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Global Nonlinear Sensitivity Analysis Using Walsh Functions

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A new global nonlinear sensitivity analysis method is developed to investigate the sensitivity of solutions of mathematical models to large uncertainties in the parameters of the model. The method is exact for discrete models where the parameter variation is intrinsically two valued, and exact for continuous models where a two valued parameter variation is sufficient. The analysis involves statistical characterizations of sensitivity similar of those of a previous Fourier expansion method, FAST (R. I. Cukier, C. M. Fortuin, K. E. Shuler, A. G. Petschek, and J. H. Schaibly, *J. Chem. Phys.* **59** (1973), 3873. J. H. Schaibly and K. E. Shuler, *J. Chem. Phys.* **59** (1973), 3879; R. I. Cukier, J. H. Schaibly, and K. E. Shuler, *J. Chem. Phys.* **63** (1975), 1140). Due to the two valued parameter variation, an analysis based on Walsh function expansions is found to be appropriate here.

I. INTRODUCTION

Many complex physical phenomena are modeled by mathematical structures that depend on parameter values for the numerical values of the output functions (the solutions of the model). If these parameters are not known accurately, it is important to assess the effect of the parameter uncertainty on the output function values. This is the objective of Sensitivity Analysis.

If the model depends on a small number of parameters, then solving the model repeatedly for different values of the parameters will give the desired information. However, for many parameter models this procedure rapidly becomes unwieldy. Also, it is often the case that the sensitivity to large parameter variations is required, where a linear sensitivity aalysis would not be appropriate. We have developed [1] a Sensitivity Analysis method, FAST (Fourier Amplitude Sensitivity Test), designed to

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address the many parameter, large parameter variation problem. FAST has been applied to a variety of physical–chemical [1–4] models.

In this paper, we present a new method of Sensitivity Analysis which we will refer to as WASP (Walsh Amplitude Sensitivity Procedure). Both FAST and WASP are examples of global nonlinear sensitivity analyses, in contrast to conventional methods, which are variants of linear analysis [5]. In a linear analysis, the measure of the sensitivity of a given output function, f, which depends on a set of p parameters, $u_1, u_2, \ldots, u_p \equiv \mathbf{u}$, to the uncertainty in the αth parameter is taken to be proportional to $\partial f(u_1 \cdots u_p)/\partial u_\alpha \mid \mathbf{u} = \mathbf{u}^0$. The analysis is linear in that it represents a truncation of the Taylor expansion of the output in terms of the parameters at its linear term. Furthermore, we refer to it as local in that all the other parameters are set to their nominal value $u_\beta = u_\beta^0$ for $\beta \neq \alpha$, $\beta = 1, 2, \ldots, p$. By definition, the linear local analysis breaks down as the higher order terms in the Taylor expansion of the output function become important relative to the linear term. What is then required is a method that permits large parameter variations and does so in a way that, when the sensitivity of the output to the αth parameter is being investigated, all the other parameters are allowed to vary. This latter feature will reveal the effects on the output that arise from simultaneous excursions of a set of the parameters from their nominal values.

FAST is a global, nonlinear Sensitivity Analysis. In FAST, each parameter is described by a probability distribution chosen to characterize one's knowledge about the parameter. Averages of functions of the output function over the joint parameter space distribution are defined and statistical characterizations of the sensitivity of the output to uncertainties in each parameter are constructed. We relate the probability distribution function of each parameter to a frequency and a search parameter s which, as s varies, carries all the parameters through their ranges of variation. The output, as a function of s, is periodic and therefore can be Fourier analyzed. The Fourier coefficients of the output function are then related to the statistical characterizations of the sensitivity. An example of such a statistical sensitivity coefficient is a reduced partial variance S_α, which gives the effect on the output function of the uncertainty in the αth parameter, averaged over the joint probability distribution function of all the remaining parameters. The S_α, $\alpha = 1, 2, \ldots, p$, can be ordered to compare the importance of the p parameters on a given output function. We refer the reader to the review article [2] for a detailed account of FAST and the aims and objectives of Sensitivity Analysis.

Often, it will suffice to carry out a simple, but still global and nonlinear Sensitivity Analysis. What is desired is a parameter probability distribution which just consists of two possible values, a minimum and a maximum value. In addition, there are discrete models where this bivariate parameter variation is natural. While one can construct a FAST method with a parameter probability distribution function which approaches, as a limit, a bivariate, equally weighted distribution, it is more advantageous to reformulate the entire analysis to reflect this discrete bivariate problem. The natural orthogonal functions here are not the Fourier, but the Walsh functions [6]. Walsh functions are orthogonal step functions which form a complete set. (An example of a set of them appears in Fig. 1.) Their two-valuedness make them an ideal choice for this problem.

The Walsh sensitivity analysis that we construct here is modeled along the lines of FAST in that the same statistical characterizations of the sensitivity are used. The result is still a global, nonlinear analysis. It has certain advantages with regard to FAST. For discrete models, where the parameter distribution is actually just two valued it is exact. That is, the expressions we obtain for the statistical sensitivity measures are exact. For continuous models, if one is willing to choose just a two valued parameter variation, then the sensitivity measures are still exact. By contrast, FAST is an approximate method, and while the approximations are controllable and have been carefully investigated [1, 2], FAST does require more "skill" for its proper use.

The remainder of this paper is organized as follows. In Section II the Walsh functions are introduced and their properties catalogued. While these results are available in the literature [6], it is convenient to collect them here. Furthermore, the manipulations of the Walsh functions that we use are required for the Sensitivity Analysis. In Section III we derive the WASP method by following a procedure similar to that used in the derivation of FAST. An example of the use of WASP, along with a comparison of it to linear analysis and to FAST is presented in Section IV. The merits of WASP and its future use are discussed in Section V.

II. HADAMARD ORDERED WALSH FUNCTIONS

A Walsh function is defined in terms of two arguments, a timelike variable [7] and a sequency variable, the latter analogous to frequency in Fourier analysis. The Walsh functions form a complete orthogonal set of step functions. For our Sensitivity Analysis, it is convenient to use the Hadamard ordered Walsh functions defined by

$$\mathrm{walh}(w, t) = (-1)^{\sum_{i=1}^{q} w_i t_i},$$

$$0 \leqslant t < 1; \qquad w = 0, 1, \ldots, M-1; \qquad M = 2^q; \qquad q = 1, 2, \ldots. \tag{2.1}$$

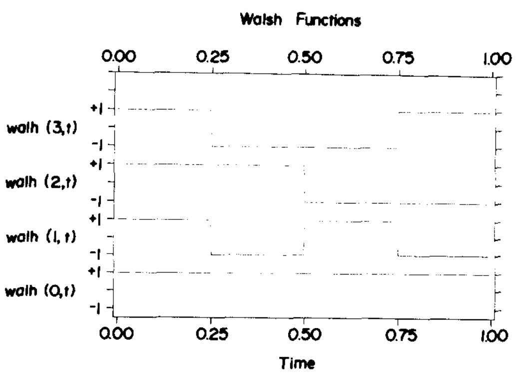

FIG. 1. The four Hadamard ordered Walsh functions for $q = 2$.

Here, the sequency variable w is represented in binary as $(w_1, w_2, ..., w_q)$ and the timelike variable t as $(t_1, t_2, ..., t_q)$. The sequency is an integer less than 2^q so it can be represented by a q digit binary number with the binary point to the right of w_q. The timelike variable is continuous on $[0, 1)$ but Eq. (2.1) only defines walh(w, t) for $t = j/M, j = 0, 1, ..., M-1$ [8]. For each value of q, a different set Q of $M = 2^q$ Walsh functions is generated by Eq. (2.1). This set, for $q = 2$, is displayed in Fig. 1.

We now list properties [6] of these sets which we will use in the Sensitivity Analysis.

1. *Multiplication.*

$$\operatorname{walh}(n, t)\operatorname{walh}(m, t) = \operatorname{walh}(n \oplus m, t) n, m \in Q, \tag{2.2}$$

where $n \oplus m$ refers to binary addition without carry, i.e., $0 \oplus 0 = 1 \oplus 1 = 0$, $1 \oplus 0 = 0 \oplus 1 = 1$. Thus,

$$\begin{aligned}\operatorname{walh}(n, t)\operatorname{walh}(m, t) &= (-1)^{\sum_{i=1}^q n_i t_i}(-1)^{\sum_{i=1}^q m_i t_i} = (-1)^{\sum_{i=1}^q (n_i + m_i) t_i} \\ &= (-1)^{\sum_{i=1}^q (n_i \oplus m_i) t_i} = \operatorname{walh}(n \oplus m, t).\end{aligned} \tag{2.3}$$

2. *Group property* [6]. If $n, m \in Q$, then $n \oplus m \in Q$.

A multiplication table for the $q = 2$ set is given in Table I. (It is instructive to compare Fig. 1 with Table I.)

TABLE I

Multiplication Table for the $q = 2$ Walsh Functions

	walh(0, t)	walh(1, t)	walh(2, t)	walh(3, t)
walh(0, t)	walh(0, t)	walh(1, t)	walh(2, t)	walh(3, t)
walh(1, t)	walh(1, t)	walh(0, t)	walh(3, t)	walh(2, t)
walh(2, t)	walh(2, t)	walh(3, t)	walh(0, t)	walh(1, t)
walh(3, t)	walh(3, t)	walh(2, t)	wahl(1, t)	walh(0, t)

3. *Scalar product.* A scalar product for functions in Q is defined as

$$\begin{aligned}\langle A(t)\, B(t)\rangle &= \int_0^1 dt A(t)\, B(t) = \frac{1}{M}\sum_{t=0}^{M-1} A(t)\, B(t) \\ &= \frac{1}{M}\sum_{t_1=0}^{1}\sum_{t_2=0}^{1}\cdots\sum_{t_q=0}^{1} A(t)\, B(t),\end{aligned} \tag{2.4}$$

where we note again that $t = j/M, j = 0, ,1, ..., M-1$, and that $t = (t_1, t_2, ..., t_q)$.

4. *Orthogonality.*

$$\begin{aligned}\langle \mathrm{walh}(n, t)\,\mathrm{walh}(m, t)\rangle &= \frac{1}{2^q} \sum_{t_1=0}^{1} \sum_{t_2=0}^{1} \cdots \sum_{t_q=0}^{1} (-1)^{\sum_{i=1}^{q} n_i t_i} (-1)^{\sum_{i=1}^{q} m_i t_i} \\ &= \frac{1}{2^q} \prod_{i=1}^{q} (1 + (-1)^{n_i + m_i}) = \prod_{i=1}^{q} \delta_{n_i m_i} = \delta_{n,m}.\end{aligned} \tag{2.5}$$

5. *Completeness* [9]. From the completeness and orthogonality properties we know that an absolutely integrable function [10] $f(t)$ can be expanded in a Walsh series as

$$f(t) = \sum_{n=0}^{\infty} c_n \,\mathrm{walh}(n, t) \tag{2.6}$$

and approximated as

$$f(t) \approx \sum_{n=0}^{M-1} c_n \,\mathrm{walh}(n, t) \qquad (M = 2^q) \tag{2.7}$$

by uniform convergence.

The error term is governed by the behavior of the c_n. As shown by Fine [11] $c_n \sim 1/n$. The coefficients c_n are given by

$$c_n = \langle f(t)\,\mathrm{walh}(n, t)\rangle, \tag{2.8}$$

using the orthogonality property.

The above results are used in the following section to construct a Walsh Sensitivity Analysis.

III. Walsh Sensitivity Analysis

We assume that a mathematical model of the physical system has been constructed and that the model can be solved to yield an output function f

$$f = f(\mathbf{u}; \boldsymbol{\tau}). \tag{3.1}$$

The output function depends on a set of p parameters $\mathbf{u} = u_1, u_2, \ldots, u_p$ which, for a given run (solution) of the model, are fixed. The model may also depend on variables $\boldsymbol{\tau} = \tau_1, \ldots, \tau_k$ which vary during the model run. For example, τ could represent the time in the solution of a physico-chemical model of a coupled hydrodynamic-chemical reaction process. In this example, the $\mathbf{u}$ could correspond to the rate and transport coefficients which are the parameters of the model.

To investigate the global sensitivity of the output to the parameters, we first introduce a transformation function g_i which relates the possible parameter values to another variable t_i as

$$u_i = g_i(t_i), \qquad i = 1, 2, \ldots, p. \tag{3.2}$$

As t_i is varied, u_i is driven over its appropriate range of variation. In accordance with the aim of this analysis, g_i will be chosen to give just two values for each u_i. Expressing $f(\mathbf{u})$, the output function, in terms of $\mathbf{t}$ by using Eq. (3.2), and expanding $f(\mathbf{t})$ [12] in a p-dimensional Walsh series, we have

$$f(\mathbf{t}) = \prod_{\alpha=1}^{p} \sum_{w^\alpha=0}^{M-1} c_{\mathbf{w}} \operatorname{walh}(w^\alpha t^\alpha) \tag{3.3a}$$

and

$$c_{\mathbf{w}} = \frac{1}{M^p} \prod_{\alpha=1}^{p} \sum_{t^\alpha=0}^{M-1} f(\mathbf{t}) \operatorname{walh}(w^\alpha t^\alpha). \tag{3.3b}$$

In Eq. (3.3) we have used the notation w^α and t^α to denote the sequency and timelike variables associated with the αth parameter, $\alpha = 1, 2, \ldots, p$. Each sequency runs over $w^\alpha = 0, 1, \ldots, M-1$ with $M = 2^q$ and $t^\alpha = j/M$, $j = 0, 1, \ldots, M-1$, as in Section II. Since only two values are required for each parameter, we use $t^\alpha = 0, 1$ for each α. That is, $M = 2$ and Eqs. (3.3) are

$$f(\mathbf{t}) = \prod_{\alpha=1}^{p} \sum_{w^\alpha=0}^{1} c_{\mathbf{w}} \operatorname{walh}(w^\alpha t^\alpha) \tag{3.4a}$$

and

$$c_{\mathbf{w}} = \frac{1}{2^p} \prod_{\alpha=1}^{p} \sum_{t^\alpha=0}^{1} f(\mathbf{t}) \operatorname{walh}(w^\alpha t^\alpha). \tag{3.4b}$$

Only one binary digit is required to represent any $\operatorname{walh}(w^\alpha t^\alpha)$ for a $Q = 1$ Walsh group. Therefore, t^α has the binary representation (t_α), where $t_\alpha = 0, 1$, and $\operatorname{walh}(w^\alpha t^\alpha) = (-1)^{w_\alpha t_\alpha}$. Note that

$$\prod_{\alpha=1}^{p} \operatorname{walh}(w^\alpha t^\alpha) = \prod_{\alpha=1}^{p} (-1)^{w_\alpha t_\alpha} = \operatorname{walh}(W, T), \tag{3.5}$$

where W and T are, respectively, the sequency and timelike variables for the p digit binary numbers $(w_p \cdots w_1)$ and $(t_p \cdots t_1)$ defined as

$$W = w_p 2^{p-1} + w_{p-1} 2^{p-2} + \cdots + w_1 2^0 \tag{3.6a}$$

and

$$T = t_p 2^{p-1} + t_{p-1} 2^{p-1} + \cdots + t_1 2^0. \tag{3.6b}$$

Thus, Eq. (3.4) can be expressed as the *one*-dimensional Walsh transform pair

$$f(T) = \sum_{W=0}^{N-1} c_W \operatorname{walh}(W, T) \tag{3.7a}$$

and

$$c_W = \frac{1}{N} \sum_{T=0}^{N-1} f(T) \operatorname{walh}(W, T) \tag{3.7b}$$

by using Eq. (3.6) and defining $N = 2^p$ [13].

The requirement of a Sensitivity Analysis is that each parameter variation shows up *uniquely* in the output function. Specifically, we require that if we assign a unique sequency to each parameter, then, in the Walsh spectrum of the output, a non-zero Walsh coefficient at a given parameter's sequency indicates a sensitivity to that particular parameter, and no other. To effect this condition we choose the set of p sequencies, one for each parameter, according to

$$\sum_{\alpha=1}^{p} b_\alpha W_\alpha \neq 0, \tag{3.8}$$

where $b_\alpha = 0$ or 1. Thus, the W_α's are "binary incommensurate." For example, for three parameters, $p = 3$, take $W_1 = 1$, $W_2 = 2$ and $W_3 = 4$. Then Eq. (3.8) is satisfied since $W_1 = 001$, $W_2 = 010$, $W_3 = 100$, $W_1 \oplus W_2 = 011$, $W_1 \oplus W_3 = 101$, $W_2 \oplus W_3 = 110$ and $W_1 \oplus W_2 \oplus W_3 = 111$; the sequencies are 1, 2, 4, 3, 5, 6 and 7, respectively. The multiplication and group properties noted in Section II show that, in general, the choice of parameter sequencies

$$W_\alpha = 2^\alpha, \qquad \alpha = 0, 1, \ldots, p-1, \tag{3.9}$$

ensures that Eq. (3.8), the binary incommensurate condition, is satisfied. With this choice of sequencies, the transformation function is given as

$$u_\alpha = g_\alpha(t_\alpha) = u_\alpha^{(0)} + \Delta_\alpha \operatorname{walh}(2^\alpha, t_\alpha 2^\alpha), \tag{3.10}$$

where $t_\alpha = 0, 1$ and $u_\alpha^{(0)}$ is the median value of u_α. Since $\operatorname{walh}(2^\alpha, t_\alpha 2^\alpha) = (-1)^{t_\alpha}$ for $t_\alpha = 0, 1$, one obtains

$$u_\alpha = u_\alpha^{(0)} \pm \Delta_\alpha, \tag{3.11}$$

with the + sign for $t_\alpha = 0$ and the − sign for $t_\alpha = 1$. Thus, the choice of the transformation function given in Eq. (3.10) generates two values of each parameter. Furthermore, it does so with equal probability since any Walsh function is either ± 1 with equal weight as t ranges on $[0, 1)$.

In summary, the transformation function of Eq. (3.10) with the parameter sequencies of Eq. (3.9) yields two equally weighted values of each parameter and each sequency provides a unique label for its assigned parameter. By examining the *one*-dimensional Walsh spectrum of the output function, cf. Eq. (3.7), the sensitivity of the output function to each parameter can be assessed.

It now remains to provide convenient and useful measures of this sensitivity for the Walsh analysis. We shall now show that the sensitivity measures used in the Fourier Sensitivity Analysis [1, 2] are also appropriate here. The scalar product defined in Eq. (2.4) is equivalent to an average over the p-dimensional parameter space probability distribution function when the transformation function of Eq. (3.10) is used, since, for some function H of the output f,

$$\langle H\rangle = \frac{1}{2^p} \prod_{\alpha=1}^{p} \sum_{t_\alpha=0}^{1} H[f(\mathbf{t})]. \tag{3.12}$$

That is, Eq. (3.12) sums over the two parameter values given by $t_\alpha = 0, 1$ via Eq. (3.10) for each parameter $\alpha = 1, 2,\ldots, p$, and the weight of each parameter value is $\frac{1}{2}$. Expanding f in a p-dimensional Walsh series yields

$$\begin{aligned}\langle f\rangle &= \frac{1}{2^p} \prod_{\alpha=1}^{p} \sum_{t^\alpha=0}^{1} \sum_{w^\alpha=0}^{1} c_{w_p\cdots w_1} \operatorname{walh}(w^\alpha t^\alpha) \\ &= \prod_{\alpha=1}^{p} \sum_{w^\alpha=0}^{1} c_{\mathbf{w}} \delta_{w_\alpha,0} = c_{\mathbf{0}} = c_{0\ldots 0},\end{aligned} \tag{3.13}$$

since

$$\sum_{t^\alpha=0}^{1} \operatorname{walh}(w^\alpha t^\alpha) = 1 + (-1)^{w^\alpha} = 2\delta_{w^\alpha,0} \qquad (w^\alpha = 0, 1), \tag{3.14}$$

as in the derivation of Eq. (2.5). Thus, the average value (over the parameter space distribution function) of the output function is its $c_{\mathbf{0}}$ Walsh coefficient. Also, by noting the correspondence of the p-dimensional Walsh transform of Eq. (3.4) (for $M = 2$) with the one-dimensional Walsh transform of Eq. (3.7), one has that

$$\langle f\rangle = \frac{1}{N} \sum_{T=0}^{N-1} \sum_{W=0}^{N-1} c_W \operatorname{walh}(W, T) = \sum_{W=0}^{N-1} c_W \delta_{W,0} = c_0 = c_{\mathbf{0}} \equiv c_{0\ldots 0}. \tag{3.15}$$

We calculate the average of f^2 by expanding f in a Walsh series, both the p- and one-dimensional forms, and using the orthogonality relation of Eq. (2.5) and obtain

$$\langle f^2\rangle = \prod_{\alpha=1}^{p} \sum_{w^\alpha=0}^{1} c_{\mathbf{w}}^2 = \sum_{W=0}^{N-1} c_W^2. \tag{3.16}$$

Thus, the total variance σ_T^2 of f induced by the simultaneous variation of *all* the parameters is

$$\sigma_T^2 = \langle f^2\rangle - \langle f\rangle^2 = \prod_{\alpha=1}^{p} \sum_{w^\alpha=0}^{1}{}' c_{\mathbf{w}}^2 = \sum_{W=1}^{N-1} c_W^2, \tag{3.17}$$

where the $'$ on the sum excludes the c_0 Walsh coefficient. This result is the analogue of Parseval's theorem of Fourier analysis.

Partial variances are constructed by averaging the output function f over all but one parameter, say the first parameter, and then calculating the variance of the result $f^*(u_1)$ with respect to the first parameter. Averaging f over $u_2 \cdots u_p$ by Walsh expansion yields

$$f^*(t_1) = \frac{1}{2^{p-1}} \prod_{\alpha=2}^{p} \sum_{t^\alpha=0}^{1} \sum_{w^\alpha=0}^{1} c_{w_p \cdots w_1} \operatorname{walh}(w^\alpha t^\alpha) = c_{w_p \cdots w_1} \operatorname{walh}(w^1 t^1). \quad (3.18)$$

The partial variance with respect to parameter one is

$$\sigma_1^2 = \langle (f^*)^2 \rangle - \langle f^* \rangle^2 = c_{00\cdots 1}^2 = c_1^2, \quad (3.19)$$

where we have noted that $\langle f^* \rangle = \langle f \rangle = c_0$. This result holds for any parameter, and we define the reduced partial variance S_α with respect to parameter α as

$$S_\alpha = C_{W_\alpha}^2 / \sigma_T^2 = \sigma_\alpha^2 / \sigma_T^2, \qquad \alpha = 1, 2, \ldots, p. \quad (3.20)$$

These partial variances are a measure of the effect that variations in a given parameter have on the output function which takes into account the simultaneous variation of all the other parameters, in an averaged sense. The S_α can be ordered to reflect the relative importance that the parameters have on a given output function.

In a similar fashion, coupled partial variances can be constructed which are formed from the Walsh coefficients whose sequency is that of the desired sequencies (parameters) added together (by binary addition without carry). Here we first average the output over all the parameters except those for the desired set, and then construct the variance with respect to this remaining set. For example, one obtains the reduced coupled partial variance for parameters α and β as

$$S_{\alpha,\beta} = \sigma_{W_\alpha \oplus W_\beta}^2 / \sigma_T^2. \quad (3.21)$$

This result is obtained by a simple generalization of the procedure leading to Eq. (3.19). The coupled partial variances are a measure of the combined effect on the output of variations in a set of parameters (α and β in Eq. (3.21)) averaged over the simultaneous variation of all the other parameters.

The sensitivity measures given above may be related to averages of the central difference formula for derivatives of a function. This connection is discussed in the Appendix.

The procedure for a Walsh Sensitivity Analysis is as follows. For a p parameter problem assign a sequency W_α to each of the parameters according to Eq. (3.9). Set $u_\alpha^{(0)}$ and Δ_α of Eqs. (3.10) and (3.11) to obtain the desired two values for each parameter. Write the output function in terms of the search variable $\mathbf{t} = T$ by use of Eq. (3.10) and evaluate its Walsh coefficients via Eq. (3.7b). From this set of N

Walsh coefficients construct the desired measures of sensitivity given by Eqs. (3.17), (3.20) and (3.21).

In the next section, an example of Walsh Sensitivity Analysis is given to illustrate the use and power of this method.

IV. An Example

In this section we present a simple example of Walsh Sensitivity Analysis to illustrate its use. Also, we compare it to linear Sensitivity Analysis and to the existing Fourier Sensitivity Analysis [1, 2].

A simple, but very common, nonlinear model output function is the exponential

$$f(u_1, u_2; \tau) = u_2 e^{u_1 \tau}.$$

The parameters are u_1 and u_2 and the variable is τ. A linear Sensitivity Analysis is obtained by truncating the Taylor expansion

$$\begin{aligned} f = f(u_1^0, u_2^0; \tau) &+ e^{u_1^0 \tau}(u_2 - u_2^0) + u_2^0 \tau e^{u_1^0 \tau}(u_1 - u_1^0) \\ &+ \tau e^{u_1^0 \tau}(u_2 - u_2^0)(u_1 - u_1^0) + u_2^0 \tau^2 e^{u_1^0 \tau}(u_1 - u_1^0)^2/2 + \cdots, \end{aligned} \tag{4.1}$$

at the first derivative terms. Define a linear Sensitivity Analysis coefficient X_α for parameter α as

$$X_\alpha = u_\alpha^0 \left. \frac{\partial f(\mathbf{u})}{\partial u_\alpha} \right|_{\mathbf{u} = \mathbf{u}^0}. \tag{4.2}$$

For the above example,

$$X_1 = u_1^0 u_2^0 \tau e^{u_1^0 \tau}, \tag{4.3a}$$

$$X_2 = u_2^0 e^{u_1^0 \tau}. \tag{4.3b}$$

The linear sensitivity coefficients are plotted in Fig. 2 with $u_1^0 = -0.25$ and $u_2^0 = 1000$ as the nominal values. From this linear analysis, one concludes that the sensitivity to u_2 is highest at small τ, while that of u_1 peaks at $u_1 \sim 4$.

To perform a Walsh Sensitivity Analysis, a range of parameter variation is required. First, let us examine the "local behavior" of the model by choosing a small variation of parameters (the Δ_α of Eq. (3.10)). In this case, the Walsh analysis should verify the linear analysis. Consider a 10% variation in both parameters, i.e., $u_1 = -0.25 \pm 0.025$ and $u_2 = 1000 \pm 100$. In Fig. 3, the average behavior of the output is plotted. The average is the normalized sum of the four simulations corresponding to the four possible combinations of parameter values. It is just the c_0 Walsh coefficient defined in Section III. The Walsh coefficients c_1 and c_2 are plotted in Fig. 4. As shown in the Appendix, $c_1(c_2)$ is the finite difference approximation to

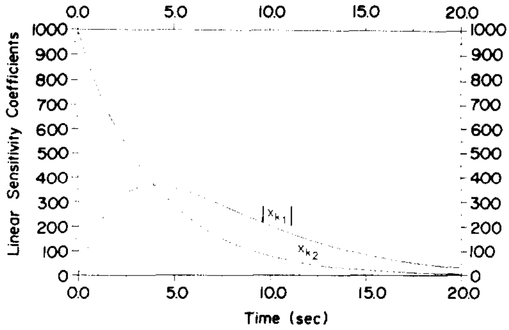

FIG. 2. Linear sensitivity coefficients defined in Eqs. (4.2) and (4.3) for the exponential model.

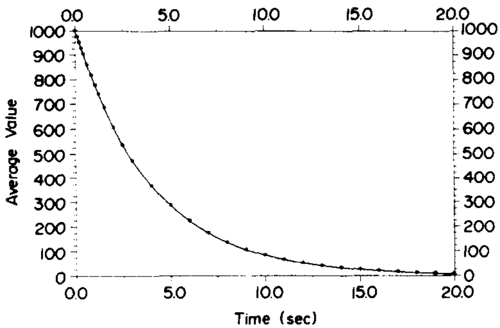

FIG. 3. Average value of the output for WASP, the C_0 Walsh coefficient; 10% variation case.

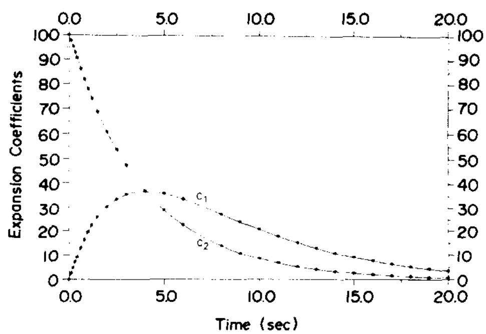

FIG. 4. The Walsh coefficients C_1 and C_2; 10% variation case.

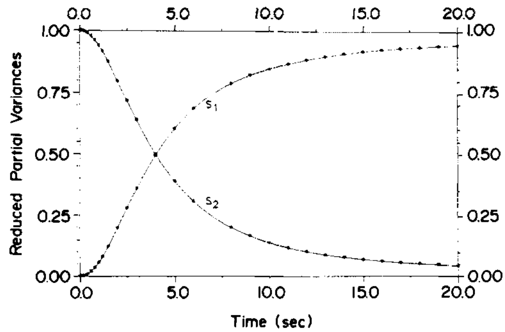

FIG. 5. The Walsh reduced partial variances S_1 and S_2 defined in Eq. (3.20); 10% variation case.

the first derivative of the output function with respect to parameter one (two) *averaged* over the probability distribution of the second (first) parameter. Comparing Fig. 2 with Fig. 4, we see that the sensitivities are the same to within a trivial scale factor, which is dependent on the transformation function $g_\alpha(t_\alpha)$. For ordering purposes it is convenient to display the reduced partial variances, S_1 and S_2, as defined in Eq. (3.20). This plot, Fig. 5, shows that the sensitivity to u_1, as measured by S_1, is increasing with τ in contrast to the peak behavior displayed by X_1 and c_1. This occurs because the standard deviation (square root of the total variance σ_T defined in Eq. (3.17)) which appears as the denominator of S_1 and S_2, is decaying with τ, which reflects the decay of the individual simulations. Another feature displayed in Fig. 5 is the lack of coupling between the parameters, as is clear from noting that $S_1(\tau) + S_2(\tau) \sim 1$. Thus, almost all the variance in the output function is assigned to S_1 or S_2. It is also instructive to plot the relative deviation, which is the standard deviation divided by the averaged output. As Fig. 6 shows, the sensitivity to the parameters can be large when measured relative to the actual simulation values which, in this case, are becoming small for large τ.

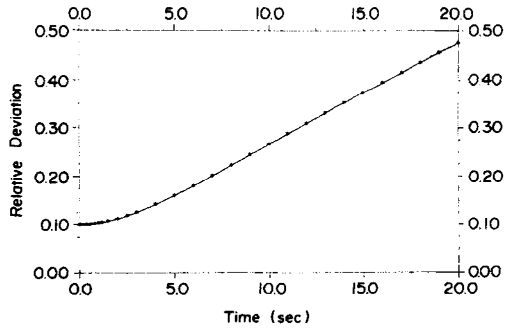

FIG. 6. Relative deviation (standard deviation/average); 10% variation case.

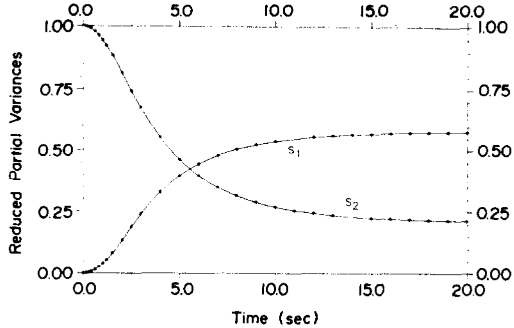

FIG. 7. The Walsh reduced partial variances; 60% variation case.

The linear or small parameter variation Walsh Sensitivity Analysis is appropriate when the output is well represented by the first derivative term of its Taylor expansion. To investigate the sensitivity properly, we must allow for a wider range of parameter variation. This is readily done in the Walsh analysis by increasing the value of Δ_1 and Δ_2. Increasing the range of variation to 60% (from the 10% variation just explored) leads to the results summarized in Fig. 7. The changes from the linear and small variation Walsh analyses are evident. They reflect the effect of the nonlinear terms in the Taylor expansion of the output. Note that now a coupling between the parameters exists since, as τ increases, $S_1(\tau) + S_2(\tau) \sim 0.8$. A larger variation of parameters would produce a greater difference with respect to the linear and small variation Walsh analyses.

If the parameter variation is increased to 100%, i.e., $u_1 = -0.25 \pm 0.25$, $u_2 = 1000 \pm 1000$, the character of the analysis changes to one of *Structural* Analysis as opposed to Sensitivity Analysis. By the term Structural Analysis we refer to changes in the model specification; here, by eliminating parameters completely. In the above example, two of the output functions are zero for all τ ($u_2 = 0$), and one is a non-zero constant ($u_1 = 0$). We present the results of this analysis in Fig. 8. There are drastic

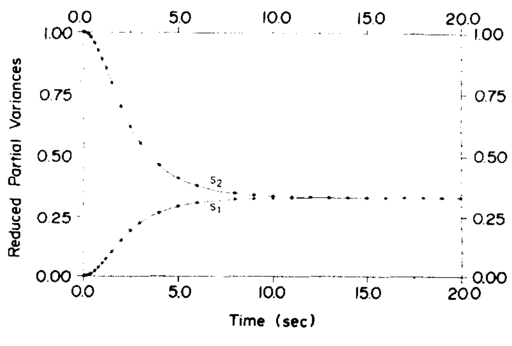

FIG. 8. The Walsh reduced partial variances; 100% variation case.

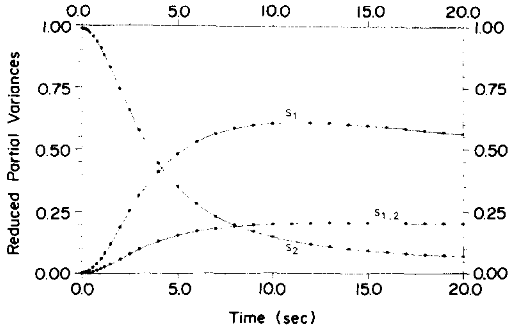

FIG. 9. The Fourier (FAST) reduced partial, and coupled partial variances (cf., Eq. (3.21)); 100% variation case.

differences with regard to the other cases treated. The average value does not decay to zero, and the reduced partial variances are totally different for large τ. The conclusion then is that Walsh analysis must be done with care to ensure that a Sensitivity Analysis as opposed to a Structural Analysis is being performed. Of course, the Walsh theory presented here is ideally suited to Structural Analysis.

We can compare the above three cases of small (essentially linear), medium and large parameter variations, with the results of FAST for these three cases. In FAST, the parameter variation is not two valued, it is obtained from a probability distribution which weights the nominal values also. The transformation function used in these FAST simulations is log-uniform (the probability distribution function of the logarithm of each parameter is uniform between finite limits and zero otherwise). For the small parameter variation case, the Fourier Sensitivity Analysis yields essentially the same results as the linear and small variation Walsh Sensitivity Analysis. The medium variation case also reproduces the Walsh analysis. For the large variation case, Fig. 9 shows that a Sensitivity, not Structural, Analysis is being done. The plots reveal the increasing influence of the nonlinear terms in the Taylor expansion of the output function on the sensitivity coefficients. At large τ the reduced partial variances, S_1 and S_2, and coupled partial variance $S_{1,2}$ sum to $\sim$0.8. This indicates even greater coupling among the parameters than in the medium variation case, and is in great contrast to the lack of coupling displayed by the linear and small variation Walsh analyses.

V. DISCUSSION

When it is sufficient to carry out a Sensitivity Analysis where each parameter takes on only two values, then the Walsh analysis developed here will be appropriate. The parameter range can be adjusted, for each parameter, to reflect ones knowledge (or lack thereof) about each parameter's possible values. The use of extreme values, a minimum and maximum, may be thought of as providing an upper limit on the model's sensitivity, with respect to other choices of parameter distribution functions.

WASP has the virtue of being an exact global nonlinear Sensitivity Analysis for models where two valued parameter distributions are appropriate. The expressions for the total, reduced partial and reduced coupled variances given in Eqs. (3.17), (3.20) and (3.21), respectively, are exact. By contrast, the analogous expressions in FAST [1, 2] are approximate. The number of simulations required for a Sensitivity Analysis of a given accuracy increases for an increase in accuracy. Since the computational expense is determined by the number of required simulations, a compromise between accuracy and cost is involved. This issue does not arise in WASP since the number of simulations N is simply related to the number of parameters p as $N = 2^p$.

We have not discussed the implementation of WASP so far [4]. It is quite straightforward. All that is required is a method to calculate Walsh coefficients of a given output function. FAST Walsh transform codes exist (analogous to FAST Fourier transform codes), which require $N \log_2 N$ operations. Thus, in almost all cases, the limiting factor in WASP is the time required to run one simulation of the model, not the Walsh transform of the N output functions.

The WASP example of Section IV with the large parameter variation illustrates the possibility of using WASP as a *Structural* Analysis method. If we consider a bivariate parameter distribution with values zero or one, the either a given parameter is missing from the model, or it is present. WASP then provides a method of assessing the sensitivity of a model to changes in its structure. This important possibility for WASP is currently being explored.

Appendix

In this Appendix we relate WASP to averaged central difference approximations of derivatives of the output function.

A two parameter example will illustrate the connection between Walsh coefficients and central difference approximations. There are $4 = 2^2$ Walsh coefficients c_0, c_1, c_2 and c_3. Reference to Eq. (3.7) shows that the c_2's are generated from the four output functions as

$$\begin{pmatrix} c_0 \\ c_1 \\ c_2 \\ c_3 \end{pmatrix} = 2^{-1/2} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{pmatrix} \begin{pmatrix} f_0 \\ f_1 \\ f_2 \\ f_3 \end{pmatrix}, \tag{A.1}$$

where the f_i denote the four values of the output function $f_0 = f(00)$, $f_1 = f(01)$, $f_2 = f(10)$ and $f_3 = f(11)$. From Eq. (A.1),

$$c_1 = \frac{1}{2}\left[\frac{f_0 - f_1}{2} + \frac{f_2 - f_1}{2}\right], \tag{A.2}$$

which is the average over the second parameter of the two central difference approximations to the first derivative with respect to the first parameter. That is, if

$$\left.\frac{\Delta f}{\Delta u_1}\right|_{u_2} = \frac{f(0u_2) - f(1u_2)}{2}, \tag{A.3}$$

then

$$c_1 = c_{01} = \left\langle \frac{\Delta f}{\Delta u_1} \right\rangle_2. \tag{A.4}$$

By a similar argument, c_2 is the averaged (over parameter one) central difference approximation to the first derivative of f with respect to u_2. Also, $c_3 = c_{11}$, from Eq. (A.1), is given by

$$c_3 = \frac{\Delta^2 f}{\Delta u_1 \, \Delta u_2}. \tag{A.5}$$

The general result is given by the succession of relations

$$c_{0\cdots 1_\alpha \cdots 0} = \left\langle \frac{\Delta f}{\Delta u_\alpha} \right\rangle_{\neq \alpha}, \tag{A.6}$$

$$c_{0\cdots 1_\alpha \cdots 1_\beta \cdots 0} = \left\langle \frac{\Delta^2 f}{\Delta u_\alpha \, \Delta u_\beta} \right\rangle_{\neq \alpha, \beta}, \tag{A.7}$$

etc.

Acknowledgments

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12. Here, and in the following development, we use the same symbol f even though the independent variable has changed.
13. This one dimensional transform pair corresponds to the s space search curve and associated s-space Fourier analysis of FAST (cf. Ref. [2]).