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Abstract. *Covariance decomposition of output variance is used in this paper to take account of interactions between non-orthogonal components in anchored ANOVA method. Results show this approach is less sensitive to the anchor reference point than existing method. Covariance-based sensitivity indices (SI) are also used, compared to variance-based SI. Furthermore, we emphasize covariance decomposition can be generalized in a straightforward way to decompose high order moments.*

1 INTRODUCTION

The Analysis of Variance (ANOVA) expansion is an elegant and very useful way to represent multivariate functions $f(\mathbf{x})$ in high dimensions, for instance, when estimating the sensitivity indices via variance-based approaches. For independent random inputs, ANOVA from standard definition consists in a unique orthogonal decomposition of $f(\mathbf{x})$. Each component function provides its best approximation to $f(\mathbf{x})$ in a least-square sense. From computational point of view, standard orthogonal ANOVA can be very expensive when encountering very high dimensional problems and complicated multivariate functions. Indeed, the drawback of standard ANOVA consists in the need to compute the high-dimensional integrals (often requiring Monte Carlo type sampling methods). Even the zeroth-order component function requires a full-dimensional integration in the stochastic space. Alternatively, anchored ANOVA decomposition [6, 4, 11, 10] gives a computationally efficient way for the numerical evaluation of component functions in ANOVA expansion, and therefore the estimation of mean and variance of multivariate functions often become computationally much cheaper. In particular, [10] presents some adaptive

criteria as dimension reduction techniques, which can be applied to problems with a very high number of stochastic variables. One main drawback appears in such a decomposition: the accuracy of approximation is found to be very sensitive to the choice of the "anchor point". [7] show that a bad choice of the anchor point can lead to an unacceptable approximation error. This paper analyzes the reason of this sensitivity to anchor point, and proposes to use the covariance decomposition capable of evaluating very accurately the output variance of multivariate function in the framework of anchored ANOVA. This technique can be extended to compute statistical moments of arbitrary order. It is found that different (arbitrary) choices of "anchor point" lead to very close approximations. Numerical results show that the numerical solution converges very quickly to the exact solution.

The paper is organized as follows: Section 2 recalls some basic notions on the standard version of the ANOVA decomposition; we then introduce in Section 3 the anchored version of ANOVA; Section 4 is devoted to the approach proposed in this paper: a covariance decomposition of the output variance. Moreover, some covariance-based sensitivity indices are introduced. Section 5 illustrates several numerical results. Finally, conclusions are drawn and some perspectives are outlined.

2 SOME DEFINITIONS: ANOVA AND VARIANCE DECOMPOSITION

Let us introduce some notations. The upper-case letters, $\mathbf{X}$ and $\mathbf{Y}$, denote the independent random input variables and random output, respectively; the lower-case letters $\mathbf{x}$ and $\mathbf{y}$ represent the realizations. Let us suppose that the response of a given system can be represented by a N-dimensional integrable function $f(\mathbf{x})$

$$y = f(\mathbf{x}) = f(x_1, x_2, \cdots, x_N). \tag{1}$$

We consider it in its functional expansion form as follows

$$y = f_0 + \sum_{1 \leqslant i \leqslant N}^{N} f_i(x_i) + \sum_{1 \leqslant i < j \leqslant N}^{N} f_{ij}(x_i, x_j) + \cdots + f_{1,2,\cdots,N}(x_1, x_2, \cdots, x_N),$$

or in compact form using a multi index system:

$$y = f_{s_0} + \sum_{j=1}^{2^N-1} f_{s_j}(\mathbf{x}_{s_j}). \tag{2}$$

The representation (2) is called ANOVA (Analysis Of Variance) decomposition [1] of $f(\mathbf{x})$, if

$$E_{X_i}(f_{s_j}(\mathbf{X}_{s_j})) = 0 \text{ for any element variable } X_i \text{ in } \mathbf{X}_{s_j}. \tag{3}$$

It follows from (3) the orthogonality of ANOVA component terms, namely

$$E(f_{s_j} f_{s_k}) = 0, \tag{4}$$

if $j \neq k$. Note that the terms in the ANOVA decomposition can be expressed as integrals of $f(\mathbf{x})$. Indeed,

$$\begin{aligned} &E(Y) = f_0, \\ &E(Y|x_i) = f_0 + f_i(x_i), \\ &E(Y|x_i, x_j) = f_0 + f_i(x_i) + f_j(x_j) + f_{ij}(x_i, x_j), \end{aligned} \tag{5}$$

and so on. We thus observe the ANOVA terms can be computed as follows:

$$f_{s_j}(\mathbf{x}_{s_j}) = E(Y|\mathbf{x}_{s_j}) - \sum_{s_k \subset s_j} f_{s_k}, \tag{6}$$

with s_k a subset multi-index of s_j.

By integrating f^2 and exploiting the orthogonality property of component functions, the variance of f can be written as follows:

$$V(Y) = \sum_{j=1}^{\mathscr{N}} E(f_{s_j}^2(\mathbf{X}_{s_j})) = \sum_{j=1}^{\mathscr{N}} V_{s_j}, \tag{7}$$

which is in fact the sum of the variances of all the decomposition terms. Here, we have denoted $V_{s_j} = V(f_{s_j}(\mathbf{X}_{s_j}))$.

3 ANCHORED ANOVA BASED METHOD

It is noted the constant term from (5) and higher order terms from (6) can be very expensive to be computed for very high dimensional and complicated $f(\mathbf{x})$. Hence, the so-called "anchored-ANOVA" method [10, 11, 12, 6, 9] appears as a good candidate to reduce the computational cost. In this case, the Dirac measure is used instead of Lebesgue measure in integrations as follows:

$$\mathrm{d}\mu(\mathbf{x}) = \delta(\mathbf{x} - \mathbf{c})\,\mathrm{d}\mathbf{x}. \tag{8}$$

The point $\mathbf{c}$ is called "anchor point". Hence, the constant term can be expressed in a very succinct way:

$$f_0 = f(\mathbf{c}). \tag{9}$$

We refer to [11, 12] for issues related to the choices of anchor points. Generally speaking, one can arbitrarily choose this reference point. We point out that a good approximation to f should be as less sensitive as possible to this anchor point $\mathbf{c}$.

Inserting (8) into (6) leads to the result of high order terms such that:

$$f_{s_i}(\mathbf{x}_{s_i}) = f(\mathbf{c}|\mathbf{x}_{s_i}) - \sum_{s_j \subset s_i} f_{s_j}(\mathbf{x}_{s_j}). \tag{10}$$

Here $f(\mathbf{c}|\mathbf{x}_{s_i})$ represents the value of $f(\mathbf{x})$ evaluated at anchor point $\mathbf{c}$ except for the variables involved in $\mathbf{x}_{s_i}$.

Equation (10) means that only values of deterministic solver f evaluated on sampling points are needed in order to approximate the component function f_{s_i}, while with (6) one needs to evaluate multi-dimensional integrations.

Integrating (2) leads to the formula for the mean computation of $f(\mathbf{x})$:

$$E(Y) = \sum_{i=0}^{\mathscr{N}} E(f_{s_i}(\mathbf{X}_{s_i})), \tag{11}$$

which is the sum of the means of all the component functions. Indeed, $E(f_{s_i})$ can be easily evaluated by Gaussian quadrature method (see [10] for more details).

In [10] (for instance in Section *A.3. A simple example*, pages 1612-1614), they evaluate the variance of f by the sum of the variances of all the component functions, similarly as for $E(Y)$:

$$V(Y) = \sum_{i=1}^{\mathscr{N}} V_{s_i} = \sum_{i=1}^{\mathscr{N}} E([f_{s_i}(\mathbf{X}_{s_i}) - E(f_{s_i})]^2), \tag{12}$$

with V_{s_i} calculated by Gaussian quadrature rule. (12) is in fact a direct generation of (7) from the standard version of ANOVA.

4 COVARIANCE DECOMPOSITION OF THE VARIANCE $V(Y)$ AND COVARIANCE-BASED SENSITIVITY INDICES

We emphasize that the way of evaluating variance $V(f)$ in (12) can be efficient and accurate enough for a good choice of anchor point $\mathbf{c}$ [10, 11, 12, 6, 9]. However, for an arbitrary choice of $\mathbf{c}$, as we will show later in the Section devoted to numerical experiments, (12) generally gives unacceptable errors.

In this paper, we propose a more flexible way to compute the variance $V(f)$. Let us observe that the formula (12) comes from (7) which is based on standard (non-anchored) ANOVA decomposition of f. Unfortunately, in anchored ANOVA decomposition, the orthogonality property of component functions is no longer valid. That is, in general:

$$E(f_{s_i}(\mathbf{X}_{s_i}) f_{s_j}(\mathbf{X}_{s_j})) \neq 0, \text{ for } i \neq j. \tag{13}$$

In other words, for anchored decomposition, (7) should be modified in order to take (13) into account. Integrating $(Y - E(Y))^2$, variance $V(Y)$ can be computed as the sum of the covariances:

$$\begin{aligned} V(Y) &= E[(Y - E(Y))^2] = E[(\textstyle\sum_{i=1}^{\mathscr{N}} f_{s_i} - \sum_{i=1}^{\mathscr{N}} E(f_{s_i}))^2] \\ &= \textstyle\sum_{i=1}^{\mathscr{N}} [V(f_{s_i}) + \underbrace{\sum_{j=1, j\neq i}^{\mathscr{N}} \mathrm{Cov}(f_{s_i}, f_{s_j})}_{(a)}] = \sum_{i=1}^{\mathscr{N}} [\mathrm{Cov}(f_{s_i}, \textstyle\sum_{j=1}^{\mathscr{N}} f_{s_j})]. \end{aligned} \tag{14}$$

Comparing the covariance decomposition of $V(Y)$ in (14) and the variance evaluation in (12), we see the term (a) in (14) is neglected in (12), while its contribution can be

significant in general with an anchored decomposition. Indeed, the key difference of the two approaches lies in the fact that the covariance term $\mathrm{Cov}(f_{s_i}, \sum_{j=1}^{\mathscr{N}} f_{s_j})$ in (14) can even be negative. Moreover, it is observed that the covariance decomposition of the unconditional variance $V(Y)$ (14) is general. As a consequence, the result should not be sensitive to the choice of anchor point. In fact, different anchor points can lead to extremely different covariance decompositions. For this reason, methods become sensitive to anchor points, if taking account only the positive part $V(f_{s_i})$ in $\mathrm{Cov}(f_{s_i}, \sum_{j=1}^{\mathscr{N}} f_{s_j})$. As a matter of fact, these methods do not converge to the exact solution. However, a good choice of the anchor point can reduce the difference $\mathrm{Cov}(f_{s_i}, \sum_{j=1}^{\mathscr{N}} f_{s_j}) - V(f_{s_i})$, thus providing acceptable results.

Note that in the case of standard orthogonal ANOVA, where

$$\mathrm{Cov}(f_{s_i}, \sum_{j=1}^{\mathscr{N}} f_{s_j}) = V(f_{s_j}),$$

(14) degenerates into (7) or (12).

Note that a similar covariance decomposition has been considered previously, e.g. in [5], where the correlated inputs are studied and covariance decomposition is used to account for correlations among inputs. We emphasize the use of (14) in this work in the framework of anchored ANOVA for independent variables is nevertheless new.

Note the approach of covariance decomposition (14) of unconditional variance $V(Y)$ can be generalized to the decompositions of higher order statistical moments, namely skewness and kurtosis. We refer to [8] for more details.

4.1 Covariance-based sensitivity estimates using anchored ANOVA decomposition

As already mentioned, the covariance decomposition given by (14) is general for any expansion of $y = f(\mathbf{x})$ with the form (2). The variance decomposition given in (7) is in fact a special case when all component functions satisfy (3), i.e. when they are mutually orthogonal.

As similarly done in [5], three sensitivity indices are defined for a single or group of inputs $\mathbf{X}_{s_i}$:

$$\mathcal{S}^a_{s_i} = \frac{V_{s_i}}{V(Y)}, \tag{15}$$

$$\mathcal{S}^b_{s_i} = \frac{\sum_{j=1, j\neq i}^{\mathscr{N}} \mathrm{Cov}(f_{s_i}, f_{s_j})}{V(Y)}, \tag{16}$$

$$\mathcal{S}_{s_i} = \frac{\mathrm{Cov}(f_{s_i}, \sum_{j=1}^{\mathscr{N}} f_{s_j})}{V(Y)} = \mathcal{S}^a_{s_i} + \mathcal{S}^b_{s_i}. \tag{17}$$

They are related to *structural*, *correlative* and *whole* contributions of $\mathbf{X}_{s_i}$, respectively. According to (14), we have

$$\sum_{i=1}^{\mathscr{N}} \mathcal{S}_{s_i} = 1. \tag{18}$$

It is emphasized that only the structural sensitivity index $\mathcal{S}_{s_i}^a$ is strictly non-negative, which means one can obtain a negative $\mathcal{S}_{s_i}$. Note also in the special case of orthogonal ANOVA expansion, we have $\mathcal{S}_{s_i}^b = 0$.

The total effects $\mathcal{S}_i^{T,a}$, $\mathcal{S}_i^{T,b}$ and $\mathcal{S}_i^T$ of the variable X_i can be evaluated by adding all the sensitivity indices containing X_i.

5 NUMERICAL RESULTS

5.1 Sobol' function test with truncated expansion and adaptivity

The purpose of this section is to show, for academic Sobol' function, that our covariance decomposition approach converges more quickly, with respect to the truncation order of anchored ANOVA expansion, than the classical variance decomposition. Furthermore, we show, when using the adaptivity strategy for instance the variance-based one in [10], that our approach can still provide more accurate results.

We consider a 8-dimensional Sobol' function:

$$y = f(\mathbf{x}) = \prod_{k=1}^{N} f^{(k)}(x_k),\ x_k \in [0,1],\ N = 4, \tag{19}$$

where

$$f^{(k)}(x_k) = \frac{|4x_k - 2| + a_k}{1 + a_k}, a_k = k^2. \tag{20}$$

If not otherwise mentioned, 4 quadrature points for 2 elements per dimension are used. Let us choose the anchor point $\mathbf{c}_1$ as follows

$$\left\{\mathbf{c}_1 | f^{(k)}(c_k) = (V^{(k)} + (E^{(k)})^2)/E^{(k)}\right\}. \tag{21}$$

Note that (21) has been used in [10]. With blue line, Fig. 1 illustrates the relative error of mean, variance, skewness and kurtosis, obtained with our approach, as a function of the truncation order. We observe that the error is very small from order 2 except for kurtosis. However, when increasing the number of quadrature points per dimension, we see the error for kurtosis is also decreasing very fast. The red line is the variance result obtained using classical variance decomposition approach. It shows that the error does not decrease, and from order 2 it remains quasi-constant with a value of 6.75%.

Let us now evaluate our numerical approach by using a variance-based adaptivity strategy [10]. It can be found that the contributions of the first 5 components represent nearly 99% of the total first-order variance. Thus, we retain them as active dimensions from order 2. Fig. 2 presents the results for mean and variance. For the covariance decomposition of the output variance, we observe that the error is slightly bigger (constant value of 0.14% from order 2) than in Fig. 1, while the error of variance decomposition approach is more or less the same as before.

When a second anchor point $\mathbf{c}_2$ is chosen as follows

$$\{\mathbf{c}_2 | c_k = 0.5\}, \tag{22}$$

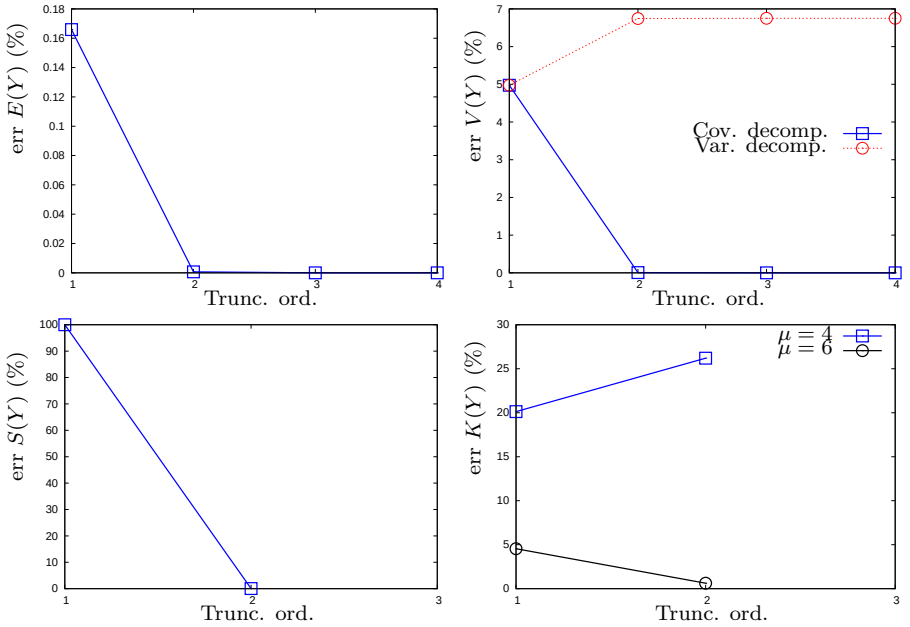

Figure 1: 8-dimensional Sobol' function test. Anchor point $\mathbf{c}_1$. Relative error of four statistics in function of truncation order of anchored ANOVA expansion.

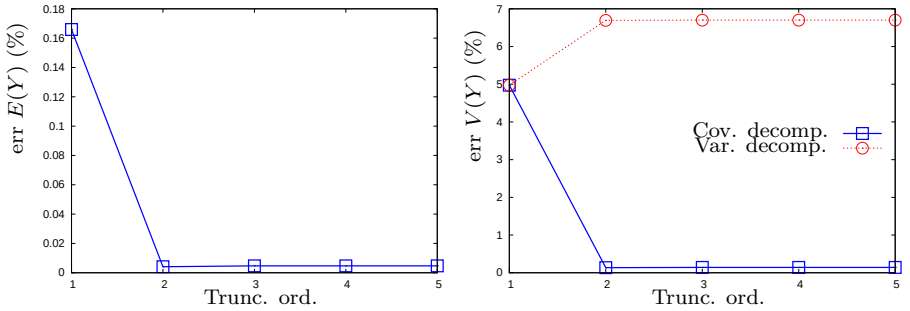

Figure 2: 8-dimensional Sobol' function test. Anchor point $\mathbf{c}_1$. Variance-based adaptive strategy is used [10]. 5 active dimensions are retained. Relative error of mean and variance in function of truncation order of anchored ANOVA expansion.

results are shown in Fig. 3. In general, mean and variance error of both approaches increases. The classical variance decomposition gives a constant error of 61.6% from order 2, while our approach for variance provides a decreasing error from order 2, with a final value of 12.2% at the 5^{th} order.

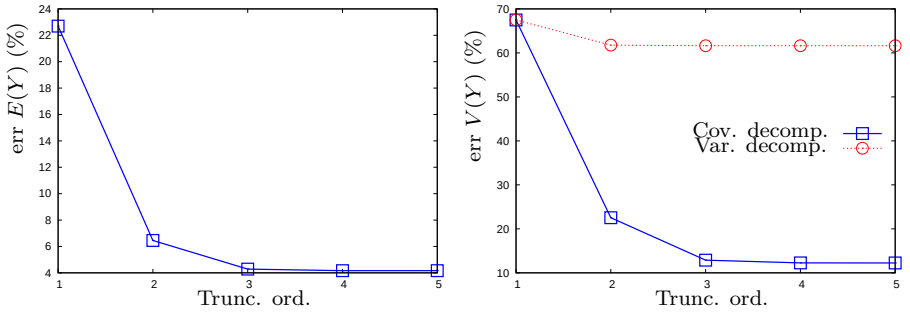

Figure 3: 8-dimensional Sobol' function test. Anchor point $\mathbf{c}_2$. Variance-based adaptive strategy is used [10]. 5 active dimensions are retained. Relative error of mean and variance in function of truncation order of anchored ANOVA expansion.

5.2 Application to the chemical reaction uncertainties during an atmospheric reentry

When considering the design of a reentry vehicle, estimating kinetic and radiative processes variability in the flow is of fundamental importance for yielding an efficient design. During the reentry phase, the spacecraft is decelerated by converting a large amount of kinetic energy into thermal energy and by inducing a strong bow shock in front of the vehicle nose. The significant increase in the gas temperature promotes strong collisions among the gas particles, changes in the chemical composition of the gas, excitation of its internal energy modes, and emission of radiation.

We focused here on the reaction rate coefficients, that are usually very uncertain, since they are difficult to measure experimentally or to estimate accurately from ab initio calculations. Detailed chemical mechanisms are necessary for an accurate heat-flux prediction but these models increase a lot the dimensionality of the stochastic space (number of uncertain parameters) with respect to conventional multi-temperature models. For this reason, efficient and low-cost uncertainty quantification methods are necessary in order to compute the most important uncertainties and to reduce the model.

One point of the heat flux trajectory is taken into account (flight path angle =-12.5^o). The stand-off distance of the shock wave is taken equal to 0.022 m. A low pressure point is considered (typically at a free stream pressure of 0.1 Torr) at high altitude and high velocity, where the ionization rate is important. Flow is taken in radiative non equilibrium (for more details see [2]).

Using this condition of the trajectory, the uncertainties on the radiative heat-flux is considered. Then, we study the interactions between the chemical reactions and their influence on the error of the radiative heat flux. The quantity of interest is the radiative heat flux at a distance corresponding to the stand-off distance for the ERC capsule.

The reaction rate coefficients of ten reactions were considered as unknown, the first six were excitation reactions and the next four were ionization. Reactions for which the rate coefficients (X_i) are considered uncertain ($\log_{10} X_i \sim \mathscr{U}(\log_{10} \min_i, \log_{10} \max_i)$) are

Reaction	ID	$\min_i$	nominal_i	$\max_i$
$N(1) + e^- \rightleftharpoons N(2) + e^-$	1	1.4476e+15	1.4476e+16	1.4476e+17
$N(1) + e^- \rightleftharpoons N(3) + e^-$	2	3.8673e+14	3.8673e+15	3.8673e+16
$N(2) + e^- \rightleftharpoons N(3) + e^-$	3	3.6169e+14	3.6169e+15	3.6169e+16
$O(1) + e^- \rightleftharpoons O(2) + e^-$	4	8.2744e+11	8.2744e+12	8.2744e+13
$O(1) + e^- \rightleftharpoons O(3) + e^-$	5	5.6319e+10	5.6319e+11	5.6319e+12
$O(2) + e^- \rightleftharpoons O(3) + e^-$	6	2.704881e+13	2.704881e+14	2.704881e+15
$N(1) + e^- \rightleftharpoons N^+ + e^- + e^-$	7	5.1688e+13	5.1688e+14	5.1688e+15
$N(2) + e^- \rightleftharpoons N^+ + e^- + e^-$	8	4.6563e+11	4.6563e+12	4.6563e+13
$O(1) + e^- \rightleftharpoons O^+ + e^- + e^-$	9	3.2477e+11	3.2477e+12	3.2477e+13
$O(2) + e^- \rightleftharpoons O^+ + e^- + e^-$	10	5.1616e+11	5.1616e+12	5.1616e+13

Table 1: Ten reactions are considered uncertain. The reaction rates are log-uniformly distributed between the minimum and maximum values.

reported in Table 1.

For simplicity, we show our results for ANOVA expansion truncated at order 2. Let us simply choose the nominal values as the anchor point. First of all, the first-order component variances can be easily computed, once the necessary deterministic sampling outputs are obtained. The results are presented in Fig. 4 (on the left). Obviously, since the ten reaction rates are considered as independent, covariance product between any two first-order component functions vanishes. Next, we can employ the variance-based adaptive criterion (see [10] for more details) in order to retain the active dimensions. Fig. 4 (on the right) shows the component variances in the descending order by comparing their contributions. We observe that the first six dimensions

$$\{X_1, X_4, X_2, X_5, X_8, X_7\} \tag{23}$$

represent about 99.9% of the total first-order variance. According to [10], these six dimensions are selected as active ones, and they are further used to calculate second-order

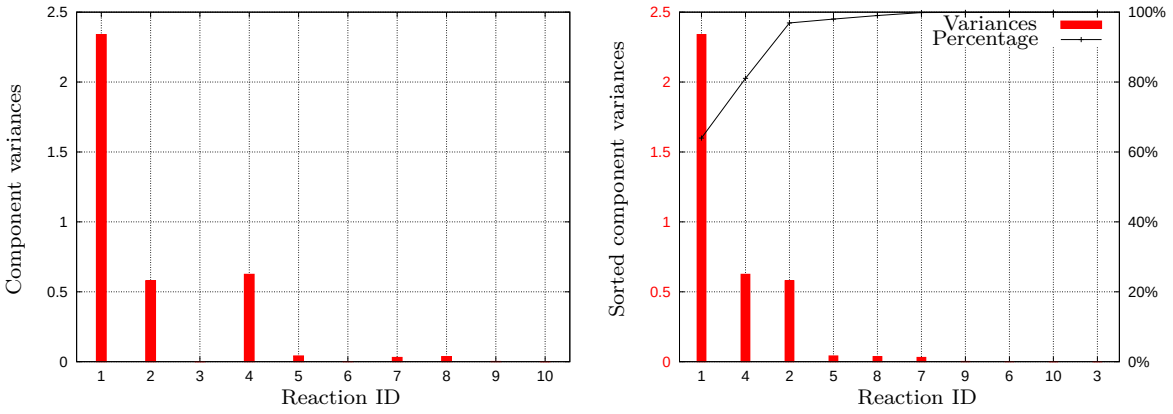

Figure 4: First-order component variances in the chemical reaction problem. On the right, the reaction ID is sorted in the descending order regarding the significance of the corresponding variance. The black line illustrates the percentage of the cumulative variance over the total first-order variance.

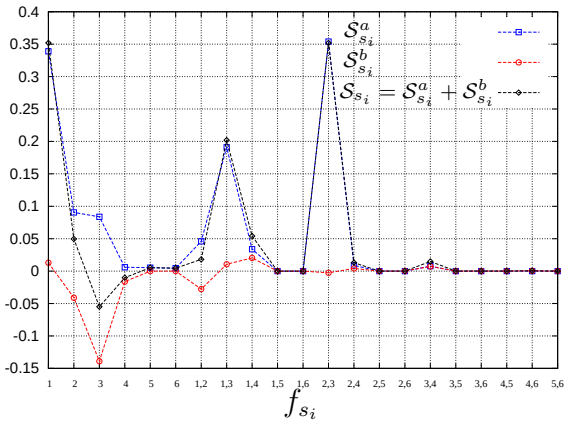

Figure 5: Covariance-based sensitivity indices for the chemical reaction problem. Only first- and second-order component functions are considered. We emphasize, in this figure, only the six active dimensions are taken into account, and there is $\sum \mathcal{S}_{s_i} = 1$. The numbering in the axis of abscissas follows (26).

interaction terms.

After computing the 10 first-order component functions and 15 second-order component functions, one can obtain the following statistics using the covariance decomposition:

$$E(Y) = 1965.42 \text{ kW/m}^2, \ V_{\text{cov}}(Y) = 6.911 \text{ (kW/m}^2)^2. \tag{24}$$

On the other hand, with the classical variance decomposition approach, the output variance is found to be

$$V_{\text{var}}(Y) = 8.090 \text{ (kW/m}^2)^2. \tag{25}$$

Note that in Section 5.1, we show that, for the academic Sobol' function, the covariance decomposition approach combined with *truncated* anchored ANOVA expansion gives more accurate results than the classical variance decomposition. As also shown in Section 5.1, this still remains true when an *adaptivity* strategy is applied in order to reduce the number of second-order component functions.

In order to better understand the difference between (24) and (25), let us focus only on six active dimensions (23). Using the new ordering of reaction rates as expressed in (26),

$$\{X'_1, X'_2, X'_3, X'_4, X'_5, X'_6\} = \{X_1, X_4, X_2, X_5, X_8, X_7\}, \tag{26}$$

Fig. 5 presents the covariance-based sensitivity indices of six active dimensions (including 6 first-order component-based indices and 15 second-order indices). We observe the second-order interaction terms

$$(X'_1, X'_3) \ = \ (X_1, X_2), \quad (X'_2, X'_3) \ = \ (X_4, X_2) \tag{27}$$

are shown to be very important compared to first-order indices. The blue line illustrates the structural indices $\mathcal{S}^a_{s_i}$ leading to the result of (25), while the black line illustrates

the whole indices $\mathcal{S}_{s_i}$ linked to the result of (24). Note finally the correlative indices $\mathcal{S}^b_{s_i}$ represented by the red line is in fact related to the difference between (24) and (25). It is observed the difference is significant for the indices corresponding to the following variables and group:

$$\begin{array}{lcl} X'_2 & = & X_4, \\ X'_3 & = & X_2, \\ (X'_1, X'_2) & = & (X_1, X_4). \end{array} \tag{28}$$

For the specific case of anchor point chosen as nominal values, classical variance decomposition approach that neglects correlative indices for (28) provides output variance quite different from covariance approach.

Finally, we have checked that the computed output variance (24) is less sensitive to anchor point than (25). For the sake of conciseness, results with other anchor points are not shown in this paper.

6 CONCLUSIONS AND PERSPECTIVES

In this paper, the standard and anchored versions of ANOVA decomposition have been reviewed. Both of them are an exact expansion of model output. Anchored ANOVA is computationally more feasible, since only sampling outputs are needed to evaluate the component functions, while numerical multi-dimensional integrations must be computed when using standard ANOVA method.

Concerning the computation of the output variance, the covariance decomposition, though requiring to resolve more integrals, provides a general exact approach which is not sensitive to the choice of anchor point, compared to the one in [10]. The covariance-based sensitivity indices are then introduced to estimate the importances of variables.

The decomposition of high order statistics can be done using anchored ANOVA without any theoretical difficulty, but is generally very prohibitive in terms of computational cost. The number of component functions $\mathscr{N}$ in ANOVA decomposition (thus also the number of statistics decomposition terms $\mathscr{M}$) increases exponentially with respect to the dimension N of deterministic solver. In order to reduce the computational cost, future work will be directed towards new adaptive criteria aiming to retain the active dimensions and the effective terms that give the most significant contributions.

Another perspective consists in proposing moment-independent sensitivity indices (see for instance [3]) within the anchored ANOVA framework.

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