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VERIFICATION AND VALIDATION OF SIMULATION MODELS

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Simulation Models

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Verification and validation of simulation models

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Abstract: This paper gives a survey of techniques used for the verification and validation of models, especially simulation models. Moreover, this paper introduces a novel way of applying basic regression analysis to validate a model.

Keywords: simulation, statistics, time series, methodology.

1. Introduction

Once we have programmed a simulation model, we must verify that no programming errors have been made. Next we must ask if the model is a valid representation of reality. Unfortunately, there are no perfect solutions for the problems of verification and validation. Note that these problems occur not only in simulation models.

Sargent (1991) states "the *conceptual model* is the mathematical/logical/verbal representation (mimic) of the problem entity developed for a particular study; and the *computerized model* is the conceptual model implemented on a computer. The conceptual model is developed through an *analysis and modelling phase*, the computerized model is developed through a *computer programming and implementation phase*, and inferences about the problem entity are obtained by conducting computer experiments on the computerized model in the *experimentation phase*."

This paper is based on Kleijnen and Van Groenendaal (1992). It is organized as follows. In Sector 2 we discuss verification, that is, how to discover programming errors? In Section 3 we examine validation: how to investigate whether the model is a good representation of reality? In Section 4, we give conclusions, followed by a substantial list of references.

2. Verification

Once we have programmed the simulation model, we may try to check whether any mistakes have been made, as follows.

(i) We can calculate some results manually, and compare these data with results of the simulation program. Getting all intermediate results from a computer program is called *tracing*. Even if we do not wish to calculate intermediate results by hand, we can still 'eyeball' the program's trace and look for 'bugs'. Simulation software provides tracing facilities and more advanced 'debuggers'; see Pegden, Shannon, and Sadowski (1990, pp. 137-148).

Moreover, we may verify certain *modules* of the simulation program. For example, we may check the pseudorandom number generator, if we had to program it ourselves or if we do not trust the software supplier's expertise (Kleijnen and Van Groenendaal, 1992, discuss pseudorandom numbers in detail). GPSS/H automatically computes chi-square statistics to test the hypothesis that the pseudorandom numbers used are uniformly distributed; see Schriber (1991, p. 317). We may compute the average of a sampled input variable such as service time, and compare that average with its expected value. Random deviations between average and expectation can be used to improve the estimated output, which leads to the variance reduction technique known as control variates. Systematic deviations between the (observed) average and the (theoretical) mean may be tested through the t test. Such systematic deviations occur when the user mixes up the variance and the standard deviation of the normal distribution. The user may further specify the wrong unit of measurement, for example, seconds instead of minutes (so the results are wrong by a factor 60). Instead of testing the mean, we can test the whole distribution through a goodness-of-fit test such as the well-known chi-square test.

(ii) The final output of the simulation program may result only after (say) a hundred thousand customers have been processed and the steady state has been reached. That result can be verified by running a simplified version of the program with a known *analytical solution*, provided we can find such a version. Any textbook on queuing theory presents steady state expectations for several output measures of the M/M/n model. For certain queuing networks we can compute steady state solutions numerically (see Lavenberg, 1983). In the steady state the system is still stochastic (but the probability law that governs the stochastic process no longer depends on the initial state). So we should use mathematical statistics to test that the expected value of (say) $\underline{\overline{x}}$, the simulation program's average output, equals the computed steady state expectation μ :

$$H_o : E(\underline{\overline{x}}) = \mu \quad . \tag{1}$$

Note that we underline random variables. To test this hypothesis we often assume normality, and estimate the variance $\underline{\overline{x}}$. Kleijnen and Van Groenendaal (1992) explain how to estimate this variance. If, for example, we use m subruns to compute the estimated variance $s^2_{\overline{x}}$ of $\overline{x}$, then the test statistic becomes

$$\underline{t}_{m-1} = \frac{\underline{\overline{x}} - \mu}{\underline{s}_{\overline{x}}} = \frac{\underline{\overline{x}} - \mu}{\underline{s}_x / \sqrt{m}} \quad . \tag{2}$$

If the simulation has multiple responses (as is usually the case), then we can apply Bonferroni's inequality to preserve the overall 'experimentwise' error rate. Multivariate techniques are alternatives to the combination of univariate techniques and Bonferroni's inequality; see Balci and Sargent (1984b) and Kleijnen and Van Groenendaal (1992). We shall return to error rates in the discussion of (3).

In Monte Carlo studies on the performance of statistical procedures, we often know the analytic solution, provided distributions are normal or sample sizes are large. For example, Kleijnen and Van Groenendaal (1992) show how to verify parts of a Monte Carlo computer program, applying (2). For some models we know the theoretical output, provided the inputs are deterministic. Examples are the economic models in Kleijnen and Van Groenendaal (1992). In that case we can verify the correctness of the simulation program, at least for one set of inputs.

(iii) To verify the computer program of a dynamic system we may use *animation*. So we present the user a moving picture of the simulated system. The user is well qualified to detect errors in the simulated behavior. These errors may be either programming errors or modeling errors; the latter type will be discussed below.

Kleijnen and Van Groenendaal (1992) present the following exercise. Simulate average waiting time (say) $\bar{\underline{w}}$ of the M/M/1 model, starting the simulation in the empty state. To test the validity of the simulation, test the null-hypothesis $H_o : E(\bar{\underline{w}}) = \mu_w$, where μ_w denotes the analytically computed steady-state mean waiting time. Eight cases result from combining (i) 'long' versus 'short' simulation runs (steady-state versus transient simulation); (ii) 'light' versus 'heavy' traffic (short versus long warm-up period); (iii) a 'few' versus 'many' metareplications (low versus high power of the validation test).

Simulation programs have special problems and opportunities. Software engineers have developed procedures for writing good computer programs and for verifying software in general: modular programming, chief programmer's approach, structured walk-throughs, correctness proofs, and so on; see Baber (1987), DeMillo, McCracken, Martin, and Passafiume (1987), and Whitner and Balci (1989). The book by DeMillo et al. has a comprehensive bibliography.

3 Validation

Once we believe that the simulation model is programmed correctly, we ask: is this a *valid* model? By definition, a valid model gives a 'good' representation of reality. This raises several questions. Some of these questions are quite philosophical; for example, do we really know reality or do we have only flickering images of reality (as Plato stated)? Ignoring these philosophical questions, it is obvious that we must make our knowledge of reality 'operational'; that is, we must explicitly formulate the laws that we think govern the simulated system, and we should measure inputs and outputs of the real system (the system concept implies that we subjectively decide on the boundary of the system and on the attributes we want to quantify). Sometimes it is difficult or impossible to obtain these measurements. For example, in a simulation of the recovery of the US economy after a nuclear attack, it is (fortunately) impossible to get these data. In simulation we often examine several system variants (in order to select a 'good' variant), but usually we have data only on the existing variant or on a few historical variants. In the military, however, it is usual to conduct field tests in order to obtain data on *future* variants. Kleijnen and Alink (1992) present a case study. Shannon (1975, pp. 231-233) briefly discusses field tests, too. Sometimes simulation is meant to predict not relative responses, which correspond to different system variants, but absolute responses. In the latter case, validation is more difficult.

To validate the simulation model, we feed it real-life input data in historical order (assuming that those data are indeed available); this is sometimes called 'trace driven' simulation. We run the simulation program, obtain the simulation output, and compare that output to the real-life output of the existing system. So we do not sample the simulation input (from the - raw or smoothed - histogram of real-life input values); instead we use the historical values in historical order: ($(x_{-T}, x_{-T+1}, \ldots, x_{-1}, x_0)$ where T+1 denotes the size of the historical sample. The further we go back into the past, the more data we get and the more powerful the validation test will be, unless we go so far back that different laws governed the system. For example, in many econometric models we do not use data prior to 1945. The output data of the real system and the simulated system can be plotted such that the horizontal axis denotes time ($t=-T,-T+1,\ldots,-1,0$) and the vertical axis denotes the observed and simulated values respectively. We usually 'eyeball' these timepaths to decide whether the simulation model adequately reflects the phenomena of interest. For example, do the simulation data indicate an economic downturn in a business cycle study; do the simulation data show saturation behavior (such as exploding queulengths) in a queuing study?

Instead of eyeballing the time series, we can use mathematical statistics. The problem with the statistical analysis of simulation output data is that these data form a time series, whereas elementary statistical procedures assume identically and independently distributed (i.i.d.) observations. Kleijnen and Van Groenendaal (1992) show how to derive independent observations, so that elementary statistical theory can be applied. For example, let us denote the *average* waiting time on day i in the simulated and the real system by $\underline{w}_i$ and $\underline{v}_i$ respectively, with i = 1,...,n. Suppose further that we use the historical arrival times to drive the simulation model (Kleijnen and Alink, 1992, discuss a case study in which there are no historical inputs available). Hence we can define the 'paired' differences $\underline{d}_i = \underline{w}_i - \underline{v}_i$. Then the t statistic is

$$\underline{t}_{n-1} = \frac{\bar{\underline{d}} - \delta}{\underline{s}_d / \sqrt{n}} , \tag{3}$$

where $\bar{\underline{d}}$ is the average and $\underline{s}_d$ is the estimated standard deviation of $\underline{d}$ (so $\bar{\underline{d}}$ is the average of the difference between two average waiting times per day). If for $\delta = 0$ the calculated value of $\underline{t}_{n-1}$ is significant, then we reject the model. If $\delta = 0$ gives a non-significant $\underline{t}_{n-1}$ then we conclude that the simulated and the real means are 'practically' the same so the simulation is 'valid enough'. Strictly speaking, the simulation is only a model (not reality), so a large enough sample size n would show that δ is not exactly zero. When testing the validity of a model through statistics like (3), we can make 'type I' and 'type II' errors respectively; we may reject the model while the model is valid, and we may accept the model while the model is not valid, respectively. The type I error may be called the model builder's risk; the type II error is the model user's risk. The power of the statistical test increases as the model specification error δ increases. A significance or 'critical' level α means that the type I error equals α. Obviously the type II or β error increases as α decreases, given a fixed sample size n. To decrease both error probabilities we can increase the sample size n and decrease the variance of the simulated system, var($\underline{w}$), through variance reduction techniques. Balci and Sargent (1984b) give a theoretical tradeoff analysis among these factors (sample size, and so on).

A most stringent validation test requires not only that the means of the model and the historical observations are identical, but also that if a historical observation exceeds its mean then the corresponding model observation (that is the observation that uses the same inputs as the historical observation did) tends to exceed its mean, too. For example, $\underline{v}$ and $\underline{w}$ should not only have the same mean but also be *positively correlated*. To investigate this correlation we can plot w versus v. We can formalize this graphical approach using least squares and we can apply a test, if certain statistical assumptions hold and there are enough observations to make the test powerful enough. Testing the hypothesis of positively correlated $\underline{v}$ and $\underline{w}$ is simple if $\underline{v}$ and $\underline{w}$ are bivariate normally distributed (which is a realistic assumption in the example, because of a central limit theorem). It can be proved that such a bivariate normal distribution implies

$$E(\underline{w} \mid \underline{v} = v) = \beta_o + \beta_1 v. \tag{4}$$

So we can plot w as a function of v, and use ordinary least squares to estimate the intercept and slope of the straight line that passes through the 'cloud' of points (v_i, w_i); the formulas are given in any statistics text. Our stringent test calls the model valid if the following composite hypothesis holds:

$$H_o: \beta_o = 0 \text{ and } \beta_1 = 1, \tag{5}$$

which implies E($\underline{w}$) = E($\underline{v}$) (as tested through equation 3). Moreover it can be found in any statistics text that

$$\beta_1 = \rho \frac{\sigma_W}{\sigma_V}. \tag{6}$$

This equality implies that if $\beta_1 = 1$ and $\rho < 1$ then $\sigma_w > \sigma_v$, that is, if the model is not perfect then its variance exceeds the real variance. (If $\beta_1 = 1$ and $\sigma_w = \sigma_v$ then $\rho = 1$, which is an unrealistic case; if $\beta_1 = 1$ and $\sigma_w < \sigma_v$ then $\rho > 1$, which violates the statistical model.) To test the hypothesis of (5), we compute the Sum of Squared Errors (SSE) with and without that hypothesis (the 'reduced' and the 'full' model respectively), and compare these two values, as follows. Based on the full model (4) we compute

$$\underline{\hat{w}}_i = \underline{\hat{\beta}}_o + \underline{\hat{\beta}}_1 \underline{v}_i \ , \tag{7}$$

which yields

$$\underline{SSE}_{full} = \sum_i^n \ (\underline{w}_i - \underline{\hat{w}}_i)^2. \tag{8}$$

Next we compute the SSE under the composite hypothesis of (5) (obviously a restricted model gives a higher SSE). That hypothesis implies $\hat{w} = v$, so

$$\underline{SSE}_{reduced} = \sum_1^n (\underline{w}_i - \underline{v}_i)^2. \tag{9}$$

It can be proved that the following expression is an F statistic with degrees of freedom 2 (the number of parameters in the hypothesis of equation 5) and n - 2 (the degrees of freedom of the SSE for the full model, where the factor 2 occurs because two parameters are estimated in that model):

$$\underline{F}_{2,n-2} = \frac{(\underline{SSE}_{reduced} - \underline{SSE}_{full})/2}{\underline{SSE}_{full}/(n-2)} . \tag{10}$$

If the computed F statistic is significantly high, we reject the hypothesis in (5) and conclude that the model is not valid. For details on this F test we refer to Kleijnen (1987, pp.156-157).

We may formulate a less stringent validation requirement: the means are not necessarily equal, but the model and the real responses are positively correlated. This requirement makes sense if the model is used to predict relative responses (as in sensitivity analysis), not absolute responses. To test this hypothesis we formulate the null-hypothesis

$$H_o: \beta_1 \leq 0. \tag{11}$$

To test this null-hypothesis we use the well-known t statistic. This means that we reject the null-hypothesis of (11) and accept the model if there is strong evidence that the model and the real-life responses are *positively* correlated.

Note that statistical analyses as in (3) through (11) require many observations. In validation, however, there are often not many observations on the real system.

In a more sophisticated analysis we estimate the autocorrelation structure from the simulated and the historical time series respectively, and compare these two structures. Spectral analysis is the technique developed for the estimation of autocorrelation functions. Unfortunately, that analysis is rather sophisticated and requires long time series.

A simple technique is the *Schruben-Turing* test, which runs as follows. We present a mixture of computer output and real-life output to one or more users, and we challenge them to identify (say) the data that was generated by computer. Of course, they may correctly identify some of the data by mere chance; this, however, we can test statistically. Turing introduced this procedure to validate Artificial Intelligence computer programs: which data is generated by computer, and which is provided by humans? Schruben (1980) applied this concept to the validation of simulation models. He discusses several statistical tests and case studies.

Above we mentioned that going far back into the past may yield historical data that are not representative of the current system; that is, the old system was ruled by different laws. Similarly, a model is adequate only if the values of its input data remain within a certain area. One example is provided by metamodeling: a regression model of *first* order is a good approximation of a simulated M/M/1 system, only if the traffic load is 'low' (see Kleijnen and Van Groenendaal 1992). In practice, there are many input variables, and we should use experimental designs combined with regression analysis (or Analysis of Variance, ANOVA) to detect the important factors. For the important factors we must obtain accurate information on the values that may occur in practice. For example, we applied experimental designs and regression analysis to a model of the greenhouse effect of carbon dioxide (CO_2) and other gases. The computed sensitivity estimates should have the right signs: some factors are known to increase the global temperature. The magnitudes of the sensitivity estimates show which factors are important so accurate information must be collected or - if the factors are controllable - their emissions should be restricted. For details see Bettonvil and Kleijnen (1991), Kleijnen and Alink (1992), and Kleijnen, Rotmans, and Van Ham (1992).

Note that if a factor is qualitative, then we can estimate the effects of the quantitative factors *per* scenario. If these estimates do not vary with the scenario, then there are no interactions between the quantitative and the qualitative factors.

Some authors, for example Banks (1989), claim that a model should remain valid under 'extreme' conditions. We, however, state that a model is valid only within a certain experimental domain. For example, Bettonvil and Kleijnen's (1991) sensitivity analysis shows that the ecological simulation model is valid only if the factors range over a relatively small area. Zeigler (1976, p. 30) emphasizes the concept of *experimental frame*, which he defines as 'a limited set of circumstances under which the real system is to be observed or experimented with'. He observes that 'a model may be valid in one experimental frame but invalid in another'.

Sensitivity analysis should be applied to find out which inputs are really important. Collecting information on those inputs is worth the effort. If nevertheless it is impossible or impractical to collect reliable information on those inputs, *risk analysis* may be applied. A probability distribution of inputs is then derived from the users' expert knowledge, which yields a probability distribution of output values; see Kleijnen and Van Groenendaal (1992). The relationship between sensitivity and risk analyses requires more research; see Kleijnen (1990).

Note that model 'calibration' means that a model's parameters are adjusted such that its output resembles the real system's output. Obviously, those latter data can *not* be used to validate the model (we also refer to cross-validation, discussed in Kleijnen and Van Groenendaal, 1992).

The validation of simulation models is closely related to the validation of other mathematical models, such as models in regression analysis, inventory control, and linear programming. We have already mentioned some typical aspects of simulation models; for example, the time series character of its inputs and outputs (because simulation is dynamic), and the random noise in stochastic simulation and Monte Carlo models. Other models share some of these characteristics with simulation models. For example, an econometric model may also be dynamic and stochastic. Another typical aspect of simulation is that its models are based on common sense or on direct observation of the real-life system; that is, the latter system is not a black box. For example, a simulation model of a queuing system represents intuitive knowledge about the system: a customer arrives, looks for an idle server, and so on. Connecting the modules for system parts gives the total simulation model, which grows in complexity and - hopefully - realism (also think of financial corporate models). Such a bottom-up approach cannot be followed in other models. Note that animation may help to obtain 'face validity'. In some applications, however, the simulation model is given by the theories of a certain discipline (for example, economics), and these models may then be black-box models. The validation of black-box models is more difficult, since we can measure input and output data only. The emphasis in validation is then on prediction, not explanation.

The model's validity is determined by its assumptions. Therefore these assumptions should be stated in the model documentation. (Being explicit about one's assumptions is the difference between a scientist and a politician, we think.) In practice, however, many assumptions are left implicit. The importance of documentation is discussed at length by Fossett, Harrison, Weintrob, and Gass (1991). They define *assessment* as 'a process by which interested parties (who were not involved in a model's origins, development, and implementation) can determine, with some level of confidence, whether or not a model's result can be used in decision making' (Fossett et al., p. 711). Important components of assessment are verification and validation. They further define *credibility* as 'the level of confidence in [a simulation's] results' (Fossett et al., p. 712). They present a framework for assessing the credibility of a simulation; this framework comprises 14 factors (these factors are also discussed in this paper, explicitly or implicitly). They apply this framework to three military weapon simulations (Kleijnen and Alink, 1992 present another military case study). Gass (1984) proposes to produce four manuals, namely for analysts, users, programmers, and managers respectively.

4. Conclusion

Validation and verification of simulation models have been discussed in several textbooks, for example, Banks and Carson (1984), Law and Kelton (1991, pp. 298-324), and Pegden et al. (1990, pp. 133-162). These textbooks give many additional references. We also refer to the production-planning case study in Kleijnen (1988) and the cigarette fabrication case study in Carson (1989). Dekker, Groenendijk, and Sliggers (1990) discuss the verification and validation of models that are used to compute air pollution; these models are needed to issue permits for building new factories and the like. Validation of system dynamics models is discussed in Kleijnen (1980, pp.137) and Wolstenhome (1990, pp. 58-60). Banks (1989) proposes control charts, which are used in quality control. Reckhow (1989) discusses several more statistical techniques. Balci and Sargent (1984a) give a detailed bibliography.

Models resemble information systems. Actually, models are a key element in some types of information systems, namely Decision Support Systems (DSSs). The problems of developing 'good' information systems are notorious; see Davis and Olson (1985).

This paper demonstrates the importance of mathematical statistics in simulation. Nevertheless we believe that the developers and users of a simulation model should be convinced of its validity, not only by statistics but also in many other ways, some of which were presented above. In conclusion, modeling - including simulation - has elements of art as well as science.

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