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Metamodelling with independent and dependent inputs

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ABSTRACT

In the cases of computationally expensive models the metamodelling technique which maps inputs and outputs is a very useful and practical way of making computations tractable. A number of new techniques which improve the efficiency of the Random Sampling-High dimensional model representation (RS-HDMR) for models with independent and dependent input variables are presented. Two different metamodelling methods for models with dependent input variables are compared. Both techniques are based on a Quasi Monte Carlo variant of RS-HDMR. The first technique makes use of transformation of the dependent input vector into a Gaussian independent random vector and then applies the decomposition of the model using a tensored Hermite polynomial basis. The second approach uses a direct decomposition of the model function into a basis which consists of the marginal distributions of input components and their joint distribution. For both methods the copula formalism is used. Numerical tests prove that the developed methods are robust and efficient.

1. Introduction

Model based simulation of complex processes is an efficient approach of exploring and studying systems whose experimental analysis is costly or time-consuming. However, these methods generally require a large number of function evaluations to achieve reasonable convergence and can become impractical for large engineering problems.

One of the very important and promising developments of model analysis is the replacement of complex models and models which need to be run repeatedly on-line with metamodels (also known as surrogate models).

There are different classes of metamodelling methods. Methods which make use of a statistical framework (Kriging, Gaussian processes, Radial Basis Functions) have become very popular with practitioners [1–3]. In this paper we consider a different class of metamodelling methods based on orthogonal polynomial decompositions.

For many practical problems only low order interactions of the input variables are important. By exploiting this feature one can dramatically reduce the computational time for modeling such systems. The Random Sampling-High Dimensional Model Representation (RS-HDMR) method originally developed by Rabitz and co-authors [4,5] has become a popular tool for building metamodels [6]. Unlike other input–output mapping methods HDRM renders the original exponential difficulty to a problem of only polynomial complexity.

RS-HDMR can also be used for global sensitivity analysis (GSA). GSA methods evaluate the effect of a factor while all other factors are varied as well and thus they account for interactions between variables and do not depend on the choice of a nominal point like local sensitivity analysis methods. Reviews of different GSA methods can be found in [7–9].

RS-HDMR belongs to a wider class of methods known as polynomial chaos expansion (PCE). A good review of PCE methods can be found in [10,11].

The majority of known methods are designed only for models with independent input variables. However, in practical applications input variables are often dependent.

The objective of this work is twofold: Firstly we present a number of new techniques which improve the efficiency of the RS-HDMR method for models with independent input variables. Secondly, we present and compare two different metamodelling techniques for models with dependent input variables.

The main difference with the traditional RS-HDMR is that we use the Quasi Monte Carlo (QMC) method based on low-discrepancy sequences (LDS) instead of random numbers for numerical integration, therefore it is called Quasi Random Sampling-High Dimensional Model Representation (QRS-HDMR). We also introduce a new technique for determination of an optimal polynomial order and a required number of sampled points to achieve a given tolerance.

For models with dependent input variables we consider two different methods. The first method consists of transforming the dependent input vector into an independent random vector and then

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applying a methodology developed for the case of independent inputs. This method is applicable in the case of inputs correlated using a Gaussian copula. We present all important steps of this method including the transformation between the original values of correlation coefficients and the transformed ones (this step was not discussed in [12] where this method was first presented). The second method is based on the direct decomposition of the model function using a basis depending on the marginal distributions of the input components and their joint distribution. It can be used with any types of copula. This method was suggested in [13], however as far as we know it has never been used in practice before. We compare two methods on representational benchmark examples.

This paper is organized as follows. The next section introduces ANOVA–HDMR decomposition. Section 3 gives an overview of global sensitivity indices. Section 4 presents the polynomial approximation method for the RS-HDMR component functions. Evaluation of SI based on RS-HDMR is discussed in Section 5. Numerical recipes concerned with determination the optimal number of sampled points and the maximum order of polynomials are discussed in Section 6. Section 7 presents the PCE method for models with independent inputs. Section 8 describes two method capable of dealing with the case of dependent input variables. Truncation of the PCE is discussed in Section 9. Section 10 presents two different methods for approximating PCE expansion coefficients. The results of numerical experiments are given in Section 11. Finally, conclusions are presented in Section 12.

2. ANOVA–High Dimensional Model Representation

Consider an integrable function $f(\mathbf{x})$ defined in the unit hypercube H^d. It can be expanded in the following form:

$$f(\mathbf{x}) = f_0 + \sum_{s=1}^{d} \sum_{i_1<\cdots<i_s}^{s} f_{i_1,\ldots,i_s}(x_{i_1},\ldots,x_{i_s}). \tag{1}$$

Each of the components $f_{i_1,\ldots,i_s}(x_{i_1},\ldots,x_{i_s})$ is a function of a unique subset of variables from $\mathbf{x}$. The components $f_i(x_i)$ are called first order terms, $f_{ij}(x_i, x_j)$—second order terms and so on.

It can be proven [14] that the expansion (1) is unique if

$$\int_0^1 f_{i_1,\ldots,i_s}(x_{i_1},\ldots,x_{i_s})dx_{i_k} = 0, \quad 1 \le k \le s,\ 1 \le s \le d \tag{2}$$

in which case it is known as the ANOVA–HDMR decomposition. It follows from condition (2) that the ANOVA–HDMR decomposition is orthogonal.

Rabitz argued [4,5] that for many practical problems only the low order terms in the ANOVA–HDMR decomposition are important and $f(\mathbf{x})$ can be approximated by

$$\hat{f}(\mathbf{x}) = f_0 + \sum_{s=1}^{p} \sum_{i_1<\cdots<i_s}^{s} f_{i_1,\ldots,i_s}(x_{i_1},\ldots,x_{i_s}). \tag{3}$$

Here p is a truncation order, which for many practical problems can be equal to 2 or 3.

3. Global sensitivity indices based on the Sobol method

The ANOVA–HDMR decomposition (1) can be used to measure the sensitivity of the model output with respect to the inputs or subsets of input variables. Global sensitivity indices (SI) are defined as follows [7,15]. Assume that $f(\mathbf{x})$ is square integrable. In this case all the $f_{i_1,\ldots,i_s}$ are also square integrable. Squaring (1) and integrating over H^d the following expression can be obtained using orthogonality of the component functions:

$$\int f^2(\mathbf{x})d\mathbf{x} - f_0^2 = \sum_{s=1}^{d} \sum_{i_1<\cdots<i_s} \int f^2_{i_1,\ldots,i_s} dx_{i_1}\ldots dx_{i_s}. \tag{4}$$

The constants

$$D = \int f^2(\mathbf{x})d\mathbf{x} - f_0^2, \qquad D_{i_1,\ldots,i_s} = \int f^2_{i_1,\ldots,i_s} dx_{i_1}\ldots dx_{i_s} \tag{5}$$

are called total variance and partial variances correspondingly.

The ratios

$$S_{i_1,\ldots,i_s} = D_{i_1,\ldots,i_s}/D \tag{6}$$

are called global sensitivity indices (SI) [15]. From (4)–(6) it follows that

$$\sum_{s=1}^{d} \sum_{i_1<\cdots<i_s} S_{i_1,\ldots,i_s} = 1. \tag{7}$$

Straightforward calculation of SI using the ANOVA–HDMR decomposition would result in 2^d integral evaluations. For high dimensional problems such an approach is impractical. Homma and Saltelli [16] introduced the SI for subsets of variables and the total SI. In [15] Sobol suggested efficient formulas for calculation of SI. This approach for SI calculation is known as the Sobol method. These formulas were further improved in [13] and [17]. They allow for more accurate estimates with a lower computational cost.

4. Approximation of ANOVA–HDMR component functions

The RS-HDMR method proposed in [4,5] aims to reduce the sampling effort by approximating the component functions using an expansion in terms of a suitable set of functions such as orthonormal polynomials.

Consider piecewise smooth and continuous component functions of the ANOVA–HDMR decomposition. Using a complete basis set of orthonormal polynomials they can be expressed via the expansion:

$$f_i(x_i) = \sum_{r=1}^{\infty} \alpha_r^i \phi_r(x_i), \tag{8}$$

$$f_{ij}(x_i, x_j) = \sum_{k=1}^{\infty}\sum_{l=1}^{\infty} \beta_{kl}^{ij} \phi_{kl}(x_i, x_j), \tag{9}$$

$\ldots.$

Here $\phi_r(x_i)$, $\phi_{kl}(x_i, x_j)$ are sets of one and two-dimensional basis functions and α_r^i and β_{kl}^{ij} are coefficients of decomposition which can be determined using orthogonality of the basis functions:

$$\alpha_r^i = \int_0^1 f_i(x_i)\phi_r(x_i)dx_i, \tag{10}$$

$$\beta_{kl}^{ij} = \int_0^1\int_0^1 f_i(x_i)\phi_k(x_i)\phi_l(x_j)dx_i dx_j.$$

In practice the summation in (8) and (9) is limited to some maximum orders k_m, l_m, l'_m:

$$f_i(x_i) \approx \sum_{r=1}^{k_m} \alpha_r^i \phi_r(x_i), \tag{11}$$

$$f_{ij}(x_i, x_j) \approx \sum_{k=1}^{l_m}\sum_{l=1}^{l'_m} \beta_{kl}^{ij} \phi_{kl}(x_i, x_j), \tag{12}$$

$\ldots.$

The question of how to find maximum orders is discussed in the following sections. In this paper we use the shifted Legendre polynomials which are orthogonal in the interval [0, 1] with unit weight in the case of uniformly distributed inputs and the Hermite polynomials which are orthogonal on $\mathbb{R}$ with Gaussian weight in the case of normally distributed inputs. The higher dimensional polynomials can be expressed as the product of one dimensional ones.

4.1. Function approximation errors

Consider an approximation error $\delta(f,\hat{f})$ defined as

$$\delta(f,\hat{f}) = \frac{1}{D}\int [f(\mathbf{x}) - \hat{f}(\mathbf{x})]^2 d\mathbf{x}. \tag{13}$$

An important theorem establishing relationship between δ and the sensitivity indices in the case of independent inputs was proven in [18]: if $f(\mathbf{x})$ is approximated by a pth order RS-HDMR, then

$$\delta(f,\hat{f}) = 1 - \sum_{s=1}^{p} \sum_{i_1<\cdots<i_s} S_{i_1,\ldots,i_s}. \tag{14}$$

Consider $p = 2$, assuming that $\delta(f,\hat{f})$ is small, hence

$$\sum_i S_i + \sum_{i<j} S_{ij} \approx 1. \tag{15}$$

If higher than $p = 2$ order interactions are important, then $\delta(f,\hat{f})$ is large and condition (15) is not satisfied. In this case one should include higher order interactions ($p = 3$) and again check condition similar to (15) with inclusion of the third order SI or use a technique suggested in [19], which in principle is capable of detecting and accounting for any order interactions.

5. Evaluation of global sensitivity indices based on RS-HDMR

For a continuous function defined in the unit hypercube H^d with piecewise derivatives the following relationship exists between the square of the function and the coefficients of its decomposition c_r with respect to a complete set of orthonormal polynomials (Parseval's theorem):

$$\int_0^1 f(x)^2 dx = \sum_{r=1}^{\infty} (c_r)^2. \tag{16}$$

An application of Parseval's theorem to the component functions of ANOVA–HDMR (8)–(9) yields the following formulas for partial variances:

$$D_i = \sum_{r=1}^{\infty} (\alpha_r^i)^2, \tag{17}$$

$$D_{ij} = \sum_{k=1}^{\infty}\sum_{l=1}^{\infty} (\beta_{kl}^{ij})^2. \tag{18}$$

Consequently, in the case of independent inputs from definitions of SI (6) we obtain

$$S_i = \frac{\sum_{r=1}^{\infty} (\alpha_r^i)^2}{D}, \tag{19}$$

$$S_{ij} = \frac{\sum_{k=1}^{\infty}\sum_{l=1}^{\infty} (\beta_{kl}^{ij})^2}{D}, \tag{20}$$

where total variance D is calculated using the original function evaluations. These formulas are a direct result of polynomials orthogonality in the ANOVA–HDMR decomposition. For practical purposes, summations truncated at some maximum order of polynomials are used similarly to (11)–(12).

6. How to choose the maximum order of polynomials

An important problem is how to choose an optimal order of the orthogonal polynomials. In the majority of published works by Rabitz and co-authors the fixed order polynomials (up to the second or third order) were used. However, in some cases polynomials up to the tenth order were used (see f.e. results for the Ishigami function (47) in Section 11). Although no explanation for the choice of such high order polynomials was given.

This problem of an optimal maximum order polynomials was considered by Ziehn and Tomlin in [6]. They proposed to use an optimization method to choose the best polynomial order for each component function. Ziehn and Tomlin also suggested to exclude any component function from the HDMR expansion which do not contribute to the HDMR expansion. The overheads for using an optimization method can be considerable. We suggest a different approach to define optimal polynomial orders based on the estimated convergence of partial variances.

Another important issue is how to define a sufficient number of sampling points in MC or QMC integration of the polynomial coefficients (10)–(11). In a limit

$$\lim_{\substack{k_m\to\infty \\ N\to\infty}} \sum_{r=1}^{k_m} (\hat{\alpha}_r^i(N))^2 = D_i, \tag{21}$$

where $\hat{\alpha}_r^i(N)$ is a numerical approximation of $\alpha_r^i(N)$ (the same asymptotic rule apply for other coefficients). Practically the accuracy of coefficients approximation depends on the number of sampled points $N : \hat{\alpha}_r^i = \hat{\alpha}_r^i(N)$. Typically, the higher the order of the component function, the greater the number of sampled points required to evaluate the polynomial coefficients with sufficient accuracy [4].

Typically the values of decomposition coefficients α_r^i, β_{kl}^{ij} etc. rapidly decrease with increasing the order of r and (k,l). As a result the truncation error is dominated by the first few truncation coefficients. To determine an optimal number of points N_{opt} the variance of $\hat{\alpha}_r^i$ is calculated as a function of N. N is increased sequentially and N at which a required tolerance of the variance is reached is taken as N_{opt}. We found that in most cases it is sufficient to monitor $\hat{\alpha}_r^i(N)$ at $r = 1, 2$. Similarly, the variance of $\hat{\beta}_{kl}^{ij}(N)$ can be monitored although it makes the algorithm more complex.

After a sufficient number of function evaluations N_{opt} is made, we monitor the convergence of the first order estimated partial variances with respect to the polynomial degree. At the fixed maximum polynomial degree k

$$D_i(k) = \sum_{r=1}^{k} (\hat{\alpha}_r^i)^2. \tag{22}$$

Consider the difference between $D_i(k+1)$ and $D_i(k)$:

$$D_i(k+1) - D_i(k) = (\hat{\alpha}_{k+1}^i)^2. \tag{23}$$

The following procedure is used for determining the maximum polynomials degree required to achieve sufficiently accurate values of the partial variances D_i's: for a given accuracy ϵ find k such that

$$\frac{(\hat{\alpha}_{k+1}^i)^2}{D_i(k+1)} < \epsilon \quad \text{and} \quad \frac{(\hat{\alpha}_{k+2}^i)^2}{D_i(k+2)} < \epsilon \quad \text{if } D_i(k+1) > 10^{-3},$$

$$(\hat{\alpha}_{k+1}^i)^2 < \epsilon \quad \text{and} \quad (\hat{\alpha}_{k+2}^i)^2 < \epsilon \quad \text{if } D_i(k+1) \le 10^{-3}. \tag{24}$$

Note, that to avoid isolated zeros we check that not only contributions of α_{k+1}^i but also those of α_{k+2}^i are small. It guarantees the robustness of the algorithm for the case when the main order component has only odd or even orders of the polynomials in the decomposition (8).

For the second order component functions the procedure is more complex because it requires monitoring convergence in a 2-dimensional space of k and l polynomial orders. Details of this procedure will be presented elsewhere.

We note that an approximation error $\delta(f,\hat{f})$ (13) has other sources of errors additional to the ones caused by neglecting the terms higher than order p in the ANOVA–HDMR decomposition. These are caused by the polynomials being truncated to some

maximum order and numerical estimation of coefficients $\hat{\alpha}_r^i(N)$ and $\hat{\beta}_{kl}^{ij}(N)$ by MC/QMC integration. Further we reflect this fact in the notation $\hat{\delta} : \hat{\delta} \approx \delta(f, \hat{f})$.

7. Polynomial chaos expansion with independent random inputs

In the previous sections the input vector $\mathbf{x}$ defined in H^d was considered either deterministic or uniformly distributed. In the general context of uncertainty propagation, $\mathbf{x}$ is considered as a random vector and will be denoted $\mathbf{X}$ further. The cumulative distribution function (CDF) for each component X_i, denoted H_{X_i}, is supposed to be known. In this case the presented above RS-HDRM technique can be used after a transformation of $\mathbf{X}$ into a random input $\mathbf{U}$ uniformly distributed on H^d is made. This transformation is performed on a component by component basis, namely by applying H_{X_i} to X_i. Consequently, $U_i = H_{X_i}(X_i)$ is uniformly distributed on H^d for all i and $f(\mathbf{X}) = f[H_{X_1}^{-1}(U_1), \ldots, H_{X_d}^{-1}(U_d)]$. Finally, we apply the RS-HDMR technique to the function composed of f and the previous transformation. We notice, that the sensitivity indices derived after the transformation can directly be interpreted on the initial "physical" variables due to their independence.

The idea of the PCE technique is to expand $f(\mathbf{X})$ using a suitable Hilbertian polynomial basis (without prior ANOVA–HDMR decomposition). For instance, when the input $\boldsymbol{\xi}$ is a standard normal vector and $f(\boldsymbol{\xi})$ is square integrable then the multivariate Hermite polynomials are a suitable basis being orthogonal with respect to the Gaussian measure. In this case, $f(\boldsymbol{\xi})$ is expanded as follows:

$$f(\boldsymbol{\xi}) = \sum_{j=1}^{+\infty} a_j^{\boldsymbol{\xi}} \psi_j(\boldsymbol{\xi}), \tag{25}$$

where ψ_j are the multivariate Hermite polynomials and $a_j^{\boldsymbol{\xi}}$ are the decomposition coefficients.

If the input random vector has an arbitrary joint probability distribution function (PDF) it is in general not possible to transform it directly into a standard normal or another random vector with a known distribution. However, when the input vector has arbitrary independent random components with known CDF, it is possible to transform each component X_i into a selected random variable Z_i with the same CDF G, (i.e. $G_{Z_i} = G, \ \forall i$) and for which a Hilbertian basis ψ_i is known. Hence, the choice of the Hilbertian basis depends on the selected measure associated with G. Once the transformation is made, the transformed function can be expanded using the selected basis. Formally, $Z_i = G^{-1} \circ H_{X_i}(X_i)$ has CDF G and inversely $X_i = H_{X_i}^{-1} \circ G(Z_i)$ has CDF H_{X_i} and the PCE is given by

$$\begin{aligned} f(X_1, \ldots, X_d) &= f\left(H_{X_1}^{-1}[G(Z_1)], \ldots, H_{X_d}^{-1}[G(Z_d)]\right) \\ &= \sum_{j=1}^{+\infty} a_j^G \psi_j^{1,G}(Z_1) \ldots \psi_j^{d,G}(Z_d), \end{aligned} \tag{26}$$

where $\psi_j^{i,G}$ are the univariate polynomials orthogonal with respect to the measure given by G and a_j^G are the coefficients of the decomposition. Notice that the PCE is not performed on the function f in its original form but on the function after the transformation. This technique is known as the generalized PCE [11].

In practice, as shown in (26) the multivariate orthogonal polynomials are expressed as the product of one dimensional ones. The coefficients a_j^G can be estimated by MC, QMC or regression methods. The decomposition needs to be truncated to a suitable order, i.e. an order offering a reasonable compromise between a good approximation and a feasible computational time. More details are given in Section 8.

Notice that if for each CDF H_{X_i} a corresponding univariate orthogonal basis $\boldsymbol{\psi}^{H_i}$ is known then the PCE can be made without a transformation as follows [20]:

$$f(X_1, \ldots, X_d) = \sum_{j=1}^{+\infty} a_j^H \psi_j^{H_1}(X_1), \ldots, \psi_j^{H_d}(X_d). \tag{27}$$

8. Dependent inputs

In this section we consider two different methods for dealing with the case of dependent inputs. Further, we use the following indexation for the PCE:

$$\sum_{j=1}^{+\infty} a_j \psi_j^1(X_1), \ldots, \psi_j^d(X_d) = \sum_{\boldsymbol{\gamma} \in \mathbb{N}^d} a_{\boldsymbol{\gamma}} \psi_{\gamma_1}(X_1), \ldots, \psi_{\gamma_d}(X_d). \tag{28}$$

Similarly to the ANOVA–HDMR decomposition, all terms of the expansion indexed by $\boldsymbol{\gamma} = (\gamma_1, \ldots, \gamma_d)$ in which only one of the γ_i's is not-zero are called the first order expansion terms. All terms of the expansion indexed by $\boldsymbol{\gamma} = (\gamma_1, \ldots, \gamma_d)$ in which only two different γ_i's are not-zero at the same time are called the second order expansion terms and so on. For a given order, the degree of the polynomial $\psi_{\gamma_i}(X_i)$ is the value of the corresponding γ_i.

We note, that in the case of dependent inputs SI cannot be computed using the straightforward ANOVA decomposition and a different approach based on generalization of Sobol' formulas should be used in this case [21].

8.1. Transformation from dependent to independent input vector

The main idea of this method is to transform when possible the dependent random vector $\mathbf{X}$ into a Gaussian or a uniform vector with independent components. This transformation is feasible for instance when the marginal distributions of $\mathbf{X}$ and the correlation matrix $\Sigma^{\mathbf{X}}$ are known. The copula theory [22] is commonly used to link the structural dependence and marginal CDFs. Sklar's theorem [22] gives the following relationship

$$H_{\mathbf{X}}(\mathbf{X}) = C\big(H_1(X_1), \ldots, H_d(X_d)\big), \tag{29}$$

where $H_{\mathbf{X}}$ is the CDF of $\mathbf{X}$ and C is the copula associated with $\mathbf{X}$. $C\big(H_1(x_1), \ldots, H_d(x_d)\big)$ is a d-dimensional uniform CDF on H^d with uniformly distributed margins.

In order to get an independent Gaussian random vector the following transformation is made: define the transformation $T_1 : \mathbb{R}^d \to \mathbb{R}^d$, where Φ is a Gaussian distribution function, such that:

$$\bar{\boldsymbol{\xi}} = T_1(\mathbf{X}) = \left(\Phi^{-1}\big[H_1(X_1)\big], \ldots, \Phi^{-1}\big[H_p(X_p)\big]\right) \tag{30}$$

is a multivariate Gaussian random vector with standard random marginals. This transformation has been presented in [23] and it is known as the Nataf transformation. We denote $\Sigma^{\bar{\boldsymbol{\xi}}}$ the correlation matrix of $\bar{\boldsymbol{\xi}}$ which is supposed to be positive definite. The latter is linked to the original correlation matrix $\Sigma^{\mathbf{X}}$ via the following relationship between correlation coefficients $\rho_{i,j}^{\mathbf{X}}$ and $\rho_{i,j}^{\bar{\boldsymbol{\xi}}}$

$$\begin{aligned} \rho_{i,j}^{\mathbf{X}} = \frac{1}{\sigma_{X_i}\sigma_{X_j}} \int_{\mathbb{R}^2} &\left(H_i^{-1}\big[\Phi(\bar{\xi}_i)\big] - \mu_i^X\right) \\ &\times \left(H_j^{-1}\big[\Phi(\bar{\xi}_j)\big] - \mu_j^X\right) \varphi_2\big(\bar{\xi}_i, \bar{\xi}_j, \rho_{i,j}^{\bar{\boldsymbol{\xi}}}\big) d\bar{\xi}_i d\bar{\xi}_j. \end{aligned} \tag{31}$$

It was shown in [24] that the following relationship between both correlation coefficients can be used:

$$\rho_{i,j}^{\bar{\boldsymbol{\xi}}} = \rho_{i,j}^{\mathbf{X}} F(\rho_{i,j}^{\mathbf{X}}, \delta_i^{\mathbf{X}}, \delta_j^{\mathbf{X}}, H_i, H_j), \tag{32}$$

where $\delta_i^{\mathbf{X}}$ is the coefficient of variation of X_i and the function $F \geq 1$ is determined by the least square fitting of polynomial expressions to exact values computed by numerical integration of Eq. (31).

To obtain a standard Gaussian uncorrelated random vector we can use the transformation T_2 defined as

$$\boldsymbol{\xi} = T_2(\bar{\boldsymbol{\xi}}) = C^{-1}\bar{\boldsymbol{\xi}}, \tag{33}$$

where C is the Cholesky decomposition matrix of $\Sigma^{\bar{\boldsymbol{\xi}}}$ [25] and $\boldsymbol{\xi}$ is a standard Gaussian uncorrelated random vector. The use of the transformation into Gaussian random vector is justified here by the fact that the mathematical equivalence between uncorrelated and independent random vectors only stands for Gaussian random vectors. Hence, the transformation

$$\boldsymbol{\xi} = T_{\text{Gauss}}(\mathbf{X}) = T_2 \circ T_1(\mathbf{X}) \tag{34}$$

allows to get the standard independent Gaussian random vector $\boldsymbol{\xi}$ from the dependent random vector $\mathbf{X}$. An additional step is required in order to get an independent random vector uniformly distributed on H^d. It is given by the transformation T_{Unif} defined as:

$$T_{\text{Unif}}(\mathbf{X}) = (\Phi(\xi_1), \ldots, \Phi(\xi_d)). \tag{35}$$

Once this transformation is applied, the methodology for the independent Gaussian case presented in Section 7 can be used to get the following PCE:

$$f(\mathbf{X}) = f \circ T_{\text{Gauss}}^{-1}(\boldsymbol{\xi}) = \sum_{\boldsymbol{\gamma}\in\mathbb{N}^d} a_{\boldsymbol{\gamma}} \psi_{\gamma_1}(\xi_1), \ldots, \psi_{\gamma_d}(\xi_d). \tag{36}$$

Notice that by using the Nataf transformation we assume that the dependence structure of $\mathbf{X}$ is given by a Gaussian copula [26]. It is important to note that the Gaussian copula does not have tail dependence [27]. Therefore, this choice of copula could lead to misleading results if the real structural dependence of $\mathbf{X}$ has tail dependence [26]. In this case, other copulas such as i.e. Archimedean can be used, however the application of the method presented in this section is limited only to the Gaussian copula.

Further we will refer to the method presented in this subsection as Method I.

8.2. Method with direct expansion

A mathematical framework for developing polynomial chaos expansions of any model characterized by any square integrable function with dependent input variables was proposed in [20]. Let $\mathbf{X} = (X_1, \ldots, X_d)$ be any d-dimensional random vector associated with the distribution measure $\nu_{\mathbf{X}}$ with the joint PDF $h_{\mathbf{X}}$. The marginal distributions of random variables X_i are respectively associated with the measure $\nu_{\mathbf{X}_i}$ and the PDF h_{X_i}. We denote $L^2(\mathbb{R}^d, \mathbb{R}, \nu_{\mathbf{X}})$ the space of square integrable functions (equipped with its Borel field), from $\mathbb{R}^d$ into $\mathbb{R}$, with respect to the probability measure $\nu_{\mathbf{X}}$. Consider the standard inner product on $L^2(\mathbb{R}^d, \mathbb{R}, \nu_{\mathbf{X}})$ defined for all functions in $L^2(\mathbb{R}^d, \mathbb{R}, \nu_{\mathbf{X}})$ as

$$\mathbb{E}(g_1(\mathbf{X})g_2(\mathbf{X})) = \int g_1(\mathbf{x})g_2(\mathbf{x})d\nu_{\mathbf{X}}(\mathbf{x}). \tag{37}$$

$L^2(\mathbb{R}^d, \mathbb{R}, \nu_{\mathbf{X}})$ with the inner product (37) is a Hilbert space. We can determine a Hilbertian basis of this space, i.e. find a countable set of orthonormal functions which spans $L^2(\mathbb{R}^d, \mathbb{R}, \nu_{\mathbf{X}})$. In the same way we define $L^2(\mathbb{R}, \mathbb{R}, \nu_{X_i})$ for $i = 1, \ldots, d$ equipped with the standard inner product with respect to ν_{X_i}.

We denote $\boldsymbol{\gamma} = (\gamma_1, \ldots, \gamma_d) \in \mathbb{N}^d$ a set of indices. Then, for all $\mathbf{x}$ belonging to the support of $\nu_{\mathbf{X}}$ a Hilbertian basis $\{\Psi_{\boldsymbol{\gamma}}, \boldsymbol{\gamma} \in \mathbb{N}^d\}$ of $L^2(\mathbb{R}^d, \mathbb{R}, \nu_{\mathbf{X}})$ is given by

$$\Psi_{\boldsymbol{\gamma}}(\mathbf{x}) = \left(\frac{h_{X_1}(x_1)\ldots h_{X_d}(x_d)}{h_X(\mathbf{x})}\right)^{1/2} \psi_{\gamma_1}(x_1), \ldots, \psi_{\gamma_d}(x_d), \tag{38}$$

where $\{\psi_{\gamma_i}, \gamma_i \in \mathbb{N}\}$ is a Hilbertian basis of $L^2(\mathbb{R}, \mathbb{R}, \nu_{X_i})$. If the components of $\mathbf{X}$ are mutually independent, then the Hilbertian basis is simplified to

$$\Psi_{\boldsymbol{\gamma}}(\mathbf{x}) = \psi_{\gamma_1}(x_1), \ldots, \psi_{\gamma_d}(x_d). \tag{39}$$

The choice of the Hilbertian basis $\{\psi_{\gamma_i}, \gamma_i \in \mathbb{N}\}$ depends on the measure $\nu_{\mathbf{X}_i}$ associated with X_i.

As shown in [12], the copula formalism can be used for the explicit expression of the basis (38). In this case the basis (38) becomes

$$\Psi_{\boldsymbol{\gamma}}(\mathbf{x}) = \frac{\psi_{\gamma_1}(x_1), \ldots, \psi_{\gamma_d}(x_d)}{c\big(H_1(x_1), \ldots, H_d(x_d)\big)^{1/2}}, \tag{40}$$

where $c(u_1, \ldots, u_d) = \partial^d C(u_1, \ldots, u_d)/\partial u_1 \ldots \partial u_d$.

Using in the independent or dependent input case the proposed basis (39) or (38), respectively (or its "copula equivalent" version (40)) for any function $f \in L^2(\mathbb{R}^d, \mathbb{R}, \nu_{\mathbf{X}})$ the PCE decomposition has a form:

$$f(\mathbf{X}) = \sum_{\boldsymbol{\gamma}\in\mathbb{N}^d} a_{\boldsymbol{\gamma}} \Psi_{\boldsymbol{\gamma}}(\mathbf{X}), \tag{41}$$

where the coefficients $a_{\boldsymbol{\gamma}}$ are given by

$$a_{\boldsymbol{\gamma}} = \mathbb{E}\big(f(\mathbf{X})\Psi_{\boldsymbol{\gamma}}(\mathbf{X})\big) \tag{42}$$

due to orthonormality of the basis functions (38) with respect to the joint PDF $h_{\mathbf{X}}$.

We notice that, in the case of an independent random vector $\mathbf{X}$, the PCE can be written in the same form as the ANOVA–HDMR decomposition:

$$f(\mathbf{X}) = \sum_{u\in\mathcal{P}(\mathcal{I})} \sum_{\boldsymbol{\gamma}\in K_u} a_{\boldsymbol{\gamma}} \Psi_{\boldsymbol{\gamma}}(\mathbf{X}), \tag{43}$$

where $\mathcal{P}(\mathcal{I})$ is the power set of $\mathcal{I} = \{1, \ldots, d\}$ and

$$K_u = \big\{\boldsymbol{\gamma} \in \mathbb{N}^d,\ \gamma_i > 0 \text{ for } i \in u\big\}. \tag{44}$$

In the independent input case the ANOVA–HDMR decomposition is unique and the components of the direct ANOVA–HDMR decomposition of f are given by

$$f_u(\mathbf{X}_u) = \sum_{\boldsymbol{\gamma}\in K_u} a_{\boldsymbol{\gamma}} \Psi_{\boldsymbol{\gamma}}(\mathbf{X}). \tag{45}$$

Further we will refer to the method presented in this subsection as Method II.

9. Truncation of the polynomial chaos expansion

In practice the polynomial chaos expansion has to be truncated. Consider a nonempty finite subset $\mathcal{A}$ of $\mathbb{N}^d$, called the truncation set, with cardinality $|\mathcal{A}|$. Then, for any function $f \in L^2(\mathbb{R}^d, \mathbb{R}, \nu_{\mathbf{X}})$ the PCE approximation of f associated with the truncation $\mathcal{A}$ is given by

$$f(\mathbf{X}) \approx \sum_{\boldsymbol{\gamma}\in\mathcal{A}} a_{\boldsymbol{\gamma}} \Psi_{\boldsymbol{\gamma}}(\mathbf{X}). \tag{46}$$

Truncation can be done according to the following considerations:

- most models are principally governed by low-order expansion terms in the sense defined by (28) [12,19]. However, this assumption is problem dependent.
- PCE with high $|\mathcal{A}|$ requires computation of a large number of polynomial chaos coefficients [11,12,19]. It results in a high cumulative error brought by coefficients approximations. Computation of high order coefficients typically requires a large number of model evaluations. Thus, in the case of computationally expensive model a truncation with high cardinality can be prohibitive.

- a high-order expansion can lead to a worse approximation of f than a low-order one [12,19,28].

In Section 6 we proposed to use a truncation technique based on analysis of partial variances. All steps of the technique remain unchanged in the case of Method I as the procedure for estimation of the truncation order is applied to a system in a transformed space in which inputs are independent. For Method II we estimate the truncation order by analyzing values of coefficients a_γ using a procedure described in Section 6, although in this case partial variances do not have the same meaning as for models with independent inputs becoming just a sum of a_γ^2. Other efficient truncation algorithms were presented in [12,19].

10. Approximation of expansion coefficients

The coefficients of the PCE can be estimated by two different methods. The first one, generally known as the projection method is a direct estimation of the expectation (42) by integration schemes such as the Monte-carlo [4,6], accelerated Monte-carlo with Latin Hypercube sampling [29], Quasi Monte Carlo [30] methods, multivariate Gauss quadrature techniques and Smolyak sparse quadrature [28]. The second method, generally known as the regression method is based on estimating the PCE coefficients by minimizing the mean square error of the response approximation [11,12,19]. The details are given in the following subsections.

10.1. Projection method

The rate of convergence for the Monte Carlo method is of the order $\sigma_f/\sqrt{N}$, where σ_f is the standard deviation of $f(\mathbf{X})$ and N is the number of function evaluations. The convergence rate of MC methods does not depend on the number of variables d although it is rather slow. The accelerated Monte Carlo methods are designed to increase the rate of convergence by reducing the variance of the Monte Carlo estimator [31]. However, the rate of convergence remains to be of the order $O(1/\sqrt{N})$.

The full tensor product quadrature [32] and Smolyak sparse quadrature [28,33] in terms of the required function evaluations are more efficient than the MC methods for smooth functions of low and moderate dimensions ($d \leq 20$).

The efficiency of MC integration scheme can be improved by using LDS instead of random points for sampling. LDS are specifically designed to place sample points as uniformly as possible. LDS are also known as quasi random numbers.

For the best known LDS for functions with bounded mix variation the asymptotic rate of convergence is known to be of the order $O(1/N)$. Apparently, this rate of convergence is much faster than that archived by MC.

There are a few well-known and commonly used LDS. Different principles were used for their construction by Halton, Faure, Sobol, Niederreiter and others. Many practical studies have proven that the Sobol' LDS is in many aspects superior to other LDS [34–36].

The Sobol' LDS was constructed by following the three main requirements [37]:

1. Best uniformity of distribution as $N \to \infty$.
2. Good distribution for fairly small initial sets.
3. A very fast computational algorithm.

Points generated by the Sobol' LDS produce a very uniform filling of the space even for a rather small number of points N, which is a very important point in practice. This is why it was used in the present study.

We note, that in the projection method coefficients of decomposition are computed using MC/QMC methods, hence points used for the MC/QMC integration are not used to directly fit a metamodel unlike in other types of emulators or in the case of the regression method, so there is no danger of "overfitting".

10.2. Regression method

The PCE coefficients estimation by the regression method depends on the possibility to invert a $N \times |\mathcal{A}|$ matrix, which is invertible if the number of model evaluation is sufficiently large. Practical experience shows that $N = k|\mathcal{A}|$ with $k = 2, 3$ can be sufficient [19]. Thus the number of model evaluation is strongly dependent on $|\mathcal{A}|$.

Different methods have been proposed to build a sparse polynomial expansion in order to minimize N and the discrepancy between f and its polynomial chaos expansion approximation [19,12].

11. Numerical results

11.1. Independent case

This subsection presents the results of SI calculation using RS/QRS-HDMR methods and comparison of RS/QRS-HDMR methods with the Sobol' method for a test function with independent inputs. We also present the comparison between the exact model and its HDMR metamodels. Component functions up to the second order were used in all ANOVA–HDMR expansions.

We consider the so-called Ishigami function. It is a highly nonlinear three dimensional function proposed in [16]:

$$f(\mathbf{x}) = \sin(\pi x_1) + 7(\sin(\pi x_2))^2 + 0.1\pi^4(x_3)^4 \sin(\pi x_1). \tag{47}$$

Here x_i, $i = 1, 2, 3$ are uniformly distributed on the interval $[-1, 1]$.

The advantage of using analytical test functions is that not only SI but the values of the polynomial coefficients in (10)–(11) can be computed analytically. In this way, the relative effect of the numerical integration error and the error of the polynomial approximation can be distinguished.

If the number of sampled points used to determine the polynomial coefficients is not sufficient for the convergence, oscillations in the profiles of approximated component functions around the exact values can occur [4]. A comparison of analytical profiles for the Ishigami function with RS-HDMR profiles (left) and QRS-HDMR profiles (right) presented in Fig. 1 shows that at small N metamodel profiles indeed exhibit oscillations. These oscillations are reduced and metamodel profiles converge to analytical ones as the number of sampled points grow. The superior performance of the QMC method is clearly visible: the agreement between metamodel profiles and analytical profiles is much closer at all presented values of N. Similar results were obtained for all other variables.

Although the test function (47) is only three dimensional it nevertheless can be quite difficult for HDMR metamodelling because of its high nonlinearity. Polynomials up to the third order, which were typically used in RS-HDMR modeling in the literature, are not able to give a good mapping of the component functions.

The algorithm presented above was used to estimate the sufficient (optimal for the given threshold) number of sampled points N_{opt} and the optimal polynomial orders k for the first order component functions (8). The estimated N_{opt} for the QRS-HDMR method was equal to 1024, while for the RS-HDMR method N_{opt} was four times higher.

We note that for approximation of the same problem authors of [12] used the regression method for estimating coefficients of decomposition and in this case only 194 sampled points were needed. Indeed, the projection methods based on MC or QMC integrations are not as efficient in low dimensions as other integration methods such as quadrature formulas or the regression method.

First order SI (19) can be approximated using RS/QRS-HDMR with the numerically calculated values for α_r^i coefficients at the

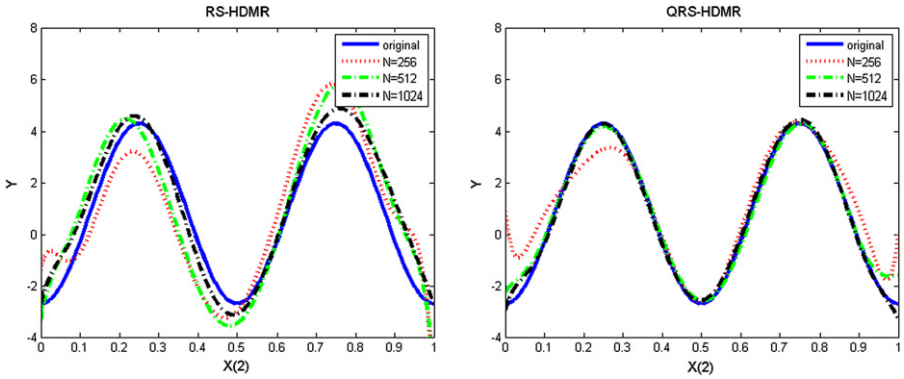

Fig. 1. The output of the HDMR model using MC (left) and QMC (right) numerical integration as a function of x_2 ($x_1 = x_3 = 0.15$). Approximations with different numbers of sampled points are used. Ishigami function. The maximum polynomial order is 8.

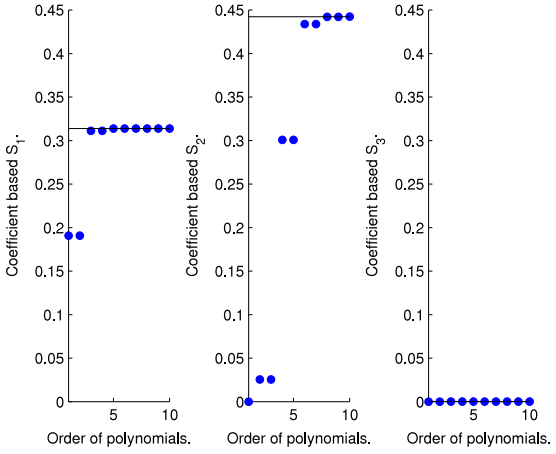

Fig. 2. First order SI $S_i(k)$ obtained using the analytical values of polynomial coefficients as functions of maximum polynomial orders k for the Ishigami function (dots). The horizontal lines show the analytical values of S_i.

fixed polynomial order k:

$$S_i(k) = \frac{\sum_{r=1}^{k} (\hat{\alpha}_r^i)^2}{D}. \tag{48}$$

$S_i(k) \leq S_i$ provided that the values of $\hat{\alpha}_r^i$ are computed with high accuracy. Fig. 2 illustrates the procedure for defining the maximum optimal polynomial orders. It can be seen that polynomials up to the third degree give acceptable results for the variable 1, up to 8–10th degree for the variable 2. Values of $S_3 = 0$, hence all $S_3(k) = 0$. Fig. 3 shows how the output of the HDMR model changes with the degree of polynomials in decomposition of $f_2(x_2)$ when all other polynomial degrees are fixed at the optimal values.

Fig. 4 compares the efficiency of the Sobol and RS/QRS-HDRM methods for evaluation of SI. The total number of function evaluations required for calculation of a full set of main effect and total SI for the Sobol method is $N_F = N(d+2)$. To compute SI using RS-HDMR or QRS-HDMR only $N_F = N$ function evaluations are required, which is $d+2$ times less than that for the original Sobol' method for the same number of sampled points. The root mean square error (RMSE) versus the number of sampled points N is calculated. To reduce the scatter in the error estimation the values of RMSE were averaged over $K = 20$ independent runs. For the MC method all runs were statistically independent. For QMC integration for each run a different part of the Sobol' sequence was used. RMSE can be approximated by a trend line $cN^{-\alpha}$. Values $(-\alpha)$ are given in brackets on the plots of RMSE versus N. Note that the values are shown as functions of model evaluations N_F, which are equal to $N(d+2)$ for the Sobol method and N for the RS/QRS-HDMR methods. It can be seen that the QMC based method has much higher convergence rates than the MC based one. The RS/QRS-HDRM methods show much faster convergence than the Sobol method. However, in practice RS-HDMR or QRS-HDMR can only provide the first and the second order SI.

11.2. Dependent case

In Sections 8.1 and 8.2 we presented two different methods to derive a PCE for dependent inputs. This subsection presents the comparison between these methods. We consider two different test functions.

11.2.1. Three dimensional hyperplane function

The first test function is the three dimensional hyperplane function defined as:

$$f(\mathbf{X}) = X_1 + X_2 + X_3, \tag{49}$$

where X_i's are Gaussian variables with zero mean and the correlation matrix $\Sigma^{\bar{H}}$. It is assumed that only $\rho^{\bar{H}}_{2,3} > 0$ while other correlation coefficients are equal to zero.

Fig. 5 shows a comparison between the original output data and the metamodel approximation using Method I. Notice that in all comparison plots sampled points used for building metamodels and for comparison purposes are different. We present the results for just one value of $\rho^{\bar{H}}_{2,3} = 0.5$. The results for other values $\rho^{\bar{H}}_{2,3} = 0.0$ and $\rho^{\bar{H}}_{2,3} = 0.9$ are very similar to those presented in Fig. 5. The points are centered around the $y = x$ axis which illustrates that a metamodel approximation is accurate. We also compute $\log_2(\hat{\delta})$ where $\hat{\delta}$ is the MC estimation of (13). For the three considered values of $\rho^{\bar{H}}_{2,3}$ $\log_2(\hat{\delta}) \sim -10$. The constructed metamodel contains only polynomials of the first order.

Fig. 6 presents the scatter plot of $\hat{f}(\mathbf{X})$ versus (X_1, X_2) for the three different values of $\rho^{\bar{H}}_{2,3}$. Variable X_1 which is independent of the two other variables, is fixed. The plot shows the approximation given by the metamodel and its dependence on $\rho^{\bar{H}}_{2,3}$.

The results for Method II are presented in Fig. 7. A Gaussian copula is used, $\rho^{\bar{H}}_{2,3}$ is fixed at 0.5. We compare the real output data versus metamodel approximation. The left plot corresponds to the case when only the first order expansion terms in the PCE are taken into account, the middle – one up to the second order and the right one – up to the third order. In this case, it is not sufficient to consider only the first or the second order expansion terms for building the metamodel. Indeed, by construction the basis (40) introduces higher order expansion terms when input variables are dependent. The $\log_2(\hat{\delta})$ values are equal to -3.4, -5.1, -6 from left

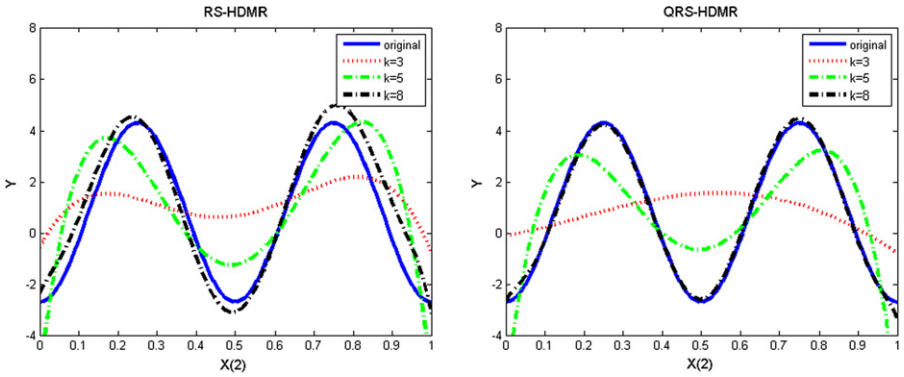

Fig. 3. The output of the HDMR model using MC (left) and QMC (right) numerical integration as a function of x_2 ($x_1 = x_3 = 0.15$) at $N = 1024$ at different orders of polynomials for $f_2(x_2)$ for the Ishigami function. Other polynomial degrees are fixed at their optimal values.

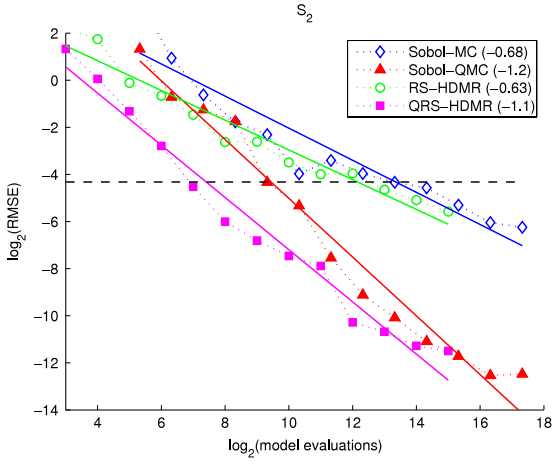

Fig. 4. RMSE of SI versus N_F for variable 2, test function (47) for the RS/QRS-HDMR and the Sobol method using MC/QMC integration. Straight lines are fitted trend lines $cN_F^{-\alpha}$. The horizontal dashed line shows the 5% threshold in the relative error.

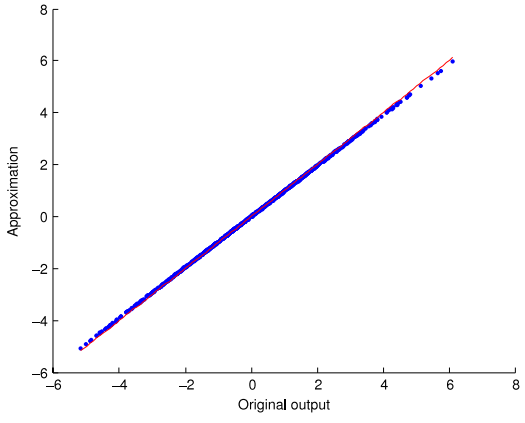

Fig. 5. Original output data versus metamodel approximations for the hyperplane test function. Method I. $N = 1024$. $\rho^{\tilde{H}}_{2,3} = 0, 0.5, 0.9$.

to right, correspondingly. We notice that the value of the lowest error is still higher than that obtained with Method I.

Fig. 8 presents the same result for $\rho^{\tilde{H}}_{2,3} = 0.9$. We observe that for the same value of N higher values of the correlation coefficients result in higher order expansion terms and higher degrees of polynomials. For the same N, the polynomial decomposition coefficients of high orders and degrees are less accurate than those for the low order ones. It results in lower accuracy of metamodel approximations. Indeed, for this case $\log_2(\hat{\delta})$ values are equal to

Table 1
$\log_2(\hat{\delta})$ for Methods I and II at different orders of expansion terms and values of the correlation coefficient ρ.

ρ	0	0.5	0.9
HM_1O_1	−10.0	−10.0	−10.0
HM_2O_1	−10.0	−3.4	−3.1
HM_2O_2	n/a	−5.1	−3.2
HM_2O_3	n/a	−6.0	−4.6
IM_1O_2	−7.0	−6.3	−7.4
IM_2O_3	−6.9	−4.3	−2.1

−3.1, −3.2, −4.6 from left to right, correspondingly. They are significantly higher than the values of $\hat{\delta}$ for the case of $\rho^{\tilde{H}}_{2,3} = 0.5$.

11.2.2. Ishigami function with dependent inputs

The second test function is the Ishigami function defined by (47) with dependent input variables and the correlation matrix $\Sigma^{\tilde{I}}$. We suppose $\rho^{\tilde{I}}_{1,3} > 0$ while all others correlation coefficients are equal to zero.

Fig. 9 presents the original output data versus metamodel built using Method I. $\rho^{\tilde{I}}_{1,3}$ is taken to be equal to 0 and 0.9. One can see that the metamodel approximation is very accurate: $\log_2(\hat{\delta})$ is equal to −7.0 and −7.4 from left to right, correspondingly. The best fit is obtained with the second order expansion terms.

Fig. 10 shows a scatterplot of $\hat{f}$ versus X_1 and X_3 at X_2 fixed at its mean value for $\rho^{\tilde{I}}_{1,3} = 0$ and 0.9. This plot shows the effect of correlation on the output.

Fig. 11 shows the original output versus metamodel built using Method II. Up to the third order expansion terms and high polynomial degrees are required. The same expansion terms and polynomial degrees have been chosen for two values of $\rho^{\tilde{I}}_{1,3}$ equal to 0.5 and 0.9. For the same value of N, the approximation is less accurate than that obtained with Method I. $\log_2(\hat{\delta})$ is equal to −4.3 and −2.15, from left to right correspondingly. When $\rho^{\tilde{I}}_{1,3}$ increases the approximation accuracy deteriorates for the same chosen expansion terms, polynomial degrees and N.

Table 1 presents the values of $\log_2(\hat{\delta})$ for different values of the correlation coefficient ρ. We denote HM_iO_j the value of $\log_2(\hat{\delta})$ for the hyperplane test function with Method i and the maximum order expansion terms $j \in \{1, 2, 3\}$. For the Ishigami function we use a similar notation with the first letter H replaced by I : IM_iO_j.

The comparison shows that Method I outperforms Method II for models of relatively simple structure such as hyperplanes. Indeed, linear or quasi-linear models do not need to account for high order expansion terms even if the inputs are correlated. The application of Method I for the hyperplane test results in a linear approximation model which makes a metamodel very efficient and

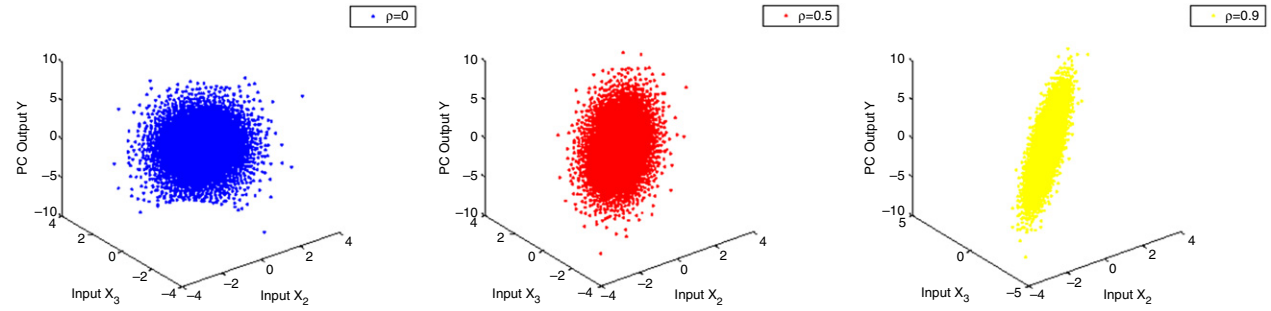

Fig. 6. Scatterplot of $\hat{f}(\mathbf{X})$ versus X_2 and X_3 for the hyperplane test function. Method I. X_1 is fixed to its mean value. $N = 1024$. $\rho^{\tilde{H}}_{2,3} = 0, 0.5, 0.9$.

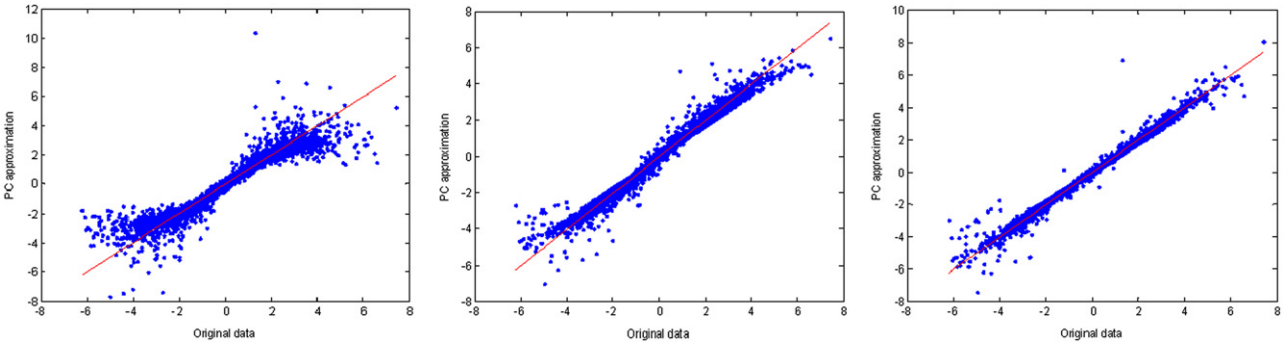

Fig. 7. Original output data versus metamodel approximations for the hyperplane test function. Method II. $N = 1024$. $\rho^{\tilde{H}}_{2,3} = 0.5$. (left) Metamodel with the first order expansion terms. (middle) Metamodel with up to the second order expansion terms. (right) Metamodel with up to the third order expansion terms.

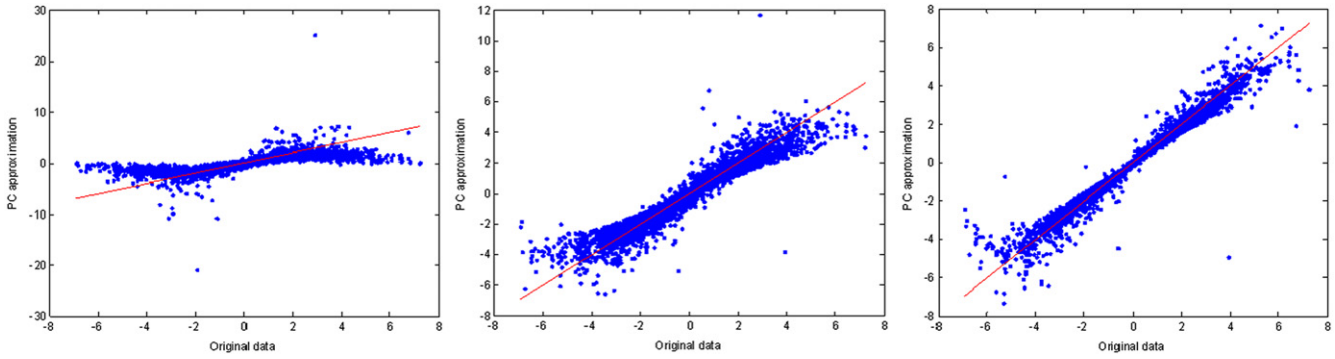

Fig. 8. Original output data versus metamodel approximations for the hyperplane test function. Method II. $N = 1024$. $\rho^{\tilde{H}}_{2,3} = 0.9$. (left) Metamodel with the first order expansion terms. (middle) Metamodel with up to the second order expansion terms. (right) Metamodel with up to the third order expansion terms.

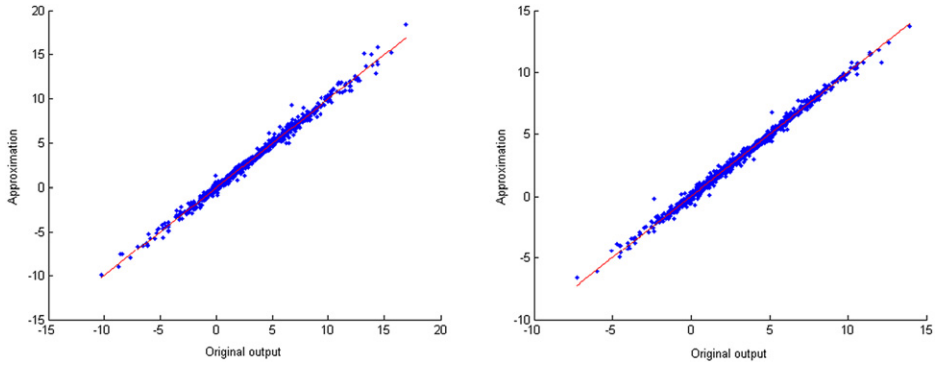

Fig. 9. Original output data versus metamodel approximations for the Ishigami test function. Method I. $N = 1024$. $\rho^{\tilde{I}}_{1,3} = 0, 0.9$.

accurate, whereas the application of Method II results in high order expansion terms in the PCE brought by the dependence structure. The second test model is highly nonlinear. Method I still performs better than Method II but the difference in efficiency between the two methods is smaller: Method II requires up to the third order expansion terms, while the Method I—up to the second order.

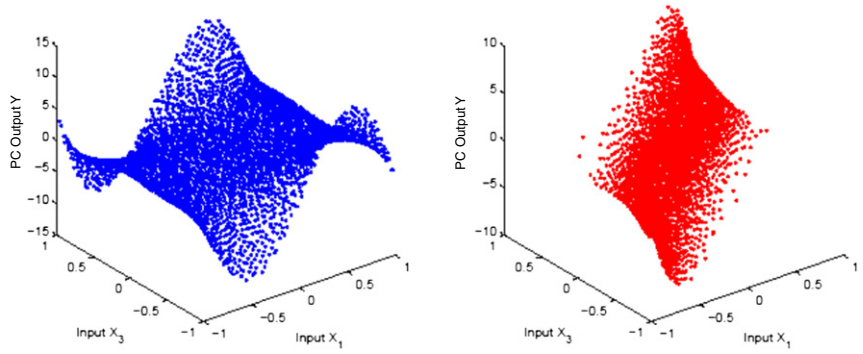

Fig. 10. Scatterplots of $\hat{f}(\mathbf{X})$ versus X_1 and X_3 for the Ishigami function. X_2 is fixed at its mean value. Method I. $N = 1024$. (left) $\rho^{\tilde{I}}_{1,3} = 0$, (right) $\rho^{\tilde{I}}_{1,3} = 0.9$.

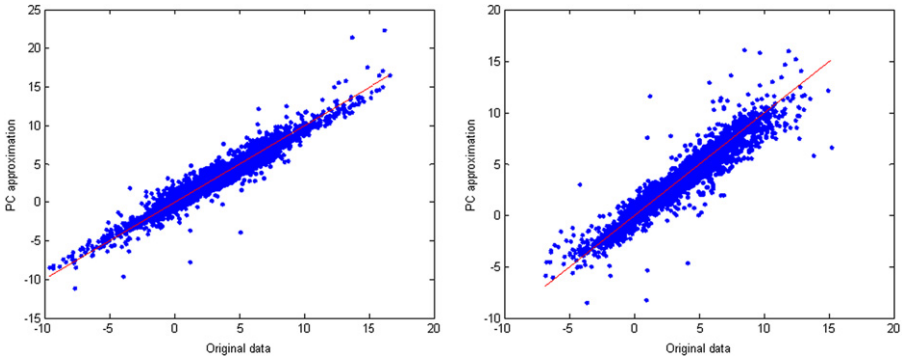

Fig. 11. Original output data versus metamodel approximations for the Ishigami test function. Method II. $N = 1024$. (left) $\rho^{\tilde{I}}_{1,3} = 0.5$, (right) $\rho^{\tilde{I}}_{1,3} = 0.9$.

12. Conclusions

A modified version of the RS-HDMR method with enhanced efficiency is presented. Comparisons shows that the QMC-HDMR method based on Sobol' sequences significantly outperforms RS-HDMR. RS/QRS-HDMR based methods are much more efficient than the Sobol method in evaluations of main effect SI. Tests also show that the developed methods for choosing optimal order of polynomials and the number of sampled points are robust and efficient. They provide good accuracy for both SI evaluations and model approximations with a reasonable number of function evaluations.

We extended the RS/QMC-HDMR methods for the case of models with dependent inputs and compared two different approaches for dealing with correlated inputs. The tests show that for models with low interaction orders the method with the transformation from dependent to independent inputs (Method I) outperforms the method with the use of the general basis functions (Method II). However, the advantage of Method I decreases for models with high interaction orders. Method I is based on the assumption that the inputs variables are linked by a Gaussian copula whereas Method II can be applied with any copula, which can be beneficial in applications where probability distribution functions have fat tails.

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References

[1] J. Oakley, A. O'Hagan, Probabilistic sensitivity analysis of complex models: a Bayesian approach, J. R. Stat. Soc. Ser. B 66 (2004) 751–769.
[2] C. Rasmussen, C. Williams, Gaussian Processes for Machine Learning, MIT Press, ISBN: 026218253X, 2006.
[3] M.D. Buhmann, Radial Basis Functions: Theory and Implementations, Cambridge University Press, ISBN: 978-0-521-63338-3, 2003.
[4] G. Li, S.-W. Wang, H. Rabitz, Practical approaches to construct RS-HDMR component functions, J. Phys. Chem. 106 (2002) 8721–8733.
[5] G. Li, S.-W. Wang, P. Georgopoulos, J. Schoendorf, H. Rabitz, Random sampling-high dimensional model representation (RS-HDMR) and orthogonality of its different order component functions, J. Phys. Chem. 110 (7) (2006) 2474–2485.
[6] T. Ziehn, A. Tomlin, Global sensitivity analysis of a 3D street canyon model—part I: the development of high dimensional model representation, Atmos environ 42 (2008) 1857–1873.
[7] A. Saltelli, S. Tarantola, F. Campolongo, M. Ratto (Eds.), Sensitivity Analysis in Practice, Wiley, 2004.
[8] A. Saltelli, M. Ratto, S. Tarantola, F. Campolongo, Sensitivity analysis for chemical models, Chem. Rev. 105 (7) (2005) 2811–2828.
[9] A. Saltelli, P. Annoni, I. Azzini, F. Campolongo, M. Ratto, S. Tarantola, Variance based sensitivity analysis of model output. Design and estimator for the total sensitivity index, Comput. Phys. Comm. 181 (2) (2010) 259–270.
[10] G. Sudret, A.D. Kiureghian, Stochastic finite elements and reliability: a state-of-the-art report, Technical Report No. UCB/SEMM-2000/08, University of California, Berkeley, 2000, p. 173.
[11] B. Sudret, Global sensitivity analysis using polynomial chaos expansions, Reliab. Eng. Syst. Saf. 93 (2008) 964–979.
[12] G. Blatman, B. Sudret, An adaptive algorithm to build up sparse polynomial chaos expansions for stochastic finite element analysis, Probab. Eng. Mech. 25 (2010) 183–197.
[13] A. Saltelli, Making best use of model evaluations to compute sensitivity indices, Comput. Phys. Comm. 145 (2002) 280–297.
[14] I. Sobol, Sensitivity estimates for nonlinear mathematical models, Math. Modeling Comput. Experiment 1 (1993) 407–414.
[15] I. Sobol, Global sensitivity indices for nonlinear mathematical models and their Monte Carlo estimates, Math. Comput. Simulation 55 (2001) 271–280.
[16] T. Homma, A. Saltelli, Importance measures in global sensitivity analysis of nonlinear models, Reliab. Eng. Syst. Saf. 52 (1996) 1–17.
[17] I. Sobol', S. Tarantola, D. Gatelli, S. Kucherenko, W. Mauntz, Estimating the approximation error when fixing unessential factors in global sensitivity analysis, Reliab. Eng. Syst. Saf. 92 (7) (2007) 957–960.
[18] I. Sobol', S. Kucherenko, Global sensitivity indices for nonlinear mathematical models. Review, Wilmott Mag. 2 (2005) 56–61.
[19] G. Blatman, B. Sudret, Adaptive sparse polynomial chaos expansion based on least angle regression, J. Comput. Phys. 230 (2011) 2345–2367.
[20] C. Soize, R. Ghanem, Physical systems with random uncertainties: chaos representations with arbitrary probability measure, SIAM J. Sci. Comput. 26 (2) (2004) 395–410.

[21] S. Kucherenko, S. Tarantola, P. Annoni, Estimation of global sensitivity indices for models with dependent variables, Comput. Phys. Comm. 183 (2012) 937–946.
[22] R. Nelsen, An Introduction to Copulas, Springer, New York, 1999.
[23] A. Nataf, Détermination des distributions de probabilités dont les marges sont données, C. R. Acad. Sci. A 225 (1962) 42–43.
[24] P. Liu, A.D. Kiureghian, Multivariate distribution models with prescribed marginals and covariances, Probab. Eng. Mech. 1 (2) (1986) 105–112.
[25] J. Gentle, Matrix Algebra: Theory, Computations and Applications to Statistics, first ed., Springer, 2007.
[26] R. Lebrun, A. Dutfoy, An innovating analysis of the nataf transformation from the copula viewpoint, Probab. Eng. Mech. 24 (3) (2009) 312–320.
[27] P. Embrechts, F. Lindskog, A. McNeil, Modelling dependence with copulas and applications to risk management, in: S. Rachev (Ed.), Handbook of Heavy Tailed Distributions in Finance, Elsevier, 2003, pp. 329–384 (Chapter 8).
[28] T. Crestaux, O.L. Maître, J.-M. Martinez, Polynomial chaos expansion for sensitivity analysis, Reliab. Eng. Syst. Saf. 94 (2009) 1161–1172.
[29] G. Blatman, Adaptive sparse polynomial chaos expansions for uncertainty propagation and sensitivity analysis, Ph.D. Thesis, Université Blaise Pascal—Clermont II, 2009.
[30] B. Feil, S. Kucherenko, N. Shah, Comparison of Monte Carlo and quasi Monte Carlo sampling methods in high dimensional model representation, in: The First International Conference on Advances in System Simulation, 2009, pp. 12–17.
[31] M. Munoz Zuniga, Méthodes stochastiques pour l'estimation contrôlée de faibles probabilités sur des mod èles physiques complexes. Application au domaine nucléaire, Ph.D. Thesis, Université Diderot—Paris VII, 2011.
[32] P. Davis, P. Rabinowits, Methods of Numerical Integration, Academic Press, 1984.
[33] T. Gerstner, M. Griebel, Numerical integration using sparse grids, Numer. Algorithms 18 (3–4) (1998) 209–232.
[34] S. Paskov, J. Traub, Faster evaluation of financial derivatives, J. Portfolio Manage. 22 (1) (1995) 113–120.
[35] P. Glasserman, Monte Carlo Methods in Financial Engineering, Springer-Verlag, New York, 2004.
[36] I. Sobol', D. Asotsky, A. Kreinin, S. Kucherenko, Construction and comparison of high-dimensional Sobol' generators, Wilmott J. (2012) 64–79.
[37] I. Sobol', On the distribution of points in a cube and the approximate evaluation of integrals, Comput. Math. Math. Phys. 7 (1967) 86–112.