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A MODEL FOR FREQUENCY DOMAIN EXPERIMENTS

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ABSTRACT

We present a meta-model which is useful for understanding simulation frequency domain experiments. This model consists of polynomial gain followed by a linear filter with additive noise. The assumptions for performing frequency domain experiments are thus made explicit. We demonstrate how the model leads to a straightforward mechanism for factor screening via statistical hypothesis testing.

1. INTRODUCTION

One topic which has interested many simulation researchers has been the construction of a mathematical model which exhibits the same behavior as a simulation. Since the simulation is itself a model, the result is known as a *simulation meta-model* (Kleijnan, Van den Burg, and Van der Ham [1979], Kleijnan [1980]). One of the difficulties in meta-modelling is the identification of terms belonging in the model. If important terms are excluded from a prospective model, then the model will suffer from a lack of fit. If too many unimportant terms are included in the prospective model, the data requirements will be unnecessarily large.

Traditional experiments have used a run of the simulation as the basic experimental unit, with each factor set at a specified value for the duration of the run. Different runs are made with different configurations of parameter values, and the response of interest is studied as a function of the location in the parameter space.

Recent work by Cogliano [1981], Schruben and Cogliano [1987], Sanchez [1987], and Schruben, Heath, and Buss [1987] has addressed the problem from a different perspective. Factors are oscillated sinusoidally within the course of a simulation run, with each factor being varied at a unique frequency. By carefully selecting the frequencies assigned to the factors, it is possible to construct an experiment in which both direct factor effects and interaction effects between factors can be identified. The advantage to this approach is that the experimental unit becomes a frequency band rather than a run of the simulation program. A simulation run produces a time series, which can be evaluated using spectral analysis. The resulting spectral estimators consist of many virtually independent frequency bands. Thus, many independent experimental units are obtained from a single run of the simulation using the spectral technique.

The spectral approach to factor identification has been empirically succesful in producing results which are comparable to those obtained via run-oriented response surface techniques (Schruben and Cogliano [1987], Sanchez [1987]). In this paper, we wish to formalize a model of the system in terms of its input/output behavior. The proposed model lends itself to evaluation in the frequency domain in a quite direct fashion, but also illustrates the strong ties between the spectral approach and more traditional response surface methods. In this model, time will be a discrete index set since our application is the study of discrete event simulations.

Spectral estimators can be obtained using least squares estimation for a basis consisting of sine and cosine functions evaluated at certain frequencies. Thus, meta-models obtained via the spectral technique are implicitly linear models, although we remark that as in the technique of linear regression, the adjective linear refers to linear in the coefficients being estimated. Over a sufficiently small range a linear model can provide a good approximation to a non-linear response surface if appropriate terms are included in the model. However, we should be concerned about potential lack of fit. In the spectral model, lack of fit may be indicated by the presence of significant effects at frequencies which do not correspond to any of the potential explanatory terms considered *a priori*.

2. THE MODEL

We will initially consider a linear model of a deterministic system which is a function of a single variable. We assume that the system is causal and time-invariant, i.e., that current system behavior does not depend on future inputs and that the function which defines the mapping of an input sequence to an output sequence does not change over time. If these assumptions are true, then the system can be modelled as

$$y(t) = \sum_{\tau=0}^{\infty} h(\tau)x(t-\tau), \qquad (1)$$

where the $x(t)$ is the input to the system at time t, and $h(\tau)$ is the impulse response function which describes the effect on the output τ time units after a unit change is made to the input.

Of course we wish to consider systems which are non-deterministic, and which may depend upon more than one term. We can generalize equation (1) to obtain an additive linear model of such a system. We first introduce multi-index notation. For a vector $\mathbf{x} = (x_1, \ldots, x_n)$, a multi-index $\alpha = (\alpha_1, \ldots, \alpha_n)$ is a vector of positive integers which operate componentwise on $\mathbf{x}$ as follows:

$$\mathbf{x}^\alpha = x_1^{\alpha_1} x_2^{\alpha_2} \ldots x_n^{\alpha_n}. \tag{2}$$

The modulus of α is the sum of its components: $|\alpha| = \alpha_1 + \ldots + \alpha_n$. To illustrate, let n=2; then for $\mathbf{x} = (x_1, x_2)$, $\mathbf{x}^{(1,0)} = x_1$ and $\mathbf{x}^{(1,2)} = x_1 x_2^2$. The modulus of $(1,3)$, say, is $|(1,3)| = 1+3 = 4$. Our model is now defined as

$$y(t) = \sum_{|\alpha| \le k} \sum_{\tau=0}^{\infty} \mathbf{x}^\alpha (t-\tau) h_\alpha(\tau) + \varepsilon(t) \tag{3}$$

where $\epsilon(t)$ is a random process, the $\mathbf{x}^\alpha$'s are potential explanatory terms, and the h_α's are impulse response functions for each respective term. This model is a generalization of a so-called Hammerstein model (Narendra and Gallman [1966]) and represents the result of passing a (multivariate) input through a memoryless polynomial followed by a (multivariate) linear filter with additive noise. Thus, both memory and nonlinearity in the system are modelled by equation (3), which are two saliant features about large scale simulations that make their analysis difficult. Equation (3) can equivalently be written as

$$y(t) = \sum_{\tau=0}^{\infty} \{h_1(\tau) z_1(t-\tau) + \ldots + h_\kappa(\tau) z_\kappa(t-\tau)\} + \varepsilon(t), \tag{4}$$

where $\kappa = \text{Cardinality}(\{|\alpha| \le k\})$, and each z_i, $i = 1, \ldots, \kappa$, corresponds to $\mathbf{x}^\alpha$ for some α.

3. THE TEST

We formulate as the null hypothesis, H_0, that term i has no effect on the outcome of the system, i.e, that $h_i(\tau) = 0$ for all τ, for $i = 1, \ldots, \kappa$. It is not evident how such a hypothesis could be tested in the time domain, but in the frequency domain we shall see that the hypothesis can be tested in a rather straightforward manner.

We now consider the frequency response:

$$Y(\omega) = H_1(\omega) Z_1(\omega) + \ldots + H_n(\omega) Z_n(\omega) + \mathcal{E}(\omega), \tag{5}$$

where $Y(\omega)$, $Z_i(\omega)$, and $\mathcal{E}(\omega)$ are the power spectra of y, h_i, z_i, and ε, respectively. (To simplify notation, frequencies ω are in radians throughout this paper.) Recall that the power spectrum is the Fourier transform of the auto-covariance function. In the case of deterministic functions, such as z_i and h_i, the auto-covariance function is defined in terms of time averages (Ljung [1987]).

Under $H_0 : h_i(\tau) = 0$ for $i = 1, \ldots, \kappa$,

$$H_i(\omega) = \sum_{\tau=-\infty}^{+\infty} 0 e^{\imath\omega\tau} = 0,$$

and hence

$$Y(\omega) = \mathcal{E}(\omega). \tag{6}$$

Recall also that the periodogram $I(\omega)$ is an (inconsistent) estimator for the spectrum $f(\omega)$, which is equal to a constant times $Y^2(\omega)$. If the ε_t's have a normal distribution, then $I(\omega)$ will be proportional to a χ^2 random variable. A consistent estimator $\hat{f}(\omega)$ can be obtained using window estimation techniques, and is also proportional to a χ^2 random variable (Priestley [1981]).

The normality assumption for the ε_t's is not required if the ε_t's can be obtained by passing iid random variables through a linear filter:

$$\varepsilon_t = \sum_{\tau=0}^{\infty} \zeta_{t-\tau} g_\tau \tag{7}$$

where the filter g_τ is such that

$$\sum_{\tau=0}^{\infty} g_\tau^2 < \infty. \tag{8}$$

Under these assumptions, the smoothed periodogram estimator $\hat{f}_N(\omega)$ is asymptotically proportional to a χ^2 random variable (Priestley [1981], pp. 466-467).

We can test the hypothesis H_0 under quite general circumstances in the following way. First, a run of the experiment is conducted in which the factors are all held at nominal values. This is designated as the *noise run*. Since all factors are being held constant, their Fourier transforms will all be zero for $\omega \neq 0$, i.e., $Z_i(\omega) = 0$ for $i = 1, \ldots, \kappa$. It follows immediately from equation (5) that the Fourier transform of the noise run, $Y_N(\omega)$, is given by the relationship

$$Y_N(\omega) = \mathcal{E}(\omega) \qquad \forall \omega \neq 0. \tag{9}$$

Next, a run of the experiment is made in which the factors are varied according to an appropriate frequency selection scheme. Since the $x_i(t)$'s are being oscillated, there will be some set of $\omega > 0$ such that $Z_i(\omega) \neq 0$. However, under H_0, all of the corresponding transfer functions $H_i(\omega)$ will be equal to zero, with the result that the Fourier transform of the signal run, $Y_S(\omega)$, is given by

$$Y_S(\omega) = \mathcal{E}(\omega) \qquad \forall \omega. \tag{10}$$

Thus, under the null hypothesis, both $\hat{f}_N(\omega)$ and $\hat{f}_S(\omega)$ will be proportional to χ^2 random variables. Also, if H_0 is true, they will have the same spectrum for $\omega \neq 0$, and hence

$$\frac{\hat{f}_S(\omega)}{\hat{f}_N(\omega)} = \frac{\hat{f}_S(\omega)/f(\omega)}{\hat{f}_N(\omega)/f(\omega)} \sim \frac{\chi^2_{\nu_S}/\nu_S}{\chi^2_{\nu_N}/\nu_N} \sim F_{\nu_S,\nu_N} \tag{11}$$

for $\omega \neq 0$, where ν_N is the appropriate degrees of freedom for the spectral estimator of the noise run, and ν_S is the appropriate degrees of freedom for the spectral estimator of the signal run. In other words, we can test H_0 by comparing the spectral ratios of the signal and noise runs to an F value with ν_S and ν_N degrees of freedom.

Actually, H_0 is both stricter and less informative than necessary. Rather than require that all κ transfer functions must be simultaneously zero, we can construct the experiment so that no two distinct terms have non-zero Fourier transform at the same frequency, i.e., $Z_i(\omega')Z_j(\omega') = 0$ for all $i \neq j$, and for all ω'. Thus the Fourier transform of each explanatory term will occur in a set of frequency bands which does not overlap with the frequency bands utilized by any other term. This is done by varying each factor at a carefully chosen frequency.

In principle each prospective term in equation (4) may be present. The driving frequencies for factors x_i, $i = 1, \ldots, n$ should be chosen so that output frequencies corresponding to distinct terms z_j, $j = 1, \ldots, \kappa$, are not equal. For a given order polynomial this can always be done (Jacobson, Schruben, and Buss [1986]; Schruben and Cogliano [1987]). The elements of the set of output frequencies corresponding to a particular term are called the term indicator frequencies. It is desirable to maximize the bandwidth (i.e. the minimum distance between two distinct term indicator frequencies) so that spectral estimates at adjacent frequencies are as independent as possible.

The term indicator frequency corresponding to a linear term is the driving frequency for that term. Term indicator frequencies for quadratic terms are the sum and difference of the respective driving frequencies. This can be seen by observing that for $x_i(t) = A_i \cos(\omega_i t)$, $i = 1, 2$, the product can be written

$$x_1(t)x_2(t) = \frac{1}{2}A_1A_2\left[\cos((\omega_1+\omega_2)t) + \cos((\omega_1-\omega_2)t)\right]. \tag{12}$$

Thus, there will be δ-functions in the frequency response at $\omega_1 + \omega_2$ and $\omega_1 - \omega_2$. (Recall that a well defined spectral estimator still exists because it is the change in the distribution function over a range which is estimated.)

This provides a mechanism for testing a hypothesis about each term, independently of what is going on with any other terms in our model. For example, consider a model with two factors, x_1 and x_2, which are assigned driving frequencies of ω_1 and ω_2, respectively. We might then construct the model to contain three terms: $z_1 = x_1$, $z_2 = x_2$, and $z_3 = x_1x_2$. The indicator frequencies corresponding to those terms would be $\{\omega_1\}$, $\{\omega_2\}$, and $\{\omega_1 + \omega_2, \omega_1 - \omega_2\}$. Our goal is to choose values for ω_1 and ω_2 so that the sets are non-overlapping and preferably have maximal distance between the elements. (For the situation described by equation (12), the desired spacing is over the interval $(0, \pi)$. If the problem was specified in terms of cycles/observation, the desired spacing would be over the range $(0, 0.5)$.)

Now consider the null hypothesis for term z_1. In the frequency domain, the Fourier transforms Z_i, $i = 2, 3$, of all other terms in the model would be zero at frequency ω_1 *by construction.* As a result, the Fourier transform of the output of the signal run at frequency ω_1 would be a function of only term z_1 and the randomness,

$$Y_S(\omega_1) = H_1(\omega_1)Z_1(\omega_1) + \mathcal{E}(\omega_1). \tag{13}$$

If the hypothesis that there is no factor effect for z_1 is true, then $H_1(\omega) = 0$ for all ω, including ω_1, and the result is that the ratio of the signal and noise spectra has an F distribution, just as in equation (11).

4. DISCUSSION

Some remarks about the procedure described here are in order. First, no assumptions were made about the independence of the y's. In fact, under the model described by equations (1), (3), and (4) the y's may be highly serially correlated. We do require a stationarity assumption, however.

Next note that the model certainly allows for the presence of time lags, but that any time lags which may occur in the model do not affect our analysis since the Fourier spectrum is lag invariant. In fact, the model specified in equations (3) and (4) is the sort of model which we would construct for a traditional response surface model if we knew the duration of time lags in the system. Time lags must be taken into account in that we must observe the output for a sufficiently long time to observe the results of our changes to the inputs. Given that we observe the system for a sufficiently long time, however, spectral analysis does not rely on prior knowledge of lag durations.

Finally, the technique will work under quite general circumstances. Priestley [1981, p. 466] states, "In fact, these asymptotic [χ^2] distributions still hold for any *fixed* number of frequencies if the residuals $\{\varepsilon_t\}$ are independent but not necessarily Gaussian...". Thus, to analyze the model in equations (3) and (4) we need to assume a sufficiently large sample and independent error terms.

The result is a technique which can be used to identify a set of factors which are significant determinants of the system outcome. The technique works in the presence of serial correlation and constant lags of unknown duration, under quite general assumptions. This gives us the capability to screen the set of potential explanatory factors and select a subset which

affects the outcome with some pre-determined statistical level of significance. The subset to be selected is not of fixed size, and the data need not meet the classical assumptions of being independent, identically distributed normal random variables with no delay between an input and its effect upon the system.

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