the reversed conventions and the omissions of rate-to-level influence links, particularly so if s/he has access only to the formal diagrammatic model as is the case in Forrester's *World Dynamics* [7] or *Urban Dynamics* [13].

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Regression Metamodels for Generalizing Simulation Results

JACK P. C. KLEIJNEN

Abstract—**Generalization of simulation results is needed for sensitivity analysis, optimization, "what-if" questions, etc. To meet these needs, several types of metamodels are presented. One type is discussed in detail, namely, linear regression models. These models can represent interactions among input variables of the simulation program and can be validated through statistical tests. Experimental designs can be utilized for efficient and systematic exploration of possible system variants. The approach is compared to Meisel and Collins' piecewise linear models. References to practical applications are included.**

I. INTRODUCTION

Simulation is the technique most applied to practical problems in operations research, systems analysis, and the like. However, a major disadvantage is its ad hoc character. In this correspondence, we present a methodology for generalizing simulation results. Our approach is based on the familiar regression analysis technique. This technique further enables us to measure the (statistical) accuracy of our generalization. The exploration of the great many systems that could be simulated is systematized and made more efficient by means of the experimental design technique.

The regression model serves as a *metamodel*, i.e., as a model of a model. Such an auxiliary model is useful for understanding the intricate simulation model itself. During the construction of the simulation program, we gain much knowledge about the details of the real-life system and its model, but not about the system as a whole. Running the simulation program for a number of situations (different parameters, variables, structural relationships), we hope to arrive at an *understanding* of the system, i.e., its simulation model. Such an interpretation and generalization enables us to meet a number of demands: sensitivity analysis, answering what-if questions, and optimization. Finding the input values which yield a desired fixed output (control) requires extensive trial and error without a metamodel; see [13], [20]–[22]. "Selling" the simulation results to the user may be facilitated if we have a simplified model of the complicated simulation model. A simplified analytical model might be derived after the most important variables in the simulation have been identified; for examples, see [8], [19]. Several authors have emphasized the need for a metamodel in order to meet the above demands; see [2], [3], [5], [16], [18], [21].

Different types of metamodels can be used.

1) *Common Sense Graphical Approach:* Change one variable, say x. Observe the resulting output y. Repeat this procedure a number of times. Plot the (x, y) combinations. Fit a curve by hand, and conclude whether x has an important effect on y. Our approach actually formalizes such hand fitting applying the least squares algorithm. It extends the procedure into multiple dimensions, and it systematizes the various steps.

2) *Explicit Formal Metamodels:* Several models can be found in the literature.

a) Meisel and Collins [16] propose *piecewise linear* approximations, which replace the handfitted curve of approach 1); see [4] for algorithms. They apply least squares for the computation of parameters [16, p. 353]. Applications can be found in [6], [7]. In Section IV, we shall return to their approach.

b) *Linear regression models:* Instead of piecewise linear functions, we use functions that are linear in the parameters. Linear regression analysis has the great advantage of being a familiar technique. Regression models have been extensively applied to interpret and generalize results in agricultural, chemical, and engineering experimentation. Here these models are also known as *analysis of variance* (ANOVA) and include "main effects" and "interactions"; see the next section. Regression metamodels in simulation have been advocated by a few other authors. For instance, in [22] main effects and interactions are estimated and "control" questions answered in a job shop simulation. In [14], a steel plant simulation is analyzed by means of a regression metamodel.

II. REGRESSION METAMODELS

Let x_j denote a factor j influencing the outputs of the *real-world* system ($j = 1, 2, \cdots, m$). A factor may be qualitative or quantitative, continuous or discrete; in [10, p. 300] it is shown how a qualitative factor can be represented by dummy variables. The response of the real-world system is a time series. We shall concentrate on a single-response variable; for multiple outputs, we apply our procedure to each variable separately. In order to compare system configurations, we characterize a time path by one or a few measures such as its average or the slope of a fitted trend. Let y denote a measure characterizing a time path of the real-world system. Hence the response variable y is a function of the factors x:

$$y = f_1(x_1, x_2, \cdots, x_m). \tag{1}$$

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This system is approximated by a simulation model. Here y is a function of k factors x_j ($j = 1, \cdots, k$), plus a vector of random numbers r, or

$$y = f_2(x_1, x_2, \cdots, x_k, r) \tag{2}$$

where k is much smaller than the unknown m and r symbolizes the effect of all factors x in (1) not explicitly represented in (2). Note that the metamodel approach also holds if no sampling is used so that r vanishes. The simulation model is specified by a computer program denoted by f_2. This model may be approximated in turn by a metamodel (within a specific experimental area E; see below). We propose a metamodel that is *linear* in its parameters β, but not necessarily in its independent variables since terms like x^2 can be utilized. A very simple metamodel to express the effects of the k factors would be

$$y_i = \beta_0 + \beta_1 x_{i1} + \cdots + \beta_k x_{ik} + e_i, \qquad i = 1, \cdots, n \tag{3}$$

where in simulation run i (or observation i) factor j has the value x_{ij} ($j = 1, \cdots, k$). These values are assumed to determine y_i linearly except for e_i, the noise which has expectation zero. Such a simple metamodel implies that a *change* in x_j has a constant effect (viz. β_j) on the expected response $\mathscr{E}(y)$. Such a (simplistic) model was used for sensitivity analysis of medical services in [15]. A more general metamodel postulates that the effect of a factor j also depends on the values of the other factors. This can be formalized as in (4) where for illustration purposes we take $k = 3$:

$$y_i = \beta_0 + (\beta_1 x_{i1} + \beta_2 x_{i2} + \beta_3 x_{i3}) + (\beta_{12} x_{i1} x_{12} + \beta_{13} x_{i1} x_{13} + \beta_{23} x_{i2} x_{i3}) + e_i. \tag{4}$$

Here the parameters (coefficients) β_{12}, β_{13}, and β_{23} denote *interactions* between the factors 1 and 2, 1 and 3, and 2 and 3. A graphical illustration of interaction in the case of two factors is shown in Fig. 1. In Fig. 1(a), the curves are parallel, i.e., the effect of x_2 on $\mathscr{E}(y)$ does not depend on the level of x_1. In Fig. 1(b), the interaction is positive (complementary factors) so that the increase in $\mathscr{E}(y)$ is stimulated when the increase of x_2 is accompanied by an increase in x_1. In Fig. 1(c), the marginal output of x_2 is much smaller when more of x_1 is available to be substituted for x_2; see also [9, p. 240]. The need to consider interactions is demonstrated by a practical steel plant simulation [14].

If all factors are quantitative continuous variables, then we add "purely quadratic" effects β_{jj}. This yields

$$y_i = \beta_0 + \sum_{j=1}^{3} \beta_j x_{ij} + \sum_{j}^{2} \sum_{<j'}^{3} \beta_{jj'} x_{ij} x_{ij'} + \sum_{l}^{3} \beta_{jj} x_{ij}^2 + e_i, \tag{5}$$

which represents the Taylor series expansion of (2), cut off after the second-degree terms. In practice, it is rare that all factors are quantitative (yet it is possible [16]). Hence we shall concentrate on the metamodel, with k main effects β_j, $k(k-1)/2$, interactions $\beta_{jj'}$, and the general mean β_0 or

$$y_i = \beta_0 + \sum_{j=1}^{k} \beta_j x_{ij} + \sum_{j}^{k-1} \sum_{<j'}^{k} \beta_{jj'} x_{ij} x_{ij'} + e_i, \qquad i = 1, \cdots, n. \tag{6}$$

We start by postulating a metamodel such as (6), but next we test statistically whether this assumption was realistic! Two statistical tests can be used.

1) Generate some new observations y from the simulation model. Use a t-statistic to compare these observations y to the predicted value $\hat{y}$ based on the regression metamodel estimated from the old observations. The "new" observations may correspond to the "center" of the design ($x_j = 0$), in order to check whether purely quadratic effects are zero.

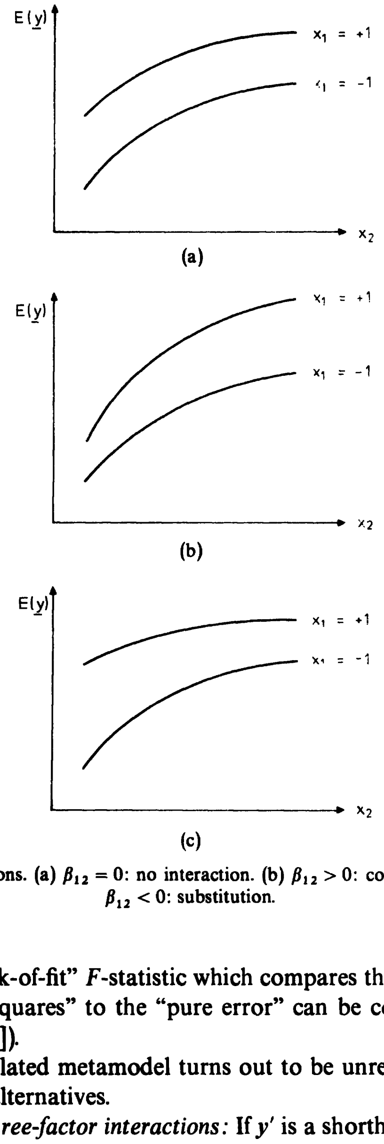

Fig. 1. Interactions. (a) $\beta_{12} = 0$: no interaction. (b) $\beta_{12} > 0$: complementary. (c) $\beta_{12} < 0$: substitution.

2) The "lack-of-fit" F-statistic which compares the "mean residual sum of squares" to the "pure error" can be computed (for details see [13]).

If the postulated metamodel turns out to be unreasonable, we have several alternatives.

a) Add three-factor interactions: If y' is a shorthand notation for y in (4), then this equation may be expanded to

$$y_i = y_i' + \beta_{123} x_{i1} x_{i2} x_{i3}. \tag{7}$$

Three-factor interactions are difficult to interpret intuitively and increase the number of parameters. More parameters means noisy insignificant estimators. Moreover, science's goal is to explain a phenomenon parsimonously.

b) Look for transformations: For instance, if y denotes waiting time and x_1 and x_2 denote mean arrival and service rate, then we suggest the transformation $x' = x_1/x_2$. In [13], we found that the response variable (average storage of containers in a harbor simulation) reacted nonlinearly to the ships' interarrival time x. However, the simple transformation $1/x$ (interarrival rate) resulted in a linear response function. A popular transformation in econometrics is $x' = \log x$ and $y' = \log y$ so that the parameters β represent elasticity coefficients. A more complicated example can be found in [23]. We strongly recommend to look for appropriate transformations from the very beginning of the study. If all else fails, we may proceed to option (3).

c) Reduce the experimental area E: This option limits the generality of our conclusions. However, if the only purpose of the metamodel is to find the optimum x-values, then a small area E can be used, a metamodel fitted, and the direction of better x-values determined. See [17] for details on this so-called response surface methodology (RSM) and [10] for a bibliography.

Note that our specification of the metamodel is based on intuition, prior experimentation, theoretical background, etc. A systematic procedure to derive the structure of the metamodel, based on pattern recognition, is explored in [1].

The parameters β can be estimated and tested for significance, using regression analysis with either ordinary or generalized least squares (see [13]). So statistical tests (F- and t-tests) can be used to determine objectively whether the metamodel is "correct" and which factors are "important;" see the methodological problems raised in [21, p. 79].

III. Experimental Design

Next consider the selection of the values x_{ij} for the independent variables j to be used as input into run i of the simulation program. This selection is the domain of experimental design. Such designs have been developed since the 1920's and have been widely applied to experiments in agriculture, chemistry, etc. In sociotechnical systems, the scientific design of experiments is difficult and expensive (disruption of the organization). However, in a simulation model of such a system, the experimental factors are completely under the scientist's control.

In [13], we studied six factors in a complicated harbor simulation. We started by letting each factor assume only two (extreme) values. Simulating all $2^6 = 64$ factor combinations would take very much computer time. Moreover, we conjectured that, in the metamodel, only 13 effects are important, namely, the six main effects and six particular interactions (plus the overall mean). To estimate these 13 effects we need much less than 64 combinations (system variants). Using experimental design methodology we selected only 16 combinations for actual simulation. In [12], seven factors were examined in an inventory-management system, viz., IBM's package IMPACT. Only 16 combinations (runs) gave us an idea of the main effects and possible interactions of these seven factors. Summarizing, experimental design can handle the exponential growth of factor combinations as the number of factors increases.

IV. Regression Versus Piecewise Linear Metamodels

Let us briefly compare our metamodels to the Meisel and Collins piecewise linear approximations. They claim that polynomial models "extrapolate very poorly" and "often interpolate poorly" [16, p. 354]. We would argue that there should be no need for extrapolation since we select the x-values such that they represent extreme conditions. If nevertheless it would turn out that these "extremes" are not extreme enough, then our models do not become high-degree polynomials like the fifth-order polynomial mentioned in [16, p. 351]. Our metamodels are indeed cruder than piecewise linear models as illustrated in Fig. 2. Nevertheless, they are useful auxiliary models for sensitivity studies and the like, as shown by [12]–[14], [22]. For optimation, our approach may be extended by RSM, mentioned in Section II. The advantages of our cruder metamodel are easy intuitive interpretation (main effects and interactions) and very limited experimentation. Meisel and Collins present case studies involving only two or three variables, but using 42 and 450 factor combinations, respectively!

V. Conclusion

How can we apply a metamodel such as (4)?

1) Select n combinations of the factors x_1, x_2, x_3. This selection fixes x_{ij} $(i = 1, \cdots, n)$ $(j = 1, \cdots, 3)$.

2) Use the original simulation model to compute the output y_i for each combination i.

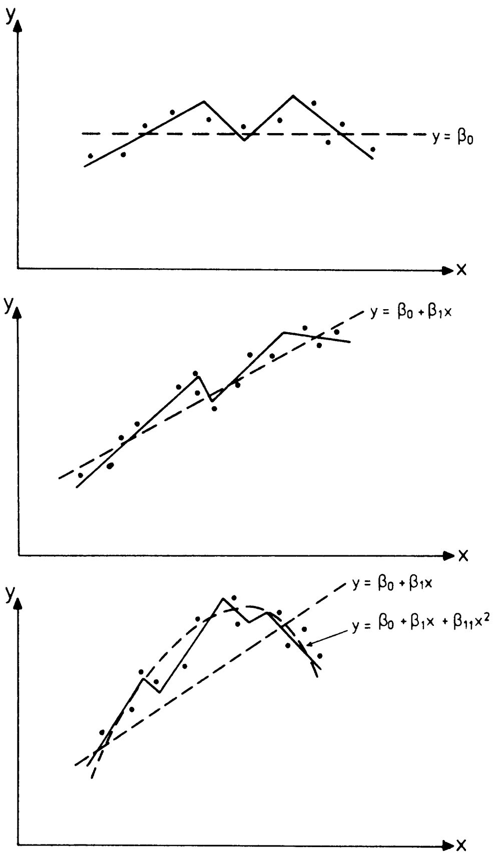

Fig. 2. Piecewise linear versus polynomial metamodels.

3) Use the n observations on the output y (step 2) together with the corresponding values of the input variables x_j (step 1), in order to estimate the effects β_1, β_{12}, etc., in (4). We can use simple regression analysis since (4) is linear in its parameters β.

4) Test whether the postulated metamodel of (4) is indeed an adequate description of the changes in y as the x_j vary! The validity of the metamodel may be tested by predicting y for some *new* combination of the x_j using the metamodel with estimated parameters $\hat{\beta}$ and comparing the prediction $\hat{y}$ to the value y obtained from the original simulation model.

5) If the metamodel does not pass the test of 4), we may try other specifications for the metamodel.

6) If the metamodel is accepted, we may proceed as follows. If the output is sensitive to specific *assumptions*, we may spend more time on the determination of the exact values of these model parameters. If the exact values cannot be determined, we may provide solutions for a variety of parameter values. When trying to optimize (or just improve) the criterion, we can concentrate on the important factors. The signs of their estimated coefficients $\hat{\beta}$ tell us in which direction these factors should be changed. Relative values like $\hat{\beta}_1/\hat{\beta}_2$ show us the relative magnitudes of the changes in the various factors.

The above approach has shown its merits in several practical applications: inventory, harbor, steel plant, job shop simulations [12]–[14], [22].

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A Simple Technique for the Generation of Correlated Random Number Sequences

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Abstract—**A simple technique, based on the theory of optimal linear prediction, is presented for the generation of cross-correlated random number sequences. The method is essentially a computer simulation of the process of linear prediction with the error of prediction playing an important role. The algorithm rearranges a random number sequence with reference to another so as to obtain the desired correlation between the two. With no specifications on the distribution of the random number sequence (linear prediction does not assume knowledge of the probability law of the random variables) the method should therefore be applicable to all continuous distributions. The validity of the algorithm has been justified through the derivations of the expressions for the expectation and variance of the correlation coefficient. Satisfactory results have been obtained for three typical distributions, viz., normal, uniform, and exponential. The assumptions made regarding the behavior of the error of prediction have been verified through computations. The method is expected to find applications in various disciplines.**

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INTRODUCTION

Monte Carlo simulation provides a convenient means for the qualitative investigation of the behavior of a stochastic system. The scope of this method is determined by the extent to which the statistical characteristics of the random number generator resemble those of the system variables. There are many well-known techniques by which it is possible to generate random numbers having the required distribution characteristics [1], [2].

In some cases, the system variables display statistical interdependence. As an example, consider the problem of reliability analysis of a power system. In this case, failure of one of the power transmission links may cause overloading of another, thereby increasing its failure probability. While simulating such a system, it becomes necessary to generate sequences of random numbers having the prescribed mutual cross correlations among them.

It is well-known that a multivariate normal sample can be generated through appropriate linear combinations of independent normal random variables. These techniques are applicable only to the case of the normal distribution. Moreover, they involve problems like computation of the square root of the covariance matrix or the solution of a system of nonlinear algebraic equations [3].

Li and Hammond [4] suggest a procedure for generating correlated random variables with specified nonnormal probability distribution functions. In this procedure, a multivariate nonnormal sample is obtained through appropriate nonlinear transformation of a multivariate normal sample. The method involves operations like "predistortion" of the desired correlation matrix (in order to compensate for the distortion during the nonlinear transformation), evaluation of the square root of the correlation matrix (for the generation of multivariate normal sample), and transformation from normal to the desired distribution. Although standard procedures are available for all these operations, the overall procedure is quite tedious. If the inverse of the desired distribution is not known in closed form, the transformation is performed by numerical methods. In such a case, the method is prone to quantization errors at two stages. (Evaluation of the error function is equivalent to transformation from normal (Gaussian) to a uniform distribution). Moreover, this method fails if the required correlation matrix does not yield a positive semidefinite predistorted correlation matrix. We propose a simple alternative approach to the same problem.

The problem to be considered in this correspondence is that of the generation of two random number sequences $[X_N]$ and $[Y_N]$ of sample size N, to represent the two jointly distributed (not necessarily normal) random variables X and Y, respectively. The marginal distributions of X and Y are assumed to be known. The marginal distributions of $[X_N]$ and $[Y_N]$, when averaged over the entire sample size, are so adjusted as to match those of X and Y, respectively. (The elements of $[Y_N]$, in general, do not have the