

Variance-based sensitivity analysis in the presence of correlated input variables

Thomas Most

*Dynardo – Dynamic Software and Engineering GmbH, Weimar, Germany
thomas.most@dynardo.de*

Abstract. In this paper we propose an extension of the classical Sobol' estimator for the estimation of variance based sensitivity indices. The approach assumes a linear correlation model between the input variables which is used to decompose the contribution of an input variable into a correlated and an uncorrelated part. This method provides sampling matrices following the original joint probability distribution which are used directly to compute the model output without any assumptions or approximations of the model response function.

Keywords: Sobol' indices, sensitivity analysis, correlation, regression

1. Introduction

In the assessment of computational engineering models sensitivity analysis has played an increasing role during the last two decades. For probabilistic models variance based sensitivity methods are very common. Based on the work of Sobol' (Sobol' 1993) first order indices have been extended to total indices capturing higher order coupling effects between the input variables (Homma and Saltelli 1996). Based on this early work a large number of extensions and improvements have been developed. A precise overview of existing variance based methods and their background is given in (Saltelli et al. 2008). As stated in (Saltelli et al. 2010) the total effect sensitivity index has become a prestigious measure to quantify higher order effects of input variables which is necessary for model simplification by variable fixing. However, the basic formulation of the variance decomposition and the common estimation procedures require so far independent input variables.

In practical applications often input variables are correlated, therefore, an increased interest in extending the classical methods for correlated inputs is marked in the recent years. In several investigations, assumptions about the model output or approximations up to a certain degree are necessary (Oakley and O'Hagan 2004), (Xu and Gertner 2008), (DaVeiga et al. 2009). Complete model independent approaches for the estimation of total effect indices are not available so far. In (Jacques et al. 2006) classical estimators have been used by grouping the correlated inputs which results in independent groups of parameters. However, even this approach is not useful for more complex models where almost all variables are coupled with each other.

In this paper we propose an extension of the classical Sobol' estimator. The basics of this method have been developed in (Most et al. 2010), where a variable decomposition similar to (Xu and Gertner 2008) was realized. The general idea has been adapted in (Mara and Tarantola 2012) for normally distributed random variables. In our approach we assume a linear correlation model between the input variables, which is used

to decompose the samples into a correlated and an uncorrelated part with respect to a certain variable. This was realized in (Mara and Tarantola2012) by an orthogonalization schemes which may lead to non-unique solution depending on the variable order. In our approach we decompose the contribution of the input variables directly by using the correlation information of the standard normal space. This decomposition results in a unique solution. For non-normal distributions the Nataf model (Nataf1962) is applied to transform the original space and the correlation information to the standard normal space. The proposed method finally provides modified sampling matrices following the original joint probability distribution while keeping the samples of a certain variable unchanged. These samples are used directly to compute the model output without any assumptions or approximations of the model response function which makes the proposed method model independent. Additionally, reduced polynomial models are presented which are used to estimate the variance contribution of single variables.

Alternatively to the decomposition approach, in (Most et al.2010) a reordering approach has been proposed. In this method the investigated variable has been taken as the first one in the variables set for the Cholesky decomposition in the standard normal space. With this approach the samples required for the estimation of the sensitivity indices can be directly determined. This method has been adapted in (Kucherenko et al.2012). In our paper we do not discuss this approach, since the implementation is much more complicated compared to the decomposition approach.

2. Variance based sensitivity analysis

2.1. FIRST ORDER AND TOTAL EFFECT SENSITIVITY INDICES

Assuming a model with a scalar output Y as a function of a given set of m random input parameters X_i

$$Y = f(X_1, X_2, \dots, X_m), \quad (1)$$

the first order sensitivity measure was introduced as (Sobol'1993)

$$S_i = \frac{V_{X_i}(E_{\mathbf{X}_{\sim i}}(Y|X_i))}{V(Y)}, \quad (2)$$

where $V(Y)$ is the unconditional variance of the model output and $V_{X_i}(E_{\mathbf{X}_{\sim i}}(Y|X_i))$ is named the *variance of conditional expectation* with $\mathbf{X}_{\sim i}$ denoting the matrix of all factors but X_i . $V_{X_i}(E_{\mathbf{X}_{\sim i}}(Y|X_i))$ measures the first order effect of X_i on the model output.

Since first order sensitivity indices measure only the decoupled influence of each variable an extension for higher order coupling terms is necessary. For this purpose total effect sensitivity indices have been introduced (Homma and Saltelli1996)

$$S_{Ti} = 1 - \frac{V_{\mathbf{X}_{\sim i}}(E_{X_i}(Y|\mathbf{X}_{\sim i}))}{V(Y)}, \quad (3)$$

where $V_{\mathbf{X}_{\sim i}}(E_{X_i}(Y|\mathbf{X}_{\sim i}))$ measures the first order effect of $\mathbf{X}_{\sim i}$ on the model output which does not contain any effect corresponding to X_i .

2.2. SAMPLING BASED ESTIMATES

One of the most simple procedures to estimate the first order indices is to sample a set of n samples of the input parameter set $\mathbf{X} = [X_1, X_2, \dots, X_m]$ according to their joint probability distribution and compute for each sample \mathbf{x}_j the model output y_j . A scatter plot is obtained if the model output values are plotted against the values of a single variable as shown in Figure 1. Then the sample values are sorted according to a single

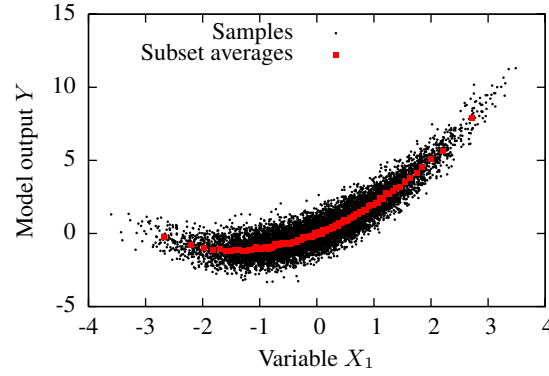


Figure 1. Scatter plot of a single input variable with the model output including subset averages of sorted sample subsets

input variable X_i and subdivided in a number of subsets. For each subset the average value is computed which is equivalent to $E_{\mathbf{X}_{\sim i}}(Y|X_i)$. By calculating the variance of the subset averages, an estimate of $V_{X_i}(E_{\mathbf{X}_{\sim i}}(Y|X_i))$ is obtained, which can directly be used to estimate the first order sensitivity index. This procedure has the advantage that it gives suitable estimates for independent and dependent input parameters. However, an extension for the total sensitivity indices does not exist so far since a sorting concerning $\mathbf{X}_{\sim i}$ seems not possible.

In order to compute the first order and total sensitivity indices using sampling methods, a matrix combination approach is very common in sensitivity analysis. In this procedure two independent sampling matrices \mathbf{A} and \mathbf{B} are generated according to the joint probability density function of the input parameters and recombined in a matrix \mathbf{C}_i , where \mathbf{C}_i contains the entries of matrix \mathbf{B} except the i -th column which is taken from \mathbf{A} . The estimates of the sensitivity indices can be obtained following (Saltelli et al.2008) as

$$\hat{S}_i = \frac{\mathbf{y}_\mathbf{A}^T \mathbf{y}_{\mathbf{C}_i} - n(\bar{y}_\mathbf{A})^2}{\mathbf{y}_\mathbf{A}^T \mathbf{y}_\mathbf{A} - n(\bar{y}_\mathbf{A})^2}, \quad \hat{S}_{T_i} = 1 - \frac{\mathbf{y}_\mathbf{B}^T \mathbf{y}_{\mathbf{C}_i} - n(\bar{y}_\mathbf{B})^2}{\mathbf{y}_\mathbf{B}^T \mathbf{y}_\mathbf{B} - n(\bar{y}_\mathbf{B})^2}, \quad (4)$$

where $\mathbf{y}_\mathbf{A}$, $\mathbf{y}_\mathbf{B}$ and $\mathbf{y}_{\mathbf{C}_i}$ are vectors containing the model outputs of the sampling matrices and $\bar{y}_\mathbf{A}$ and $\bar{y}_\mathbf{B}$ are the corresponding mean value estimates. Instead of the estimators in Eq. (4) other approaches exist as discussed in (Saltelli et al.2010). However all of these methods are based on the generation of the sampling matrices \mathbf{A} , \mathbf{B} and \mathbf{C}_i . Due to the combination of independent columns of \mathbf{A} and \mathbf{B} the matrices \mathbf{C}_i follow the joint probability density function of \mathbf{A} and \mathbf{B} only if the input variables are independent. In case of dependent parameters X_k and X_l the k -th and l -th columns of the matrices \mathbf{C}_k and \mathbf{C}_l are independent due to the independence of \mathbf{A} and \mathbf{B} . Correlations between X_i and the remaining variables are lost in \mathbf{C}_i , see the first two plots in Figure 2. For the correlated case only a grouping of the dependent parameters according to

(Jacques et al.2006) would lead to equivalent probability density functions, but this would limit the method to special cases where the grouping is possible.

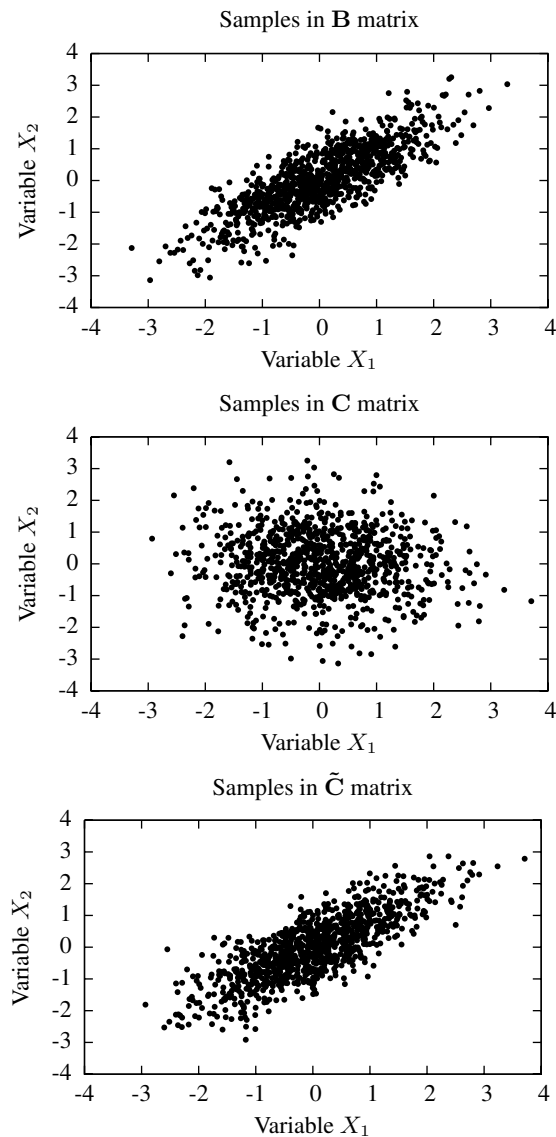


Figure 2. Original and modified joint probability distributions of two correlated variables using the original and the extended matrix combination approach

2.3. REGRESSION BASED ESTIMATES

In order to decrease the numerical effort of a probabilistic analysis often surrogate models are used to approximate the model output instead of evaluating the real sophisticated model. For this purpose, the model

output is replaced mainly by a continuous function, which can be evaluated quite fast compared to a real model call. A very common method is polynomial regression, where the model response Y is generally approximated by a polynomial basis function

$$\mathbf{p}_{\mathbf{X}}^T(\mathbf{x}) = [1 \ x_1 \ x_2 \ x_3 \ \dots \ x_1^2 \ x_2^2 \ x_3^2 \ \dots \ x_1 x_2 \ x_1 x_3 \ \dots \ x_2 x_3 \ \dots] \quad (5)$$

of linear or quadratic order with or without linear coupling terms. The model output y_j for a given sample \mathbf{x}_j of the input parameters \mathbf{X} can be formulated as the sum of the approximated value \hat{y}_j and an error term ϵ_j

$$y(\mathbf{x}_j) = \hat{y}_j(\mathbf{x}_j) + \epsilon_j = \mathbf{p}_{\mathbf{X}}^T(\mathbf{x}_j)\boldsymbol{\beta}_Y + \epsilon_j, \quad (6)$$

where $\boldsymbol{\beta}_Y$ is a vector containing the unknown regression coefficients. These coefficients are generally estimated from a given set of sampled support points by assuming independent errors with equal variance at each point. By using a matrix notation the resulting least squares solution reads (Myers and Montgomery2002)

$$\hat{\boldsymbol{\beta}}_Y = (\mathbf{P}_{\mathbf{X}}^T \mathbf{P}_{\mathbf{X}})^{-1} \mathbf{P}_{\mathbf{X}}^T \mathbf{Y}, \quad (7)$$

where $\mathbf{P}_{\mathbf{X}}$ is a matrix containing the basis polynomials of the support point samples.

In order to verify the approximation model the coefficient of determination is often used

$$R^2 = 1 - \frac{\sum_{j=1}^n (y_j - \hat{y}_j)^2}{\sum_{j=1}^n (y_j - \bar{y})^2}, \quad \bar{y} = \frac{1}{n} \sum_{j=1}^n y_j. \quad (8)$$

Generally, R^2 is interpreted as the fraction of the variance of the true model represented by the approximation model. This can be used to estimate total sensitivity indices based on the multivariate regression model (Bucher2009)

$$\hat{S}_{T_i}^R = R_{\mathbf{X}}^2 - R_{\mathbf{X}_{\sim i}}^2, \quad (9)$$

where $R_{\mathbf{X}}^2$ is obtained using the full parameter set to build up the regression model and $R_{\mathbf{X}_{\sim i}}^2$ is estimated for a regression model with a reduced parameter set $\mathbf{X}_{\sim i}$.

First order sensitivity indices can be estimated by using only these polynomial basis terms which belong to the investigated variable X_i . The resulting one-dimensional coefficient of determination is a direct estimate of first order indices

$$\hat{S}_i^R = R_{X_i}^2. \quad (10)$$

3. Correlated input variables

3.1. REPRESENTATION OF NON-NORMAL JOINT DISTRIBUTION FUNCTIONS

In probabilistic models the dependency between input variables is often modeled by a linear correlation model based on the Pearson correlation coefficient representing pairwise linear correlations

$$\rho(X_i, X_j) = \frac{E[(X_i - \bar{X}_i)(X_j - \bar{X}_j)]}{\sqrt{V(X_i)V(X_j)}}, \quad (11)$$

with the mean values \bar{X}_i and \bar{X}_j .

In our study the Nataf model (Nataf1962) is used to generate multivariate joint distribution function of non-normally distributed random variables. In this model the marginal distributions of the individual random variables are transformed to standard normal densities

$$Z_i = \mathcal{T}_{X_i}(X_i), \quad (12)$$

and the resulting multivariate distribution is assumed to be jointly normal

$$f_{\mathbf{Z}}(\mathbf{z}) = \frac{1}{\sqrt{(2\pi)^m |\mathbf{C}_{\mathbf{Z}\mathbf{Z}}|}} \exp \left[-\frac{1}{2} \mathbf{z}^T \mathbf{C}_{\mathbf{Z}\mathbf{Z}}^{-1} \mathbf{z} \right], \quad (13)$$

where m is the number and $\mathbf{C}_{\mathbf{Z}\mathbf{Z}}$ is the covariance matrix of the random variables which contains in case of standard normal variables the correlation coefficients $C_{ij} = \rho(Z_i, Z_j)$. If the correlation coefficients are given in the standard normal space, the correlation coefficients in the original space can be obtained as follows

$$\rho(X_i, X_j) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{x_i - \bar{X}_i}{\sigma_{X_i}} \frac{x_j - \bar{X}_j}{\sigma_{X_j}} f_{Z_i Z_j}(z_i, z_j) dz_i dz_j, \quad (14)$$

where $f_{Z_i Z_j}(z_i, z_j)$ is a two-dimensional standard normal probability density function. Often the correlation coefficients are given in the original space. In this case the correlation coefficients in the standard normal space can be derived by solving Eq. (14) iteratively.

3.2. DECOMPOSITION OF INPUT VARIABLES

If input variables are correlated with each other, a single variable can be represented as the sum of a function of the remaining inputs (correlated) and an independent (uncorrelated) part

$$X_i = f(X_1, X_2, \dots, X_{i-1}, X_{i+1}, \dots, X_m) + X_i^{U, \mathbf{X}_{\sim i}} = X_i^{C, \mathbf{X}_{\sim i}} + X_i^{U, \mathbf{X}_{\sim i}}. \quad (15)$$

By using a linear correlation model, the correlated part of each input variable can be represented by a linear combination of the remaining variable set $\mathbf{X}_{\sim i}$

$$X_i^{C, \mathbf{X}_{\sim i}} = \beta_{X_i, 0} + \sum_{j=1, j \neq i}^m \beta_{X_i, j} X_j. \quad (16)$$

In case of standard normal and linearly correlated random variables Z_i , the coefficients

$$Z_i^{C, \mathbf{Z}_{\sim i}} = \beta_{Z_i, 0} + \sum_{j=1, j \neq i}^m \beta_{Z_i, j} Z_j, \quad (17)$$

can be directly determined from the correlation coefficients

$$\beta_{Z_i, 0} = 0, \quad \beta_{Z_i} = \mathbf{C}_{\mathbf{Z}_{\sim i} \mathbf{Z}_{\sim i}}^{-1} \boldsymbol{\rho}_{Z_i}, \quad (18)$$

where $\beta_{Z_i} = [\beta_{Z_i, 1}, \dots, \beta_{Z_i, i-1}, \beta_{Z_i, i+1}, \dots, \beta_{Z_i, m}]$ contains the coefficients belonging to $\mathbf{Z}_{\sim i}$, $\mathbf{C}_{\mathbf{Z}_{\sim i} \mathbf{Z}_{\sim i}}$ is the correlations matrix of $\mathbf{Z}_{\sim i}$ and $\boldsymbol{\rho}_{Z_i} = [\rho(Z_i, Z_1), \dots, \rho(Z_i, Z_{i-1}), \rho(Z_i, Z_{i+1}), \dots, \rho(Z_i, Z_m)]$ contains

the correlation coefficients of $\mathbf{Z}_{\sim i}$ with respect to Z_i . A derivation of Eq. (18), which is valid only in the standard normal space, can be found in the appendix.

For a given set of discrete samples of the standard normal parameter set \mathbf{Z} arranged in matrix \mathbf{M} , the uncorrelated parts of the j th column of \mathbf{M} with respect $\mathbf{Z}_{\sim i}$ can be determined as follows

$$\mathbf{M}_{(j)}^{U, \mathbf{Z}_{\sim i}} = \mathbf{M}_{(j)} - \mathbf{M}_{(j)}^{C, \mathbf{Z}_{\sim i}} \quad (19)$$

with

$$\mathbf{M}_{(j=i)}^{C, \mathbf{Z}_{\sim i}} = \sum_{k=1, k \neq i}^m \beta_{Z_i, k} \mathbf{M}_{(k)}, \quad \mathbf{M}_{(j \neq i)}^{C, \mathbf{Z}_{\sim i}} = \mathbf{M}_{(j)}. \quad (20)$$

For later use the correlated and uncorrelated parts of a single random variable with respect to only one other variable is introduced. The correlated part of X_j with respect to X_i can be formulated as follows

$$X_j^{C, X_i} = \beta_{X_j, 0}^{X_i} + \beta_{X_j, 1}^{X_i} X_i. \quad (21)$$

In the standard normal space we obtain

$$Z_j^{C, Z_i} = \beta_{Z_j, 0}^{Z_i} + \beta_{Z_j, 1}^{Z_i} Z_i, \quad \beta_{Z_j, 0}^{Z_i} = 0, \quad \beta_{Z_j, 1}^{Z_i} = \rho(Z_i, Z_j). \quad (22)$$

For a given sampling matrix \mathbf{M} the decomposition reads

$$\mathbf{M}_{(j)}^{U, Z_i} = \mathbf{M}_{(j)} - \mathbf{M}_{(j)}^{C, Z_i} = \mathbf{M}_{(j)} - \rho(Z_i, Z_j) \mathbf{M}_{(i)}. \quad (23)$$

In the second decomposition the corresponding i th column of \mathbf{M}^{C, Z_i} is equal to $\mathbf{M}_{(i)}$ and the values of the i th column of \mathbf{M}^{U, X_i} vanish.

As discussed in (Saltelli et al.2004) the conditional variance $V_{\mathbf{X}_{\sim i}}(E_{X_i}(Y|\mathbf{X}_{\sim i}))$ may decrease by introducing dependence between X_i and $\mathbf{X}_{\sim i}$. This may result in total effect indices smaller than first order indices. Furthermore, if we use a linear correlation model and increase the absolute value of the correlation coefficient between two input variables close to one, the total effect indices of both variables approach to zero. For factor fixing this relation requires a step-wise fixing of a single factor and a revaluation of the indices of the remaining variables. If only the sensitivity indices of the full model are used for factor fixing, this may result in a mistaken removing of important variables. One possibility to overcome this, is to evaluate the sensitivity indices on one side for the uncorrelated part of a single variable X_i^U and on the other side for this variable including all correlated portions of the other variables $X_j^{C, X_i}, j \neq i$. This concept was introduced for first order indices of linear models in (Xu and Gertner2008). In our study we introduce first order indices S_i^C and S_i^U as well as total effect indices $S_{T_i}^C$ and $S_{T_i}^U$ for the correlated and uncorrelated parts of a single variable X_i . Per definition S_i^C is equivalent to the original first order index and $S_{T_i}^U$ to the original total effect index. The additional measures S_i^U and especially $S_{T_i}^C$ should give us additional information for factor fixing without requiring a step-wise revaluation of the sensitivity indices.

4. Estimation of sensitivity indices for correlated input variables

4.1. EXTENSION OF THE MATRIX COMBINATION APPROACH

In the original matrix combination approach presented in section 2.2 it is intended to modify a single input variable X_i by a second random sampling set while keeping the other variables unchanged in order to add or to remove the influence of X_i from the model.

In order to calculate the correlated first order and total effect indices, not only the samples of X_i itself, but also all correlated parts of the remaining variables with respect to X_i have to be modified. By assuming a linear correlation model in the standard normal space as presented in section 3.2, a decomposition of the matrices \mathbf{A} and \mathbf{B} in an uncorrelated and correlated part with respect to X_i is performed. For this purpose both matrices are transformed to the correlated standard normal space by the marginal transformations

$$\mathcal{A}_{kl} = \Phi[F_{X_l}^{-1}(A_{kl})], \quad \mathcal{B}_{kl} = \Phi[F_{X_l}^{-1}(B_{kl})], \quad (24)$$

where $\Phi(\cdot)$ is cumulative distribution function of a standard normal random variable and $F_{X_l}^{-1}(\cdot)$ is the inverse cumulative distribution function of X_l . By using the decomposition proposed in Eq. (23) we obtain the columns of the correlated and uncorrelated sampling matrices as follows

$$\mathcal{A}_{(j)}^{C,Z_i} = \rho(Z_i, Z_j)\mathcal{A}_{(i)}, \quad \mathcal{A}_{(j)}^{U,Z_i} = \mathcal{A}_{(j)} - \mathcal{A}_{(j)}^{C,Z_i}, \quad (25)$$

$$\mathcal{B}_{(j)}^{C,Z_i} = \rho(Z_i, Z_j)\mathcal{B}_{(i)}, \quad \mathcal{B}_{(j)}^{U,Z_i} = \mathcal{B}_{(j)} - \mathcal{B}_{(j)}^{C,Z_i}. \quad (26)$$

Now a modified matrix $\tilde{\mathcal{C}}_i^C$ can be obtained, which contains the uncorrelated part of \mathcal{B} with respect to Z_i and the correlated part of \mathcal{A}

$$\tilde{\mathcal{C}}_i^C = \mathcal{C}_i^{C,Z_i} = \mathcal{B}^{U,Z_i} + \mathcal{A}^{C,Z_i}. \quad (27)$$

Finally the entries of matrix $\tilde{\mathcal{C}}_i^C$ are transformed to the original space by the individual marginal transformations

$$\tilde{\mathcal{C}}_{i,kl}^C = F_{X_l}[\Phi^{-1}(\tilde{\mathcal{C}}_{i,kl}^C)]. \quad (28)$$

Since the correlated part with respect to X_i is modified simultaneously for all variables, $\tilde{\mathcal{C}}_i^C$ follows the original joint probability distribution of \mathbf{X} as shown in Figure 2.

In order to obtain the uncorrelated first order and total effect indices we use the decomposition with respect to $\mathbf{X}_{\sim i}$. For this purpose the matrices \mathcal{A} and \mathcal{B} are decomposed following Eq. (19)

$$\mathcal{A}_{(j)}^{U,\mathbf{Z}_{\sim i}} = \mathcal{A}_{(j)} - \mathcal{A}_{(j)}^{C,\mathbf{Z}_{\sim i}}, \quad \mathcal{A}_{(j=i)}^{C,\mathbf{Z}_{\sim i}} = \sum_{k=1, k \neq i}^m \beta_{Z_i, k} \mathcal{A}_{(k)}, \quad \mathcal{A}_{(j \neq i)}^{C,\mathbf{Z}_{\sim i}} = \mathcal{A}_{(j)}, \quad (29)$$

$$\mathcal{B}_{(j)}^{U,\mathbf{Z}_{\sim i}} = \mathcal{B}_{(j)} - \mathcal{B}_{(j)}^{C,\mathbf{Z}_{\sim i}}, \quad \mathcal{B}_{(j=i)}^{C,\mathbf{Z}_{\sim i}} = \sum_{k=1, k \neq i}^m \beta_{Z_i, k} \mathcal{B}_{(k)}, \quad \mathcal{B}_{(j \neq i)}^{C,\mathbf{Z}_{\sim i}} = \mathcal{B}_{(j)}. \quad (30)$$

The resulting $\tilde{\mathcal{C}}_i^U$ contains the uncorrelated part of Z_i from matrix \mathcal{A} and the correlated part with respect to $\mathbf{Z}_{\sim i}$ from matrix \mathcal{B}

$$\tilde{\mathcal{C}}_i^U = \mathcal{C}_i^{U,\mathbf{Z}_{\sim i}} = \mathcal{A}^{U,\mathbf{Z}_{\sim i}} + \mathcal{B}^{C,\mathbf{Z}_{\sim i}}. \quad (31)$$

Analogous to the correlated part, $\tilde{\mathbf{C}}_i^U$ is obtained by transforming the entries of $\tilde{\mathbf{C}}_i^U$ back to the origin space.

4.2. EXTENSION FOR REGRESSION BASED INDICES

The regression based indices presented in section 2.3 can be directly applied for correlated input variables. However, the one-dimensional coefficient of determination is an estimate of the first order index of a single variable including all correlated parts of the other variables. Using a matrix \mathbf{Z} containing the support points of the regression in the standard normal space, the first order index reads

$$\hat{S}_i^{R,C} = R_{\mathbf{Z},Z_i}^2. \quad (32)$$

The estimate for the total effect index given in Eq. (9) quantifies the total variance contribution of the uncorrelated part Z_i^U of variable Z_i

$$\hat{S}_{T_i}^{R,U} = R_{\mathbf{Z},\mathbf{Z}}^2 - R_{\mathbf{Z},\mathbf{Z}_{\sim i}}^2. \quad (33)$$

The correlated part of Z_i can be represented by the other variables and thus the explained variation of the reduced model is decreased by the contribution of Z_i^U only. The total effect of the variable Z_i including all correlated parts of the other variables can be estimated analogously to the matrix combination approach: The sampling matrix \mathbf{Z} is decomposed in a correlated and uncorrelated part with respect to Z_i according to Eq. (31). Then the uncorrelated part of the samples \mathbf{Z}^{U,Z_i} is used for the reduced model within the estimate of the total effect index

$$\hat{S}_{T_i}^{R,C} = R_{\mathbf{Z},\mathbf{Z}}^2 - R_{\mathbf{Z}^{U,Z_i},\mathbf{Z}_{\sim i}}^2. \quad (34)$$

In order to estimate the first order index of the uncorrelated part of the variable Z_i with respect to all other variables, Eq. (19) is used to calculate the uncorrelated part of i th column of the sample matrix \mathbf{Z} and the corresponding first order sensitivity index is obtained

$$\hat{S}_i^{R,U} = R_{\mathbf{Z}^{U,Z_i},\mathbf{Z}_{\sim i}}^2. \quad (35)$$

With the four measures $\hat{S}_i^{R,U}$, $\hat{S}_i^{R,C}$, $\hat{S}_{T_i}^{R,U}$ and $\hat{S}_{T_i}^{R,C}$ regression based sensitivity indices are introduced, which give similar results as the model independent measures proposed in section 4.1, but only if the regression model can represent the underlying investigated model. If this is not the case, e.g. if complex nonlinearities and interactions describe the model response Y in terms of the input variables \mathbf{X} , the polynomial based measures quantify only the contribution which is represented by the basis function. The total contribution of higher order and unexplained dependencies, which are not represented by the regression model, can be estimated using the full regression basis

$$\hat{S}_{T_i}^{U_{unexplained}} = 1 - R_{\mathbf{Z},\mathbf{Z}}^2. \quad (36)$$

Since the introduced sensitivity measures investigate the influence of a single variable including all correlated parts of the other variables, it can not be distinguished, if the influence of this variable is caused by its contribution within the model or if it is caused by its correlation with other important variables. This fact shall be clarified by a simple example: A purely additive model with three inputs is given

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3. \quad (37)$$

The input variables are normally distributed, have zero mean and the covariance

$$\Gamma = \begin{bmatrix} \sigma_{X_1}^2 & 0 & 0 \\ 0 & \sigma_{X_2}^2 & \rho\sigma_{X_2}\sigma_{X_3} \\ 0 & \rho\sigma_{X_2}\sigma_{X_3} & \sigma_{X_3}^2 \end{bmatrix}, \quad (38)$$

where ρ is the linear correlation between X_2 and X_3 .

The first order and total effect indices of this problem can be derived analytically as follows: X_3 can be formulated with respect to X_2 and vice versa as

$$\begin{aligned} X_3 &= \rho \frac{\sigma_{X_3}}{\sigma_{X_2}} X_2 + \sqrt{1 - \rho^2} X_3^U, \\ X_2 &= \rho \frac{\sigma_{X_2}}{\sigma_{X_3}} X_3 + \sqrt{1 - \rho^2} X_2^U, \end{aligned} \quad (39)$$

with X_2^U and X_3^U having the same variances as X_2 and X_3 , respectively. Since X_2 and X_3^U as well as X_3 and X_2^U are independent, we can calculate the variance contribution of the inputs as follows

$$\begin{aligned} V_{X_1^C}(Y) &= V_{X_1^U}(Y) = \beta_1^2 \sigma_{X_1}^2, \\ V_{X_2^C}(Y) &= (\beta_2 \sigma_{X_2} + \rho \beta_3 \sigma_{X_3})^2, \\ V_{X_2^U}(Y) &= (1 - \rho^2) \beta_2^2 \sigma_{X_2}^2, \\ V_{X_3^C}(Y) &= (\beta_3 \sigma_{X_3} + \rho \beta_2 \sigma_{X_2})^2, \\ V_{X_3^U}(Y) &= (1 - \rho^2) \beta_3^2 \sigma_{X_3}^2. \end{aligned} \quad (40)$$

With help of the total variance

$$V(Y) = V_{X_1}(Y) + V_{X_2^C}(Y) + V_{X_3^U}(Y) = V_{X_1}(Y) + V_{X_2^U}(Y) + V_{X_3^C}(Y), \quad (41)$$

the sensitivity indices can be determined

$$S_i^C = S_{T_i}^C = \frac{V_{X_i^C}(Y)}{V(Y)}, \quad S_i^U = S_{T_i}^U = \frac{V_{X_i^U}(Y)}{V(Y)}. \quad (42)$$

From Eq. (40) it follows, that the variance contribution of the uncorrelated parts of X_2 and X_3 vanish if the correlation coefficient tends to one or minus one. On the other hand it can be seen, that if one of the variable factors β_2 or β_3 is zero, the corresponding variance contribution and thus the sensitivity index of the correlated part is not zero, due to the remaining influence of the other variable.

In order to distinguish between the variance contribution due to the correlation and the contribution by the model parameters, an effective variance contribution is defined

$$V_{X_i}^{eff}(Y) = \beta_i^2 \sigma_{X_i}^2. \quad (43)$$

For the general polynomial regression case, the following procedure is proposed: First the full regression model is build up in the standard normal space and the regression coefficients $\hat{\beta}$ are determined. Then the

first order effects are estimated by using only the linear and quadratic coefficients of the full model, which belong to the investigated variable Z_i ,

$$\hat{S}_i^\beta = \frac{V_{\beta_{Z_i}}(Y)}{V(Y)}, \quad (44)$$

where $V_{\beta_{Z_i}}(Y)$ is the resulting variance if only the first order regression terms of Z_i are considered. Total effects can be estimated similarly

$$\hat{S}_{T_i}^\beta = 1 - \frac{V_{\beta_{\mathbf{Z}_{\sim i}}}(Y)}{V(Y)}, \quad (45)$$

where $V_{\beta_{\mathbf{Z}_{\sim i}}}(Y)$ is estimated by using the regression model without all coefficients, first order and interaction, which belong to Z_i . The definition of \hat{S}_i^β and $\hat{S}_{T_i}^\beta$ is not following the general definition of the first order and total effect sensitivity indices, where the variance of conditional expectation is used. Nevertheless, this measures may be used to give additional information about the unknown underlying model.

However, for strongly correlated random variables the accuracy of the estimated regression coefficients may be very poor. In such a case the estimated sensitivity measures \hat{S}_i^β and $\hat{S}_{T_i}^\beta$ may have very low accuracy. In the first numerical example, this problem is investigated.

5. Numerical examples

5.1. ADDITIVE LINEAR MODEL

In the first example a purely additive model is investigated

$$Y = X_1 + X_2 + X_3. \quad (46)$$

The input variables are normally distributed, have zero mean and the covariance

$$\Gamma = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 2\rho \\ 0 & 2\rho & 4 \end{bmatrix}. \quad (47)$$

Different cases with $\rho = 0.0, 0.8, 0.99999, -0.8, -0.5$ are investigated with the sampling based approach and the regression based approach. The sampling based sensitivity indices are calculated using the subset averaging and the proposed matrix recombination method with 10.000 Latin Hypercube samples. In Table I the estimated sensitivity indices are compared to the analytical solution obtained with Eq. (40). The table indicates a very good agreement of all estimated indices with the reference values for the uncorrelated and the correlated cases. In the uncorrelated case, the sensitivity indices of an additive model sum up to one. By considering correlated inputs this is not the case, since coupling terms caused by the correlations are introduced indirectly into the model. This can result in a sum larger than one (correlated formulation with $\rho = 0.8$) and also smaller than one (correlated formulation with $\rho = -0.5$, uncorrelated formulation with $\rho = 0.8$). Interestingly the influence of a variable seems to vanish looking only on the correlated or uncorrelated formulation of the total effect indices which is observed for variable X_2 in the correlated formulation with $\rho = -0.5$ and X_2 and X_3 in the uncorrelated formulation with $\rho = 1.0$. However, if both

Table I. Sensitivity indices of the additive model assuming uncorrelated and correlated inputs

	Analytical		Subset	Matrix combination						Regression			
	$S_i^C, S_{T_i}^C$	$S_i^U, S_{T_i}^U$	\hat{S}_i	\tilde{S}_i^C	$\tilde{S}_{T_i}^C$	\tilde{S}_i^U	$\tilde{S}_{T_i}^U$	$\hat{S}_i^{R,C}$	$\hat{S}_{T_i}^{R,C}$	$\hat{S}_i^{R,U}$	$\hat{S}_{T_i}^{R,U}$	\hat{S}_i^β	$\hat{S}_{T_i}^\beta$
$\rho = 0.0$													
X_1	0.167	0.167	0.177	0.157	0.168	0.157	0.166	0.155	0.155	0.168	0.168	0.168	0.155
X_2	0.167	0.167	0.177	0.154	0.164	0.153	0.163	0.168	0.168	0.169	0.168	0.168	0.168
X_3	0.667	0.667	0.674	0.667	0.673	0.669	0.672	0.670	0.670	0.672	0.672	0.672	0.670
$\rho = 0.8$													
X_1	0.109	0.109	0.118	0.117	0.108	0.118	0.107	0.110	0.110	0.109	0.108	0.109	0.110
X_2	0.735	0.039	0.742	0.738	0.727	0.050	0.039	0.735	0.735	0.040	0.039	0.109	0.456
X_3	0.852	0.157	0.861	0.858	0.848	0.169	0.157	0.853	0.853	0.156	0.156	0.434	0.783
$\rho = 0.99999$													
X_1	0.100	0.100	0.110	0.088	0.103	0.088	0.101	0.099	0.099	0.101	0.100	0.100	0.099
X_2	0.900	0.000	0.907	0.900	0.916	0.000	0.000	0.900	0.900	0.001	0.000	0.100	0.500
X_3	0.900	0.000	0.907	0.900	0.916	0.000	0.000	0.900	0.900	0.001	0.000	0.401	0.800
$\rho = -0.8$													
X_1	0.357	0.357	0.368	0.361	0.359	0.359	0.359	0.362	0.362	0.354	0.353	0.353	0.362
X_2	0.129	0.129	0.137	0.141	0.130	0.136	0.139	0.134	0.134	0.127	0.127	0.353	-0.788
X_3	0.514	0.514	0.523	0.527	0.513	0.520	0.512	0.521	0.521	0.509	0.509	1.420	0.300
$\rho = -0.5$													
X_1	0.250	0.250	0.256	0.240	0.250	0.243	0.249	0.241	0.241	0.254	0.253	0.253	0.241
X_2	0.000	0.188	0.011	0.005	0.000	0.179	0.188	0.000	0.000	0.189	0.188	0.253	-0.266
X_3	0.563	0.750	0.573	0.571	0.570	0.755	0.752	0.564	0.564	0.759	0.759	1.023	0.495

the correlated and uncorrelated formulation of the total effect indices are considered, no important variable can be misinterpreted or mistakenly removed from the model. This is not the case if either only the correlated or the uncorrelated formulation is used.

Additionally the regression based indices by using 1000 Latin Hypercube samples as support points are given in Table I. The estimates $\hat{S}_i^{R,U}$, $\hat{S}_i^{R,C}$, $\hat{S}_{T_i}^{R,U}$ and $\hat{S}_{T_i}^{R,C}$ agree very well with the analytical values. The introduced measures \hat{S}_i^β and $\hat{S}_{T_i}^\beta$, which analyze the variance contribution by coefficient removing, are equivalent for the uncorrelated case. In the correlated case, the results differ in that way, that these indices indicate how the total variance is decreased or eventually increased, if the variable X_i is removed completely from the model formulation. For this reason negative indices or values larger as one are possible in contrast to classical sensitivity indices. This measures should be considered as additional information in order to detect imaginary variable importance caused only by input correlations.

However, the accuracy of the coefficient based indices \hat{S}_i^β and $\hat{S}_{T_i}^\beta$ may be very low for highly correlated variables, if the regression model can not represent the true model perfectly. This situation is analyzed by adding to the deterministic model a random noise ϵ which is independent of the inputs

$$Y = X_1 + X_2 + X_3 + \epsilon, \quad (48)$$

where ϵ is a zero-mean normally distributed random variable with standard deviation $\sigma_\epsilon = 0.5$. In Figure 3 the standard deviation of the estimated regression coefficients of the tree inputs are shown for a set of 100 support point samples. The figure indicates an increasing error in the regression coefficients of both correlated variables if the correlation coefficient is increased, while the error in the coefficient of the uncorrelated variable is almost unchanged. This results in an inaccurate estimate of the sensitivity measures \hat{S}_i^β and $\hat{S}_{T_i}^\beta$.

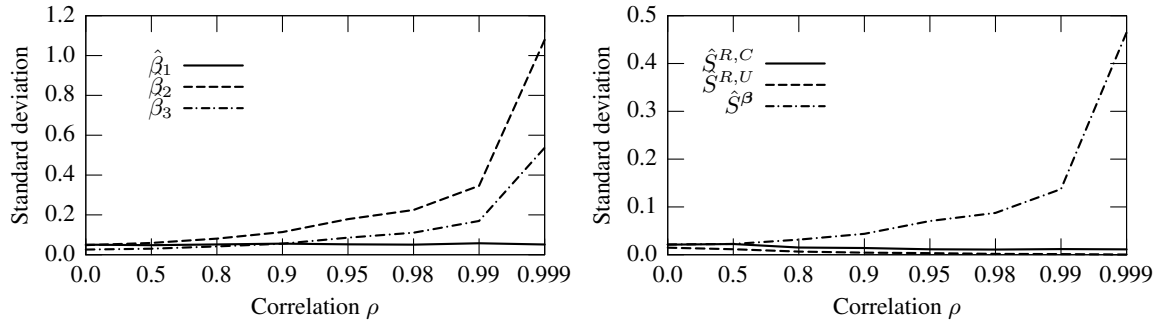


Figure 3. Standard deviation of the regression coefficients (left) and the estimated total effect sensitivity indices of X_2 (right) dependent on the correlation for the additive model including random noise

for highly correlated variables. In Figure 3 the standard deviation of the estimated index $\hat{S}_{T_2}^\beta$ is displayed additionally. Similar to the regression coefficient itself, the accuracy of the sensitivity index decreases with increasing correlation. Nevertheless, if the variables are correlated with $\rho \leq 0.9$ the error in the estimate seems acceptable. In contrast to the measure based on single regression coefficients, the accuracy of the sensitivity indices estimated as the difference of the coefficient of determination of the full and a reduced regression model is not decreased with increasing correlation. This is plotted additionally in Figure 3. Using only 100 samples, the accuracy of the estimated regression based measures seems very good.

5.2. COUPLED NONLINEAR MODEL

In the second example a nonlinear model is investigated, which contains linear, quadratic and interaction terms

$$Y = X_1 + 2X_1^2 + X_2 + X_3 + X_2X_3. \quad (49)$$

The covariance is taken analogous to the previous example. In Figure 4 the scatter plots are shown for the first two variables. In the figure a significant quadratic influence of X_1 and a significant influence of the coupling term X_2X_3 can be remarked in the uncorrelated case. If X_2 and X_3 are assumed to be correlated, the scatter plot of X_2 with Y indicates also a quadratic behavior, while in the model formulation only a linear and a coupling term appears. This quadratic influence can be explained, if we rewrite Eq. (49) by considering the decomposition of X_3 analogous to Eq. (39) as follows

$$Y = X_1 + 2X_1^2 + X_2 + \rho \frac{\sigma_{X_3}}{\sigma_{X_2}} X_2 + \sqrt{1 - \rho^2} X_3^U + \rho \frac{\sigma_{X_3}}{\sigma_{X_2}} X_2^2 + \sqrt{1 - \rho^2} X_2 X_3^U. \quad (50)$$

In Table II the corresponding sensitivity indices are given. The table indicates a good agreement of the first order indices estimated with the extended matrix combination approach and the regression based method with the indices obtained with the subset averaging. The effect seen in the scatter plots, that the influence of X_2 dominated in the uncorrelated case by the coupling term and in the correlated case by quadratic dependencies, can be observed also in the sensitivity indices. In the uncorrelated case the difference between first order and total effect indices of X_2 is more than 20%, but in the correlated case this difference decreases significantly. This example clarifies, that the proposed measures quantifying the total effect influence give useful information for model interpretation in the case of correlated inputs.

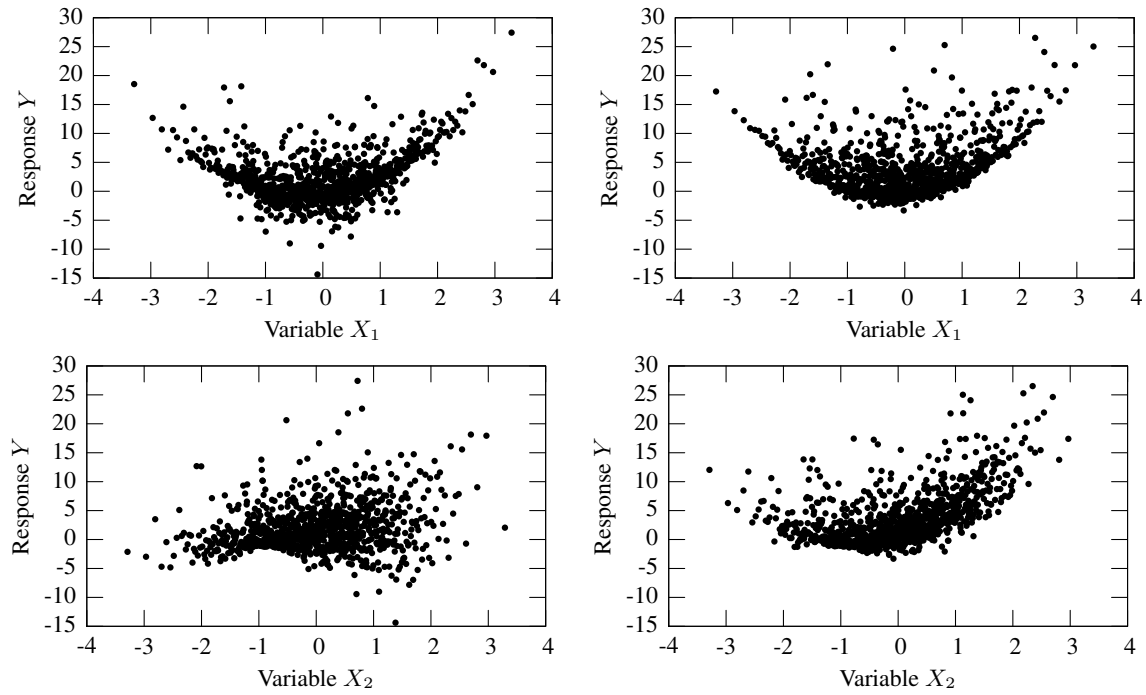


Figure 4. Anthill plots of the response of the coupled nonlinear function with respect to X_1 and X_2 by assuming $\rho = 0.0$ (left) and $\rho = 0.8$ (right)

Table II. Sensitivity indices of the coupled nonlinear model assuming uncorrelated and correlated inputs

	Subset	Matrix combination				Regression					
	\hat{S}_i	\hat{S}_i^C	$\hat{S}_{T_i}^C$	\hat{S}_i^U	$\hat{S}_{T_i}^U$	$\hat{S}_i^{R,C}$	$\hat{S}_{T_i}^{R,C}$	$\hat{S}_i^{R,U}$	$\hat{S}_{T_i}^{R,U}$	\hat{S}_i^β	$\hat{S}_{T_i}^\beta$
$\rho = 0.0$											
X_1	0.484	0.489	0.518	0.490	0.518	0.491	0.511	0.491	0.510	0.512	0.491
X_2	0.070	0.036	0.256	0.034	0.259	0.060	0.292	0.059	0.291	0.058	0.274
X_3	0.231	0.217	0.452	0.216	0.454	0.204	0.441	0.204	0.440	0.231	0.436
$\rho = 0.8$											
X_1	0.382	0.405	0.362	0.405	0.361	0.373	0.367	0.371	0.365	0.365	0.373
X_2	0.501	0.528	0.540	0.055	0.071	0.506	0.562	0.014	0.072	0.041	0.469
X_3	0.551	0.548	0.592	0.090	0.123	0.565	0.615	0.064	0.120	0.165	0.593

5.3. ISHIGAMI FUNCTION

In the final example the well-known Ishigami function (Ishigami and Homma1990) is investigated. This function was defined for independent uniformly distributed variables

$$-\pi \leq X_i \leq \pi, \quad i = 1, 2, 3, \quad (51)$$

as follows

$$Y = \sin(X_1) + a \sin^2(X_2) + bX_3^4 \sin(X_1), \quad (52)$$

with $a = 7.0$ and $b = 0.1$. The analytical first order and total sensitivity indices were derived in (Homma and Saltelli1996) and are given in Table III. The values indicate a vanishing first order influence of X_3 but a significant coupling term of X_1 and X_3 as indicated in the total effect indices.

In our analysis again the subset averaging and the matrix combination approach are applied using 10.000 Latin Hypercube samples. The regression based approach is not used due to the highly nonlinear functional behavior, which can not be represented by low order polynomials. The results of the analyses assuming uncorrelated and even correlated inputs are given additionally in Table III.

The correlation has been assumed in the second case between X_1 and X_3 as $\rho_{23} = 0.5$. In the Nataf model this correlation coefficient is transformed to $\tilde{\rho}_{23} = 0.518$ in the correlated Gaussian space using the iteration in Eq. (14). In the third case additional correlations are introduced ($\rho_{12} = 0.3$, $\rho_{23} = 0.8$, $\tilde{\rho}_{12} = 0.313$, $\tilde{\rho}_{23} = 0.814$). For the uncorrelated case the indices obtained with the different methods agree

Table III. Sensitivity indices of the Ishigami test function assuming uncorrelated and correlated inputs

	Analytical		Subset \hat{S}_i	Matrix combination			
	S_i	S_{T_i}		\hat{S}_i^C	$\hat{S}_{T_i}^C$	\hat{S}_i^U	$\hat{S}_{T_i}^U$
$\rho_{23} = 0.0$							
X_1	0.314	0.557	0.324	0.330	0.570	0.330	0.570
X_2	0.442	0.442	0.461	0.456	0.429	0.456	0.429
X_3	0.000	0.244	0.008	0.008	0.251	0.008	0.251
$\rho_{13} = 0.5$							
X_1	-	-	0.305	0.312	0.453	0.065	0.346
X_2	-	-	0.479	0.484	0.473	0.484	0.473
X_3	-	-	0.174	0.172	0.444	0.071	0.200
$\rho_{12} = 0.3, \rho_{13} = 0.5, \rho_{23} = 0.8$							
X_1	-	-	0.310	0.306	0.799	0.057	0.354
X_2	-	-	0.576	0.559	0.785	0.022	0.454
X_3	-	-	0.213	0.198	0.927	0.022	0.117

very well with the theoretical values. Interestingly for the first correlated case, the first order index of X_3 increases significantly due to the correlation.

5.4. CONCLUSIONS

In the presented paper an extension of the classical Sobol' estimator for correlated input variables has been proposed. In this method the matrix recombination is modified by changing not only the variable itself but also its coupling terms with other variables due to the correlations. For this purpose a decomposition of the sampling matrices in an uncorrelated and a correlated part is proposed. This decomposition is based on a linear correlation model between the input variables. Additionally a regression based approach is presented, which is much more efficient, if the model behavior can be represented by the regression basis. However, attention is required in both methods in order to perform the decomposition. For non-normally distributed inputs a transformation to the Gaussian space is necessary before decomposing the samples.

Appendix

In the standard normal space the correlated part of a single variable Z_i can be represented by the remaining variable set $\tilde{\mathbf{Z}} = \mathbf{Z}_{\sim i}$ as follows

$$Z_i^{C,\tilde{\mathbf{Z}}} = \beta_{Z_i,0} + \sum_{j=1}^{m-1} \beta_{Z_i,j} \tilde{Z}_j. \quad (53)$$

The intercept $\beta_{Z_i,0}$ is zero, since all variables are normally distributed with zero mean. An estimate of the coefficients β_{Z_i} can be obtained from a discrete sample matrix \mathbf{Z} by using linear regression

$$\hat{\beta}_{Z_i} = (\mathbf{P}_{\tilde{\mathbf{Z}}}^T \mathbf{P}_{\tilde{\mathbf{Z}}})^{-1} \mathbf{P}_{\tilde{\mathbf{Z}}}^T \mathbf{Z}_{(i)}, \quad (54)$$

where $\mathbf{Z}_{(i)}$ is the i th column of \mathbf{Z} and the level matrix $\mathbf{P}_{\tilde{\mathbf{Z}}}$ of the reduced variable set contains all columns of \mathbf{Z} without the i th column. The entries of $\mathbf{P}_{\tilde{\mathbf{Z}}}^T \mathbf{P}_{\tilde{\mathbf{Z}}}$ can be obtained from the reduced sample matrix $\tilde{\mathbf{Z}}$ as follows

$$(\mathbf{P}_{\tilde{\mathbf{Z}}}^T \mathbf{P}_{\tilde{\mathbf{Z}}})_{kl} = \sum_{t=1}^n \tilde{Z}_{tk} \tilde{Z}_{tl}. \quad (55)$$

In the case of standard normal variables, the sum in Eq. (55) can be formulated in terms of the estimator of the correlation coefficients as follows

$$(\mathbf{P}_{\tilde{\mathbf{Z}}}^T \mathbf{P}_{\tilde{\mathbf{Z}}})_{kl} = (n-1) \hat{\rho}(\tilde{Z}_k, \tilde{Z}_l). \quad (56)$$

Analogously, the entries of $\mathbf{P}_{\tilde{\mathbf{Z}}}^T \mathbf{Z}_{(i)}$ can be formulated as

$$(\mathbf{P}_{\tilde{\mathbf{Z}}}^T \mathbf{Z}_{(i)})_k = \sum_{t=1}^n \tilde{Z}_{tk} Z_{ti} = (n-1) \hat{\rho}(\tilde{Z}_k, Z_i), \quad (57)$$

which finally results in the estimates of the regression coefficients

$$\hat{\beta}_{Z_i} = (\hat{\mathbf{C}}_{\tilde{\mathbf{Z}}\tilde{\mathbf{Z}}})^{-1} \hat{\boldsymbol{\rho}}_{\tilde{\mathbf{Z}}, Z_i}, \quad (58)$$

where $\mathbf{C}_{\tilde{\mathbf{Z}}\tilde{\mathbf{Z}}}$ is the correlation matrix of the reduced variable set $\tilde{\mathbf{Z}}$. In order to generate samples of the full variable set \mathbf{Z} the input correlation values have to be defined. If this is the case, the predefined values instead of the estimators can be used and the regression coefficients β_{Z_i} can be exactly determined.

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