the number of experimental trials is not a function of the number of factors.

i) Since we use the error variance to test the adequacy of the fitted function and the significance of model parameters, an accurate estimate of the variance of $\bar{Y}$ is needed in order to avoid any wrong conclusion.

ii) As the steepest ascent method is affected by the size of the experimental error [7], we may try to reduce it, by selecting a minimum variance design (see section 7.2), by increasing simulation run length, and if possible, by using a variance reduction technique.

iii) If possible, provision should be made to estimate some of the higher order coefficients that were not included in the postulated model. The study of these coefficients will provide some indication of whether the assumption that these terms can be ignored is a reasonable one or not.

8.1.2 Exploring the near Stationary Region

The experimenter may arrive at a near stationary region either as the result of successive application of steepest ascent method, or because he has already found it at the begining of his investigation. In either cases, only immediate neighbourhood need be explored to determine the local nature of response function $\phi(\vec{X})$, and this may be done without excessively large number of experimental points.

Although many auther have ignored the exploration of near stationary region, and were only satisfied by finding the approximated optimum point,we think that it is an important step in case of simualtion for the following reasons:

First,it should be remembered that because of random error and possible lack of fit between fitted equation and the true response $\phi(\vec{x})$, it must not be implied immediatly that the true surface has a maximum (or minimum) at the selected point. So in practice further exploration and confirmatory runs should be performed arround the stationary point of the fitted surface.

Second, the discovery of factors dependence of a particular type may give us an idea about the cost of departure from the optimum point, if it was impossible to reach it in practice. For example, finding the direction of a stationary ridge means that we can know the different combinations of factor levels that optimize the response $\overline{Y}$. Then the choice between these alternatives can be decided according to the cost of each combination or according to an auxiliary response.

Two exploratory techniques are proposed in the statistical literature, canonical analysis [7,13] and Ridge analysis [14]. The author matched the two

techniques in a single computer program in order to have more robust conclusion. This can be done by using canonical analysis to reveal the factor dependence withen the local stationary region, then using ridge analysis to evaluate the locus of the obsolute maximum or minimum when augmenting the experimental region.

8.2. The choice between experimental alternatives

When simulation model contains qualtitative factors, as managerial polices or operating rules, the search procedure will be reduced to the optimum choice between a number of experimental alternatives. More specifically, it is required to find the combination of factor levels corresponding to the best simular response $\bar{Y}$, such that the probability of correct selection (CS) is a least P^*, given that the difference Δ between the best and the next best simular response is at least Δ^*. This may be stated formally as:

$$(26) \qquad Pr(CS/\Delta \geq \Delta^*) \geq P^*$$

where Δ^* and P^* have to be specified by the experimenter. The previous formulation of the problem permits the use of one of the multiple ranking procedures [2,30,31,35, 38,39]. Most of these methods assume normality, indepe-ndence and common known or unknown variances.

In practical simulation models, the distribution of the response $\overline{Y}$ is not known, variances are not known and tend to differ So either we manipulate simulation runs to meet these assumptions or we hope that the effect of their violation is negligible.
After consulting serveral multiple ranking procedures, the authers choosed three of them that seem to be attractive for simulation circumstances. The selected procedures are, Bechhofer and Blumenthal [2], Paulson [38], and Sasser et al[39]. Bechhofer method is the only one extensivly tested for its sensitivity to assumptions violation, it is quite robust and relatively efficient [31]. Unfortunately, it cannot capitalize on favorable configurations of population means. Paulson's procedure gives us the possibility to eliminate inferior populations, so it might be advantageous when comparing a large number of alternatives.

The authors conducted a comparative study using Monte Carlo sampling and two simulation models (see [28] pp 227-244). The results of this study indicate that paulson method is the most effecient method, specialy when the number of alternatives is large. Bechhofer method seems to be the best procedure from robustess point of view, but unfortunately it require large sample sizes when deeling with a large number of alternatives.

Sasser method, which is a heuristic version of Bechhofer, is less efficient than paulson procedure.

To conclude, the results of this empirical study(1), show that no ideal procedure that consider the particular circumstances of simulation does exist in present time. We recommend the method of Paulson when experimenter is wary about computer time and the number of alternatives is greater than 5, otherwize, Bechhofer procedure seems to be the msot robust one, and it is relatively efficient.

9. The Proposed Experimental Plan

Although no one can provide a general experimental plan for sucess in every case, it is possible to direct simulation user to some choices that most suit his experimental situation. This is achieved by the following steps which are written in an algorithmic form:(2)

1. Conduct initial simultion runs to estimate the characteristics of the generated stochastic sequence $(Y_t, t=1,2,\ldots)$. (section 3).

2. If both degree of autocorrelation "cor (Y_t, Y_{t+1})" and size of simulated system are small go to step 3. otherwize select a start up policy i.e the initial conditions and the number of observations to be deleted and go to 3. (sections 4 and 5.1).

3. If simulated model is terminating one use indepe-ndent replications method to estimate output accuracy and sample size. (sections 5.2,5.3).

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(1) See also Kleijnen. [31].
(2) An indication will be given to the corresponding sections of this paper which discuss each step

Otherwize, use independent subruns to estimate output accuracy and simulation run length (sections 5.2,5.3).

4. If number of factors or control variables is large, conduct a screening experiment in order to detect the most important subset of them (section 7.1). otherwise go to step 5.

5. Select the experimental objectives?
   If an exploratory experiment is to be conducted go to step 6.
   If an optimization " " " " " " " " " 9.

6. Postulate a mathematical model $f(\vec{x},\vec{\theta})$ representing the simular response function $\phi(\vec{x})$ in the selected subregion of the factors space (section 2).

7. If it is desired to estimate parameters or to evaluate relative effect of the experimental factors, generate an experimental design which minimizes the variance "$Var(\hat{\vec{\theta}})$", using a D-optimal algorithm or fractional factorial plan (section 7.2).
   If it is desired to explore simular response $\phi(\vec{x})$ in a subregion of the factors space,select a response surface design as central composite or Box and Behinken designs (section 7.3).

8. Use a multiple regression routine to estimate parameters and to test lack of fit and significance of parameters and go to step 10 (section 6.1).

9. If simular response function $\phi(\vec{x})$ does not contain qualitative factors:
   - Selectan initial point in factors space.
   - Search a stationary region using the steepest ascent method or a direct search method.
   - Explore the stationary region using a response surface design in order to estimate an optimal point (section 8.1).

If simular response function $\phi(\vec{x})$ contains qualitative factors use one of the multiple ranking procedures to select the best experimental alternative. Use Paulsons method if number of factors p>5, otherwize use Bechhofer's procedure (section 8.2).

10. End simulation experiment.

10. Conclusion

In the present paper, we developed a complete theoritical base for experimenting management models by simulation technique. The main effort was devoted to the adaptation of the statistical theory of experimental design to the particular circumstances of simulation studies, and to the development of the set of techniques that increase simulation output accuracy and reduce the cost of experimentation. It is our hope that the present work will direct simulation user toward the appropriate selection of a sampling plan, and the efficient design and analysis of his experiment. This work should be subjected to further modifications and perfection in order to reach a robust and integrated experimental theory for investigating systems by simulation models.

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