An alternative way to compute Fourier amplitude sensitivity test (FAST)

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Abstract

In this article we investigate the relationship between two coefficients used in sensitivity analysis of model output. One is the Fourier amplitude sensitivity test's coefficient, developed in the 1970s, and the other the Sobol' sensitivity indices, developed in the 1990s. Supposedly both methods are capable of computing the "main effect" contribution of model's input parameters to model's output variance. We discuss the equivalence of the two methods, and prove the identity of their prediction on two test cases. Relative advantage and disadvantages of the methods are also illustrated. © 1998 Elsevier Science B.V. All rights reserved.

1. Introduction

Sensitivity analysis of model output aims to quantify how a model depends on its input parameters. Global sensitivity analysis, in particular, tries to apportion the variation in the output variable(s) to the variation of the model input parameters, while local sensitivity analysis is usually concerned with the computation of the derivative of the model response with respect to the model input parameters (Saltelli and Von Maravić, 1995).

In the 1970s a new method for global sensitivity analysis (SA) of complex chemical systems was introduced, which was superior to the local SA methods used till that time for similar applications.

The new method, named Fourier amplitude sensitivity test (FAST) was based on Fourier developments of the output function, and allowed an ANOVA-like decomposition of the model output variance. FAST was superior to the local SA methods because (a) it could apportion the output variance to the variance in the input parameters and (b) It could be used to fix the non-influential parameters at their midpoint or "nominal value" (Cukier et al., 1973, 1975, 1978; Schaibly and Shuler, 1973, Koda et al., 1979; McRae et al., 1982).

FAST is superior to commonly used methods for global sensitivity analysis, such as those based on correlation or regression coefficients. When using, for instance, standardised regression coefficients (SRC, Draper and Smith, 1981) for the purpose of SA, the analysis is only as good as the fit of the regression model. If the associated model coefficient of determination R^2 is low, then the SRC-based SA is of little value. Ranking the data, and using for the analysis the standardised rank regression coefficients (SRRC), may improve the R^2 value, but the cost of the transformation is to alter the models under analysis (see Saltelli and Sobol', 1995a).

In spite of its merits, the new method was used rarely in the years subsequent to its discovery (for a review see Turanyi, 1990, or Helton, 1993). This was perhaps due to some disadvantages of the method such as (a) its computational complexity and (b) its scarce ability to compute the higher-order terms in the ANOVA-like decomposition of the model output's variance. In fact, when using FAST, one can estimate the individual contribution of each parameter to the output variance, i.e. what is known as a main effect in Statistics.

Cukier et al. (1978) recognised that if D is the total variance of the model output, this can be decomposed in terms of increasing dimensionality as

$$D = \sum_{i=1}^{n} D_i + \sum \sum_{1 \leq i \leq j \leq n} D_{ij} + \cdots + D_{12 \cdots n} \tag{1}$$

and that a first-order parameter sensitivity can be given by

$$S_i = \frac{D_i}{D}. \tag{2}$$

In principle, also the interaction terms D_{ij} and the higher-order effects may contribute to the model variance, and hence add to the sensitivity of a parameter, but those terms are not easily computed with FAST. FAST practitioners discounted the relevance of those terms observing that FAST was a good method to use when the sum of the first-order terms was at least as high as 0.6 (Liepmann and Stephanopoulos, 1985). We are not aware of applications where interaction terms were actually computed. In other words, FAST is good for (quasi-)additive models, i.e. models with no important or significative interactions among factors.

In 1990 the Russian mathematician Ilya M. Sobol' (1990a) developed a method for global SA which he defined as more general than FAST. His method also

computed ANOVA-like decomposition of the output variance, but in this case both the main effects S_i, the interaction terms S_{ij} and higher-order terms could be computed by straightforward Monte-Carlo integration of multidimensional integrals, e.g.

$$D = \int_{K^n} f^2(x)\, dx - f_0^2 \tag{3}$$

and

$$D_{i_1 \dots i_s} = \int_0^1 \cdots \int_0^1 f_{i_1 \dots i_s}^2 \, dx_{i_1} \cdots dx_{i_s}, \tag{4}$$

where $D_{i_1 \dots i_s}$ is a generic term in the series development of D and $f_{i_1 \dots i_s}$ is a term in the Sobol' decomposition of $f(x)$ into summands of increasing dimension (see Section 3).

Sobol' also claimed that his decomposition is unique. Although the two methods (FAST and Sobol's) differ considerably in their theoretical and computational features, they both allow the evaluation of the fractional contribution to the variance of $f(x)$ which is due to each individual variable (main effect). Given that these are a property of the model and of the input parameter space, the values provided by the two methods should be identical.

We have computed both measures of sensitivity and found them equal on a number of test cases, making allowance for experimental error. FAST appears to be computationally cheaper, and relatively independent of sample size once the Nyquist criterion is satisfied. Sobol' is computationally more intensive, and seems to be more dependent on sample size. It also gave more accurate results in one of the test cases.

The advantage of Sobol' with respect to FAST substantially resides in its capability to compute higher-order terms in the variance series development (1), and is hence relevant when those terms make a significant contribution to the output variance.

It should also be mentioned that FAST and Sobol' indices are not the only options in the arena of the variance-based methods. Iman and Hora (1990) have discussed an "Importance measure"; Krzykacz (1990) and McKay (1995), a "Correlation ratio". All those measures are amenable to the evaluation of the main effect in the variance decomposition scheme.

In Sections 2 and 3 we briefly recall the basis of the FAST and Sobol' methods. In Section 4 two test cases are described, one an analytical model and the other a computational one. Results are presented in Section 5 and conclusions are summarised in Section 6.

2. Fourier amplitude sensitivity test (FAST)

The FAST method allows the computation of that fraction of the variance of a given model output or function which is due to each input variable. The key idea

underlying the method is to apply the ergodic theorem as demonstrated by Weyl (1938). This hypothesis allows the computation of an integral in an n-dimensional space through a mono-dimensional integral.

Let the function

$$f(\boldsymbol{x}) = f(x_1, x_1, \ldots, x_n) \tag{5}$$

be defined in the n-dimensional unit cube:

$$K^n = (\boldsymbol{x}|0 \leq x_i \leq 1; \ i = 1, \ldots, n). \tag{6}$$

Consider the set of transformations

$$x_i = g_i(\sin(w_i \cdot s)), \quad i = 1, \ldots, n. \tag{7}$$

If a linearly independent set of frequencies $\{w_1, \ldots, w_k\}$ is chosen (no w_i may be obtained as a linear combination of the other frequencies with integer coefficients), when s varies from $-\infty$ to ∞, the vector $(x_1(s), \ldots, x_n(s))$ traces out a curve that fills the whole n-dimensional unit cube $\boldsymbol{K}^n$, so that, following Weyl (1938), the integral

$$f_0 = \int_{K^n} f(\boldsymbol{x}) \, dx_1 \cdots dx_n, \tag{8}$$

and the integral

$$\widehat{f}_0 = \lim_{T \to \infty} \frac{1}{2T} \int_{-T}^{T} f(\boldsymbol{x}(s)) \, ds \tag{9}$$

are equal.

Since the numerical computation of integrals like that in (9) is impossible for an incommensurate set of frequencies, an appropriate set of integer frequencies is used. The consequences of this change are that the curve is no longer a space-filling one, but becomes a periodic curve with period 2π, and approximate numerical integrations can be made. If these ideas are extended to the computation of variances, the variance of f may be computed through

$$D = \frac{1}{2\pi} \int_{-\pi}^{\pi} f^2(\boldsymbol{x}(s)) \, ds - \widehat{f}_0^2, \tag{10}$$

where

$$\widehat{f}_0 = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(\boldsymbol{x}(s)) \, ds. \tag{11}$$

The application of Parseval's theorem to the computation of (11) allows to reach the expression

$$\boldsymbol{D} = 2 \sum_{j=1}^{\infty} (A_j^2 + B_j^2), \tag{12}$$

where the A_j and the B_j are the common Fourier coefficients of the cosine and the sine series, respectively. After Cukier et al. (1978), the part of this variance due to each individual input variable is the part of the summatory (12) extended only to the frequency assigned to each input variable in (7) and its harmonics, so that

$$S_i = \frac{2 \sum_{p=1}^{\infty} (A_{p \cdot w_i}^2 + B_{p \cdot w_i}^2)}{2 \sum_{j=1}^{\infty} (A_j^2 + B_j^2)}, \tag{13}$$

is the fraction of the variance of f due to the input variable x_i. The summation in p is meant to include all the harmonics related to the frequency associated to the input variable considered. This coefficient is equal to what is called a "main effect" in factorial design. Unfortunately, the fraction of the total variance due to interactions, i.e. the combined effect due to two variables that cannot be resolved by the sum of individual effects, may not be computed with this technique up to the present, although Cukier et al. (1978) make some reference to the possibility of computing higher-order terms contribution (see the next section).

The computation of formula (13) for each input variable needs the evaluation of the function f at a number of points in K^n to compute each A_i and each B_i, $i = 1, \ldots, n$.

The first step in the computation of the indices is the selection of the set of integer frequencies. Cukier et al. (1975) provide an algorithm to produce those optimal sets. Those sets are optimal in the sense of being free of interferences until fourth order, and demanding a minimum sample size. This minimum is determined by the Nyquist criterion and is $2w_{max} + 1$, where w_{max} is the maximum frequency in the set. Schaibly and Shuler show (1973) that the results are independent of the assignation of frequencies to the input parameters. The selected points are equally spaced points in the one-dimensional s-space. A study of the errors due to the use of integer frequencies is in Cukier et al. (1975).

3.1. Sobol' sensitivity indices

The sensitivity indices were developed by Sobol' (1990a, translated in 1993), who based his earlier work on the Fourier Haar series (Sobol', 1969). Sobol' considered his method as a natural extension of the Fourier-based FAST approach. Let us consider again the function $f(x) = f(x_1, x_1, \ldots, x_n)$ defined in the n-dimensional unit cube. Under assumptions described in Sobol' (1990a), it is possible to decompose $f(x)$ into summands of increasing dimensions:

$$f(x_1, \ldots, x_n) = f_0 + \sum_{i=1}^{n} f_i(x_i) + \sum_{1 \le i \le j \le n} \sum f_{ij}(x_i, x_j) + \cdots + f_{12\ldots n}(x_1, x_2, \ldots, x_n), \tag{14}$$

where f_0 is a constant and the integrals of every summand over any of its own variables is zero:

$$\int_0^1 f_{i_1 \ldots i_s}(x_{i_1}, \ldots, x_{i_s}) \, dx_{i_k} = 0, \quad 1 \le k \le s. \tag{15}$$

The total variance of $f(x)$ can be written as $D = \int_{K^n} f^2(\bar{x})\,d\bar{x} - f_0^2$ while

$$D_{i_1\ldots i_s} = \int_0^1 \cdots \int_0^1 f_{i_1\ldots i_s}^2(x_{i_1}, \ldots, x_{i_s})\,dx_{i_1} \cdots dx_{i_s} \tag{16}$$

is a contribution to the total variance due to a generic term $f_{i_1\ldots i_s}$ in the series development. At this point the sensitivity estimates $S_{i_1\ldots i_s}$ can be introduced: $S_{i_1\ldots i_s} = D_{i_1\ldots i_s}/D$. Given that the relation

$$D = \sum_{i=1}^n D_i + \sum_{1 \le i \le j \le n} D_{ij} + \cdots + D_{12\ldots n} \tag{17}$$

can be proven (Sobol' 1990a, same expression as in FAST), it follows that $\sum'' S_{i_1\ldots i_s} = 1$, where the sum with inverted commas indicates sum over all the combinations of indices. This ANOVA-like decomposition is conceptually identical to the one realised in FAST. In the treatment of numerical experiments, similar decompositions are discussed in Cotter (1979), Cox (1982), Efron and Stein (1981) and Sacks et al. (1989). These articles are reviewed in Archer et al. (Submitted). The terms $S_{i_1\ldots i_s}$ can be considered as a natural sensitivity estimates, as they give the fraction of the total variance of $f(x)$ which is due to any individual parameter or combination of parameters. In this way, for example, S_1 is the main effect of parameter x_1, S_{12} is the interaction effect, i.e. that part of the output variation due to parameters x_1 and x_2 which cannot be explained by the sum of the effects of parameters x_1 and x_2. Finally, the last term $S_{123\ldots n}$ is that fraction of the output variance which cannot be explained by summing terms of lower order. When using sensitivity indices it is also possible to partition the input variables set in such a way as to compute the "variable total effect term" S_{Ti}. This gives the sum of all the $S_{i_1\ldots i_s}$ terms where at least one of the $i_1, \ldots, i_s$ is equal to i. For a function of three variables, for example

$$S_{T1} = S_1 + S_{12} + S_{13} + S_{123}. \tag{18}$$

The applicability of these sensitivity estimates is related to the possibility of evaluating the multidimensional integrals (such as Eq. (16)) using Monte-Carlo methods.

As an example, the estimates of sample mean and variance are

$$\hat{f}_0 = \frac{1}{N}\sum_{m=1}^N f(x_m); \qquad \hat{D} - \hat{f}_0^2 = \frac{1}{N}\sum_{m=1}^N f^2(x_m) \tag{19}$$

where x_m is a sampled point in the space K^n, and N the size of the sample. The partial variances needed to compute the main effects are

$$\hat{D}_i + \hat{f}_0^2 = \frac{1}{N}\sum_{m=1}^N f(u_{im}, x_{im})f(v_{im}, x_{im}) \tag{20}$$

where u and v denote different realisations of the vector $(x_1, x_2, \ldots, x_{i-1}, x_{i+1}, \ldots, x_n)$. Eq. (20) can be interpreted as follows: in order to compute the contribution to the

total variance due to parameter X_i multiply values of f obtained by sampling independently all the variables by corresponding f values obtained by resampling all the variables except X_i. If X_i is an important variable, then high values of the first "f" term in the $(f \times f)$ product will be multiplied by similarly high "f" values in the second term. Otherwise, the pairing of terms will tend to be random, high values being possibly multiplied by the lower ones, and the $\hat{D}_i$ value will in general be smaller. The higher-order interactions and the total effects terms are computed by way of integrals of the same form as (20) above.

A recent application of Sobol' indices to a test case of atmospheric chemistry can be found in Saltelli and Hjorth, (to appear).

3.2. Sample generation

Quasi-random numbers have been used for the computation of the Monte-Carlo integrals. A description of the LP_τ sequences can be found in Sobol' (1967, 1976, 1990b). As discussed in Sobol' (1990b) quasi-random numbers are characterised by an enhanced convergence under certain limitations (in the value of n; see also Bratley and Fox, 1988; Sobol' et al., 1992; Davis and Rabinowitz, 1984).

4. Test functions

4.1. Analytical test case

In order to compare the results against exact analytical values the following function is used:

$$f = \prod_{i=1}^{n} g_i(x_i), \tag{21}$$

where the function f is defined in the n-dimensional unit cube (Eq. (6)) and the a's are parameters. Fig. 1 gives plots of the g terms for different values of "a". The

$$g_i(x_i) = \frac{|4x_i - 2| + a_i}{1 + a_i}, \quad a_i \geq 0 \tag{22}$$

with all a's $= 0$, was used in Davis and Rabinowitz (1984) to test multidimensional integration. The function (21), (22) has also been used in Saltelli and Sobol (1995a, b).

For all g functions,

$$\int_0^1 g_i(x_i)\, dx_i = 1$$

and therefore

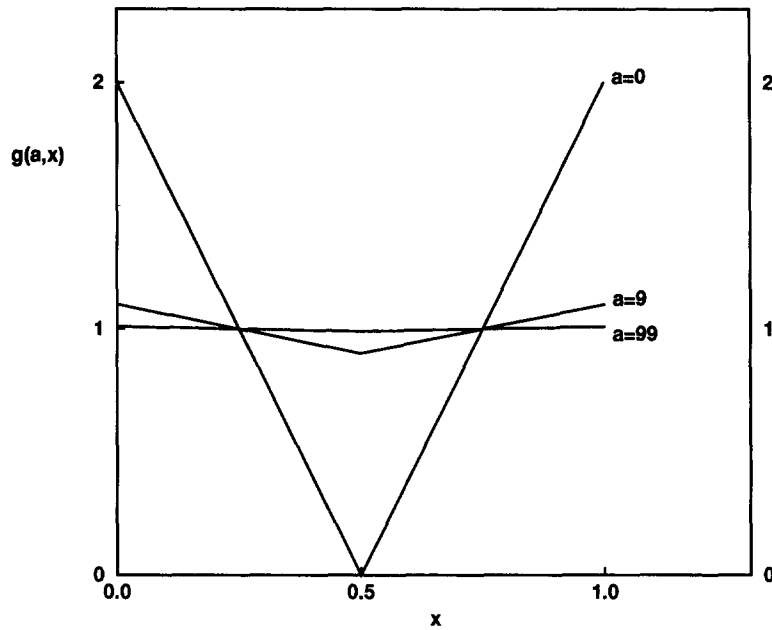$$\int_0^1 \cdots \int_0^1 f\, dx_1 \cdots dx_n = 1.$$

Fig. 1.

The function $g_i(x_i)$ varies as

$$1 - \frac{1}{1+a_i} \le g_i(x)_i \le 1 + \frac{1}{1+a_i}. \tag{23}$$

For this reason the value of the a's determine the relative importance of the input variables (the x's). For example, if $a_i = 0$,

$$0 \le g_i(x_i) \le 2$$

and x_i is an important variable. If $a_i = 9$,

$$0.9 \le g_i(x_i) \le 1.1$$

and x_i is much less important. If $a_i = 99$,

$$0.99 \le g_i(x) \le 1.01$$

and the variable x_i is insignificant. For this function the sensitivity indices can be computed analytically (Saltelli and Sobol', 1995a). The partial variances of the first-order are

$$D_i = \frac{1}{3(1+a_i)^2} \tag{24}$$

Table 1
List of input parameters and their p.d.f. for the level E exercise

Notation	Definition	Distribution	Range	Units
T	Containment time	Uniform	$[100, 1000]$	yr
k_I	Leach rate for iodine	log-uniform	$[10^{-3}, 10^{-2}]$	yr^{-1}
k_C	Leach rate for Np chain nuclides	log-uniform	$[10^{-6}, 10^{-5}]$	yr^{-1}
$v^{(1)}$	Water velocity in geosphere (first layer)	log-uniform	$[10^{-3}, 10^{-1}]$	m/yr
$l^{(1)}$	Length of geosphere (first layer)	Uniform	$[100, 500]$	m
$R_I^{(1)}$	Retention factor for I (first layer)	Uniform	$[1, 5]$	—
$R_C^{(1)}$	Factor to compute ret. coeff. for Np (first layer)	Uniform	$[3, 30]$	—
$v^{(2)}$	Water velocity in geosphere (second layer)	log-uniform	$[10^{-2}, 10^{-1}]$	m/yr
$l^{(2)}$	Length of geosphere (second layer)	Uniform	$[50, 200]$	m
$R_I^{(2)}$	Retention factor for I (second layer)	Uniform	$[1, 5]$	—
$R_C^{(2)}$	Factor to compute ret. coeff. for Np (second layer)	Uniform	$[3, 30]$	—
W	Stream flow rate	log-uniform	$[10^5, 10^7]$	m^3/yr

while the higher-order partial variances are simply the product of the lower ones, i.e.

$$D_{12} = D_1 D_2. \tag{25}$$

The total variance is given by the product of the first-order terms:

$$D = -1 + \prod_{i=1}^{n} (1 + D_i). \tag{26}$$

For the numerical computations, Sobol' LPτ sequences have been used.

4.2. Level E test case

The Level E model is a very well-known test case (OECD, 1989; Robinson and Hodgkinson, 1987). It includes 12 uncertain parameters whose inputs take the form of probability distributions (see Table 1), and simulates the transport of radionuclides from an underground nuclear waste disposal, through a geosphere made of two layers of different geochemical properties, up to the biosphere and man. The processes modeled include dispersion, advection, retention and radioactive decay for the ^{129}I isotope and the ^{237}Np, ^{233}U, ^{229}Th decay chain. The output considered in the present analysis is the annual dose to man, between $t = 0$ and 10^7 yr. The model is strongly nonlinear and nonmonotonic, as indicated by the R^2 values. Even when computed on the rank transformed data, R^2 can be as low as 0.1 at some time points. Level E input is given in OECD (1989), and an analysis of its sensitivity is given in Saltelli et al. (1993) and Saltelli and Homma (1992) and Bolado et al. (1995).

5. Results and discussion

Both test cases discussed in this article can be considered as difficult for the purpose of SA. Both are nonlinear, nonmonotonic, and nonadditive in their input parameters.

5.1. The g(x) function

A set of test cases were considered where all variables were equally important: all a_i's were set equal to either 0, or 1, or 9 or 99. According to Saltelli and Sobol' (1995a) this is the most difficult case for SA. The problem dimensionality (i.e. the number of variables n) was varied between 5 and 11. Results are given in Fig. 2. Here we have plotted:

- Sobol' average first order index $\langle S_i \rangle$ at base sample size $N = 4096$. The number of model evaluation at each n is $(n + 1)N$. The average $\langle S_i \rangle$ is taken over the n variables.
- FAST average index; the sample size, equal to the number of model evaluations, was different for each n value (see Table 2)
- The analytical value (just one number: the analytical S_i values are identical given that all the a_i's are equal).
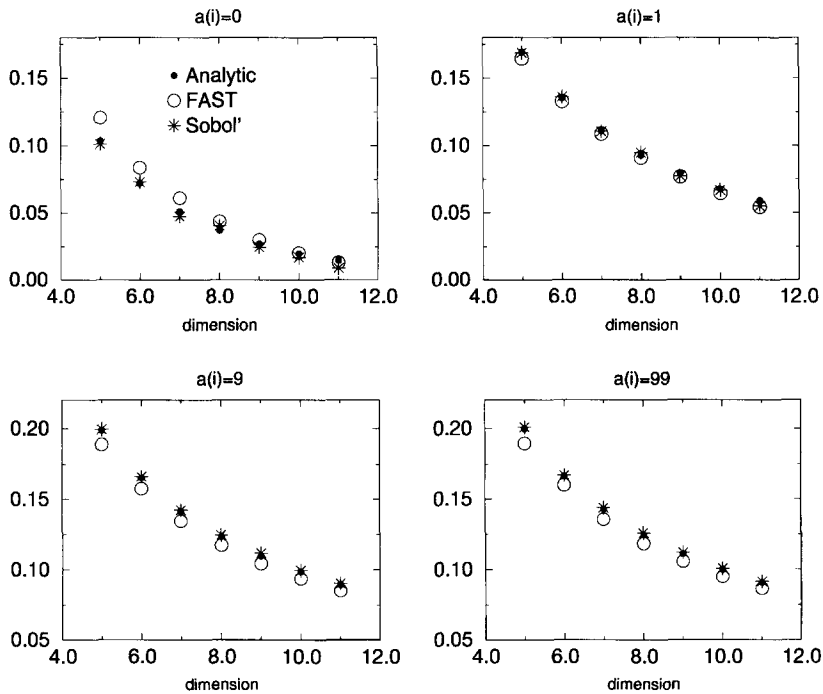

Fig. 2.

Table 2

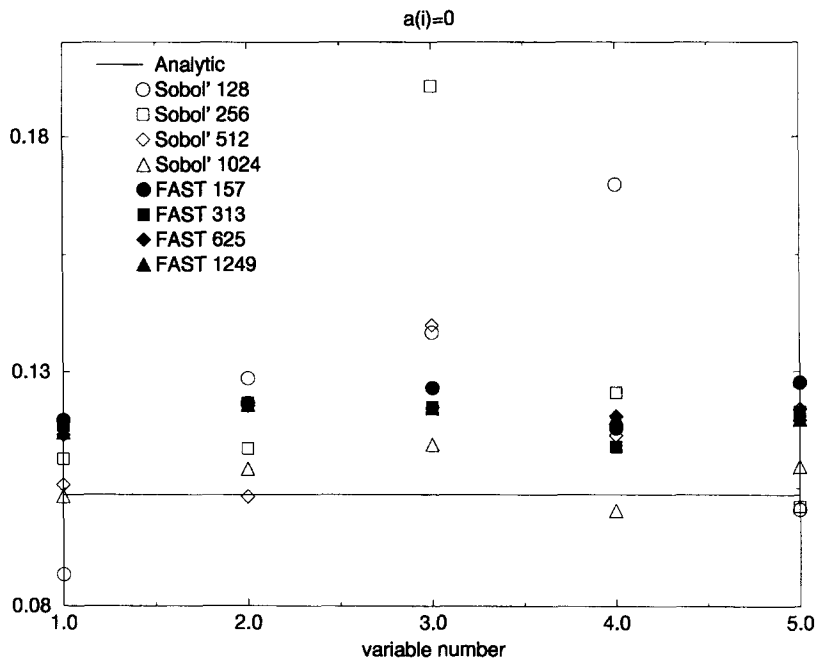| Number of variables	Sample size used	Minimum (Nyquist) size
5	313	79
6	393	99
7	697	175
8	1001	251
9	1289	323
10	1641	411
11	1977	495

Fig. 3.

There is a general agreement between the three sets of points, Sobol' giving better fit to the analytical values at such a large sample size. The effect of sample size was investigated in Fig. 3 for the $n = 5$, a_i's $= 0$ point. Here the individual indices (not averaged) are given at different sample sizes as marked in the figure. It should be kept in mind that for the computation of the Sobol' indices, the value given in the legend of Fig. 3 is N, the base sample. This must be multiplied by $(5 + 1)$ in order to obtain the total number of model evaluations. FAST appear to be fairly stable and insensitive to sample size as long as the Nyquist criterion is satisfied. FAST also shows a clear positive bias for this point (this was the worst case for FAST among those of Fig. 2). Sobol' is much more dependent on the sample size. It also appears biased toward higher values. Yet Sobol' indices converges steadily to the true value.

5.2. Level E model

The results for this test case are shown in Figs. 4 and 5. Only the four most important variables are shown, the other variables having main effect of practically zero. Sobol' was tried at base sample size $N = 1024$ and 4096. The number of model evaluations was $(12 + 1)N$, as 12 is the number of variables. FAST could be computed with as little as 587 model evaluations.

It can be seen that the main effects for this model are quite low, according to both methods. There is a general agreement between the two methods, higher for the larger Sobol' sample.

The importance of the interaction and higher-order terms for this test case is shown in Figs. 6(a)–(i), the remaining three variables being unimportant. These figures compare the main effect S_i (open circle) against the total effect S_{Ti} (full circle) for each variable.

This set of figures is particularly instructive. First, it shows that a sensitivity analysis based on the main effects alone may be misleading, especially for computational models. Unlike the experimental design settings (see e.g. Box et al., 1978), where parameters are usually varied within controlled and generally narrow ranges, in computational experiments large ranges of variation are usually explored. (A computer run is in general less expensive than a physical experiment.) The larger the range of the inputs, the lesser the model linearity and additivity.
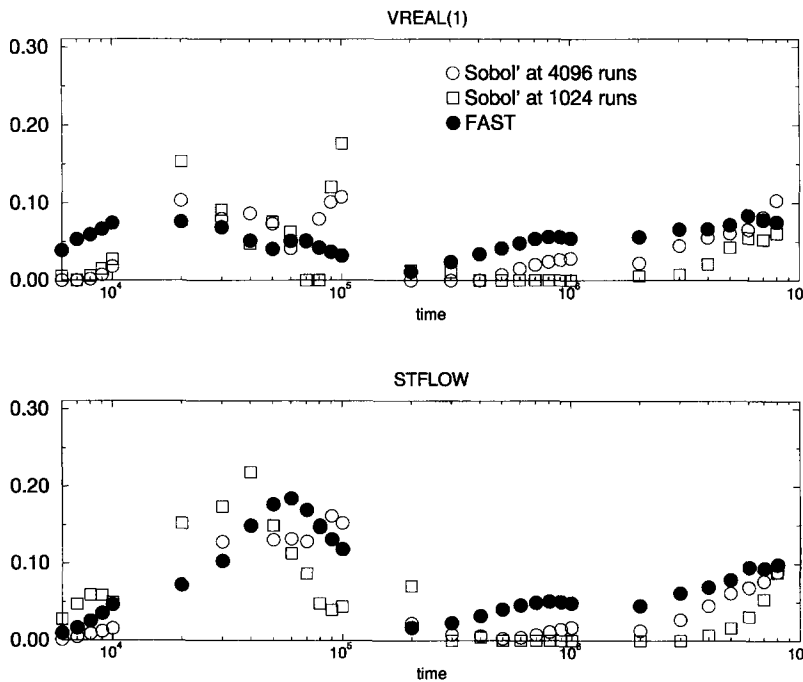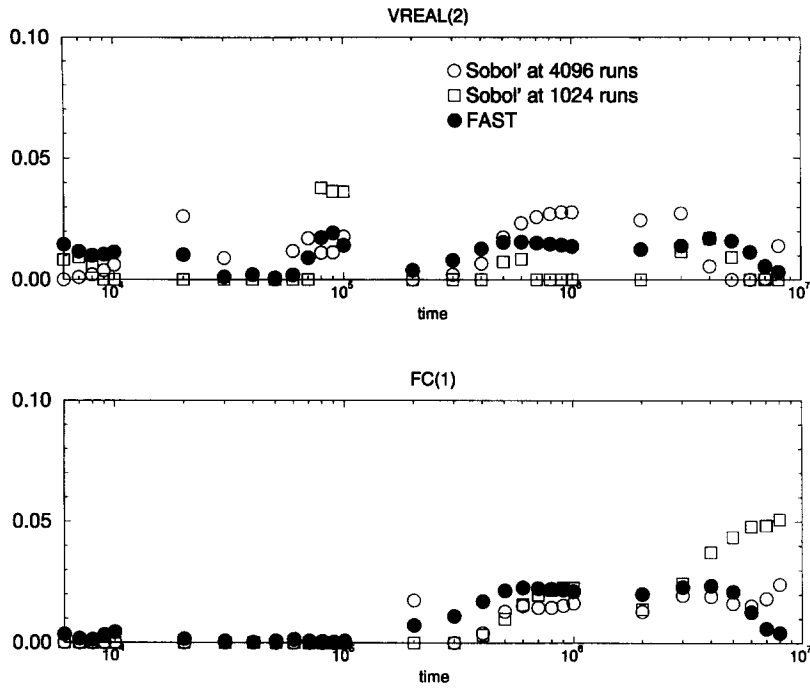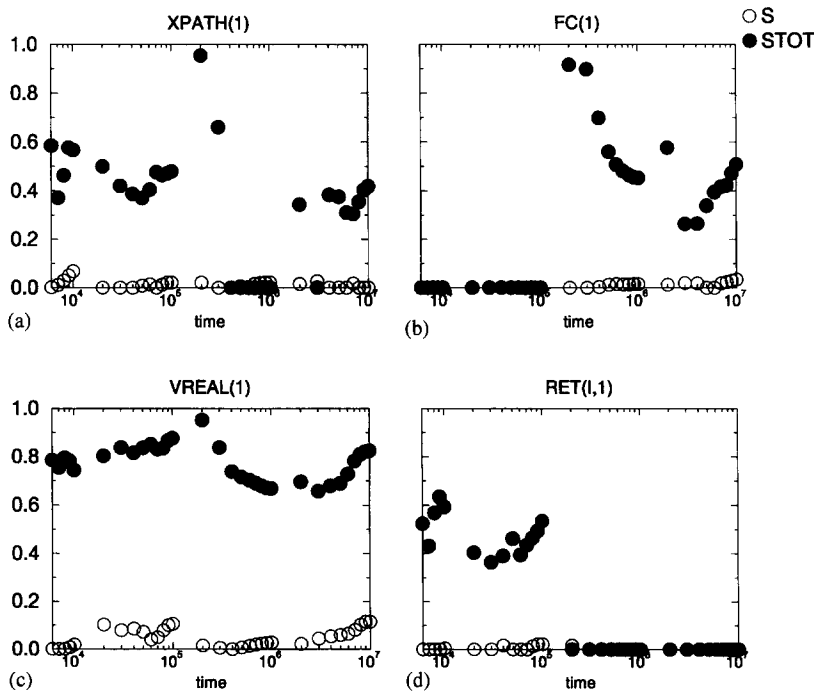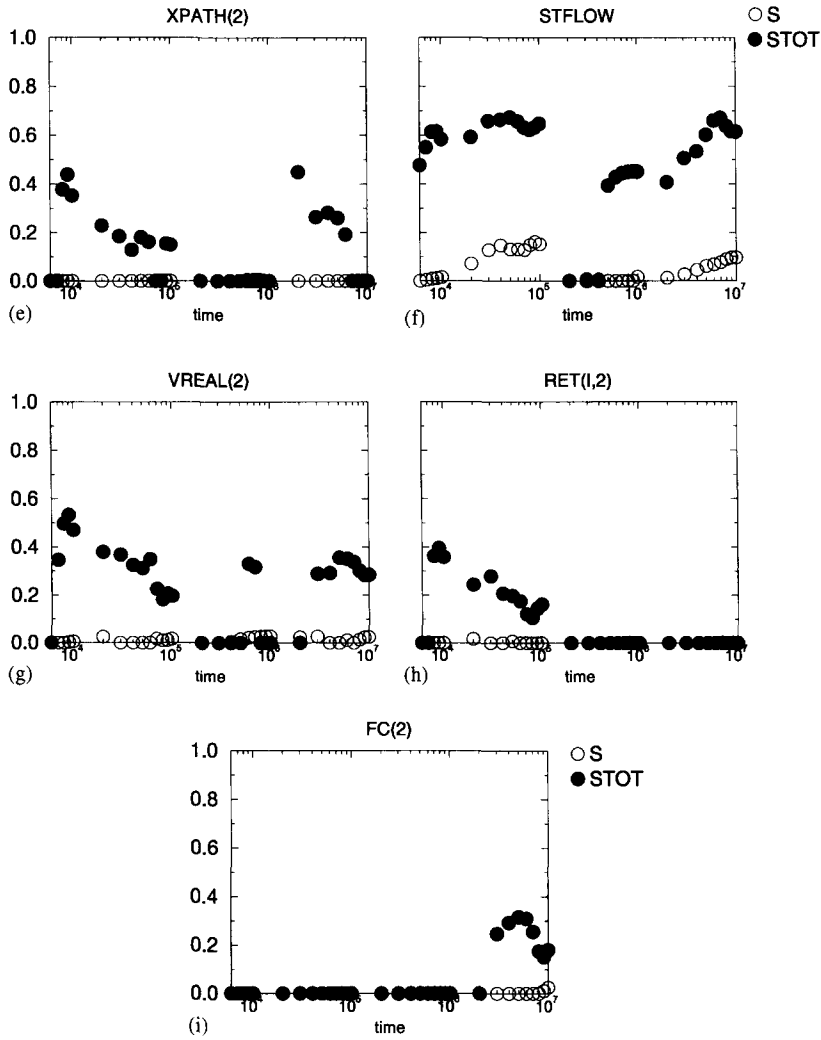

Fig. 4.

Fig. 5.

Fig. 6.

Fig. 6. (Continued)

Furthermore, a closer look at the S_{Ti} may give a considerable insight into what the important interaction (or higher-order) terms can be at the different time point. XPATH(1) at $t = 2 \times 10^5$ is likely to interact with FC(1) and VREAL(1). FC(1) interacts with STFLOW at late times, and so on.

6. Conclusions

A comparison of the predictions and of the performances of the FAST and Sobol' indices has been realised by means of a computational experiment. Both indices have been applied to two test cases at different sample sizes and/or at different problem dimensionality.

Although the computation of the two indices follow quite different routes, they can estimate the same statistical entity, i.e. the main effect contribution to the output variance decomposition in the ANOVA terminology. Our results seem to vindicate this hypothesis. The two indices tend to yield the same number when estimating the main effects.

FAST appears to be computationally more efficient, and is clearly a cheaper method to predict sensitivities associated to main effects. From the limited experience of the present study, it also seems that FAST is more prone to systematic deviations from the analytical values (bias), perhaps because of the interference problem.

Sobol' indices are computationally more expensive, although they converge to the analytical values. Furthermore, these indices provide a unique way to estimate the global effect of variables as well as interaction terms of any order.

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