1 Qualitative GSA measures for functions with correlated input parameters

This chapter explains the computation of the EE-based screening measures that are applied to the Keane and Wolpin (1994) model. First, I outline two sampling schemes that are tailored to the computation of EEs. Second, I present a simplified version of the approach to extend EEs to models with correlated parameters by Ge and Menendez (2017). Third, I develop an improvement to these measures that sustains the EE's fundamental derivative characteristic. The section concludes with the analysis of a test function. This analysis shows, first, my ability to replicate the results in Ge and Menendez (2017), and second, validates my improvement.

1.1 Sampling Schemes

In the following, I present two sampling schemes, the trajectory and the radial design. These are tailored to the computation of EEs. However, positional differences in these samples cause differences in post-processing these to compute the EEs.

According to several experiments by Campolongo et al. (2011) with common test functions, the best design is the radial design (Saltelli (2002)) and the most commonly used is the trajectory design (Morris (1991)). Both designs are comprised by a $(k+1) \times k$-dimensional matrix. The elements are generated in $[0, 1]$. Afterwards, they can potentially be transformed to the distributions of choice. The columns represent the different input parameters and each row is a complete input parameter vector. To compute the aggregate qualitative measures, a set of multiple matrices, or sample subsets, of input parameters has to be generated.

A matrix in radial design is generated the following way: Draw a vector of length $2k$ from a quasi-random sequence. The first row, or parameter vector, is the first half of the sequence. Then, copy the first row to the remaining k rows. For each row k' of the remaining 2, ..., $k+1$ rows, replace the k'-th element by the k'-th element of the second half of the vector. This generates a matrix of the following form:

$$\underset{(k+1)\times k}{\mathbf{R}} = \begin{pmatrix} a_1 & a_2 & ... & a_k \\ \mathbf{b_1} & a_2 & ... & a_k \\ a_1 & \mathbf{b_2} & ... & a_k \\ \vdots & \vdots & \ddots & \vdots \\ a_1 & a_2 & ... & \mathbf{b_k} \end{pmatrix} \tag{1}$$

Note here, that each column consists only of the respective first row element, except of in one row. From this matrix, one EE can be obtained for each parameter X_i. This is achieved by using the $(i+1)$-th row as function argument for the minuend and the first row as subtrahend in the EE formula in Equation (**??**). Then, $\Delta^{(i,j)} = b_i^{(j)} - a_i^{(j)}$. The asterisk is an index for all elements of a vector.

$$d_i = \frac{Y(\mathbf{a_{\sim i}}, b_i) - Y(\mathbf{a})}{b_i - a_i} = \frac{Y(\mathbf{R_{i+1,*}}) - Y(\mathbf{R_{1,*}})}{b_i - a_i}. \tag{2}$$

If the number of radial subsamples is high, the draws from the quasi-random sequence lead to a good and fast coverage of the input space (compared to a random sequence). The quasi-random sequence considered here is the Sobol' sequence. This sequence is comparably successful in covering the unit hypercube, but also conceptually more involved. Therefore, its presentation is beyond the scope of this work. Since this sequence is quasi-random, the sequence has to be drawn at once for all sets of radial matrices.

Next, I present the trajectory design. As we will see, it leads to a relatively representative coverage for a very small number of subsamples but also to repetitions of similar draws. I skip the equations that generate a trajectory and present the method verbally. There are different forms of trajectories. I focus on the common version presented in Morris (1991) that generates equiprobable elements. The first step is to decide the number p of equidistant grid points in interval $[0, 1]$. Then, the first row of the trajectory is composed of the lower half value of these grid points. Now, fix $\Delta = p/[2(p-1)]$. This function implies, that adding Δ to the lowest point in the lowest half results in the lowest point of the upper half of the grid points, and so on. The rest of the rows is constructed by, first, copying the row one above and, second, by adding Δ to the i-th element of the $i+1$-th row. The created matrix scheme is depicted below.

$$\underset{(k+1)\times k}{\mathbf{T}} = \begin{pmatrix} a_1 & a_2 & \dots & a_k \\ \mathbf{b_1} & a_2 & \dots & a_k \\ \mathbf{b_1} & \mathbf{b_2} & \dots & a_k \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{b_1} & \mathbf{b_2} & \dots & \mathbf{b_k} \end{pmatrix} \tag{3}$$

In contrary to the radial scheme, each b_i is copied to the subsequent row. Therefore, the EEs have to be determined by comparing each row with the row above instead of with the first row. Importantly, two random transformations are common. These are randomly switching rows and randomly interchanging the i-th column with the $(k-i)$-th column and then reversing the column. The first transformation is skipped as it does not add additional coverage and because we need the stairs-shaped design to facilitate later transformations which account for correlations between input parameters. The second transformation is adapted because it is important to also have negative steps and because it sustains the stairs shape. Yet, this implies that Δ is also parameter- and trajectory-specific. Let f

and h be additional indices representing the input parameters. The derivative formula is adapted to the trajectory design as follows:[1]

$$d_i = \frac{Y(\mathbf{b_{f \leq i}}, \mathbf{a_{h > i}}) - Y(\mathbf{b_{f < i}}, \mathbf{a_{h \geq i}})}{b_i - a_i} = \frac{Y(\mathbf{T_{i+1,*}}) - Y(\mathbf{T_{i,*}})}{b_i - a_i}. \tag{4}$$

The trajectory design involves first, a fixed grid, and second and more importantly, a fixed step Δ. s.t. $\{\Delta\} = \{\pm\Delta\}$. This implies less step variety and less space coverage vis-á-vis the radial design for more than a small number of draws.

To improve the coverage of the sample space by the trajectories, Campolongo et al. (2007) develop a post-selection approach based on distances. The approach creates enormous costs for more than a small number of trajectories. This problem is effectively mitigated by Ge and Menendez (2014). The following describes the main ideas of both contributions.

The objective is to select k trajectories from a set of N matrices. Campolongo et al. (2007) assign a distance to each pair of trajectories in the start set. To each set of pair combinations in every possible subset containing k trajectories, Campolongo et al. assign an aggregate distance based on the pair distance. Then, the optimized trajectory set is the subset with the highest aggregate distance.

This is computationally very costly, because each aggregate distance is a sum of a binomial number of pair distances[2]. To decrease the computation time, Ge and Menendez (2014) propose two improvements. First, in each iteration i, they select only $N(i) - 1$ matrices from a set containing $N(i)$ trajectories until the set size has decreased to k. Second, they compute the pair distances in each iteration based on the aggregate distances and the pair distances from the first set. Due to numerical imprecisions, their improvement does not always result in the same set as obtained from Campolongo et al. (2007). However, the sets are usually very similar in terms of the aggregate distance. This thesis only uses the first step in Ge and Menendez (2014) to post-select the trajectory set because the second step does not provide any gain.[3]

So far, we have only considered draws in [0,1]. For uncorrelated input parameters from arbitrary distributions with well-defined CDF, Φ, one would simply evaluate each element (potentially including the addition of the step) by the inverse CDF, or quantile function, Φ^{-1}, of the respective parameter. One intuition is, that Φ maps the sample space to [0,1]. Hence Φ^{-1} can be used to transform random draws in [0,1] to the sample space of the arbitrary distribution. This is a basic example of so-called inverse transform sampling which we will recall in the next section.

[1] In contrary to most authors, I also denote the step as a subtraction instead of Δ when referring to the trajectory design. This provides additional clarity.

[2] For example, $\binom{30}{15} = 155117520$.

[3] This refers only to my implementation.

1.2 The approach for correlated input parameters in Ge and Menendez (2017)

This section describes the incomplete approach by Ge and Menendez (2017) to extend the EE-based measures to input parameters that are correlated. Their main achievement is to outline a transformation of samples in radial and trajectory design that incorporates the correlation between the input parameters. This implies, that the trajectory and radial samples cannot be written as in Equation (2) and Equation (4). The reason is that the correlations of parameter X_i, to which step Δ^i is added, implies that all other parameters in the same row with non-zero correlation in $\mathbf{X_{\sim i}}$ are changed as well. Therefore, the rows cannot be denoted and compared as easily by a's and b's as in Equation (2) and (4). Transforming these matrices allows to re-define the EE-based measures accordingly, such that they sustain the main properties of the ordinary measures for uncorrelated parameters. The property is being a function of the mean derivative. Yet, Ge and Menendez (2017) fail to fully develop these measures. I explain how their measures lead to arbitrary results for correlated input parameters. This section covers their approach in a simplified form, focussing on normally distributed input parameters, and presents their measures.

The next paragraph deals with developing a recipe for transforming draws $\mathbf{u} = \{u_1, u_2, ..., u_k\}$ from $[0, 1]$ for an input parameter vector to draws $\mathbf{x} = \{x_1, x_2, ..., x_k\}$ from an arbitrary joint normal distribution. We will do this in three steps.

For this purpose, let $\mathbf{\Sigma}$ be a non-singular variance-covariance matrix and let $\boldsymbol{\mu}$ be the mean vector. The k-variate normal distribution is denoted by $\mathcal{N}_k(\boldsymbol{\mu}, \mathbf{\Sigma})$.

Creating potentially correlated draws $\mathbf{x}$ from $\mathcal{N}_k(\boldsymbol{\mu}, \mathbf{\Sigma})$ is simple. Following Gentle (2006)[4], this can be achieved the following way: Draw a k-dimensional row vector of i.i.d standard normal deviates from the *univariate* $N_1(0, 1)$ distribution, such that $\mathbf{z} = \{z_1, z_2, ..., z_k\}$, and compute the Cholesky decomposition of Σ, such that $\mathbf{\Sigma} = \mathbf{T^T T}$. The lower triangular matrix is denoted by $\mathbf{T^T}$. Then apply the operation in Equation (10) to obtain the correlated deviates from $\mathcal{N}_k(\boldsymbol{\mu}, \mathbf{\Sigma})$.

$$\mathbf{x} = \boldsymbol{\mu} + \mathbf{T^T z^T} \tag{5}$$

Intuition for the underlying mechanics is provided in Appendix A.

The next step is to understand that we can split the operation in Equation (10) into two subsequent operations. For this, let $\boldsymbol{\sigma}$ be the vector of standard deviations and let $\mathbf{R_k}$ be the correlation matrix of $\mathbf{x}$.

The first operation is to transform the standard deviates $\mathbf{z}$ to correlated standard deviates $\mathbf{z_c}$ by using $\mathbf{z_c} = \mathbf{Q^T z^T}$. In this equation, $\mathbf{Q^T}$ is the lower matrix from the

[4]See page 197

Cholesky decomposition $\mathbf{R_k} = \mathbf{Q^T Q}$. This is equivalent to the above approach in Gentle (2006) for the specific case of the multivariate standard normal distribution $\mathcal{N}_k(0, R_k)$. This is true because for multivariate standard normal deviates, the correlation matrix is equal to the covariance matrix.

The second operation is to scale the correlated standard normal deviates: $\mathbf{z} = \mathbf{z_c}(\mathbf{i})\boldsymbol{\sigma}(\mathbf{i}) + \boldsymbol{\mu}.$, where the is indicate an element-wise multiplication.

The last step to construct the final approach is to recall the inverse transform sampling method. Therewith, we can transform the input parameter draws $\mathbf{u}$ to uncorrelated standard normal draws $\mathbf{z}$. Then we will continue with the two operation in the above paragraph. The transformation from $\mathbf{u}$ to $\mathbf{z}$ is denoted by $F^{-1}(\Phi^c)$, where the c in Φ^c stand for the introduced correlation. This transformation is summarized by the following three points:

$$\left.\begin{array}{l} \textbf{Step 1: } \mathbf{z} = \boldsymbol{\Phi^{-1}}(\boldsymbol{u}) \\[2ex] \textbf{Step 2: } \mathbf{z_c} = \mathbf{Q^T z^T} \\[2ex] \textbf{Step 3: } \mathbf{x} = \boldsymbol{\mu} + \mathbf{z_c}(\mathbf{i})\boldsymbol{\sigma}(\boldsymbol{i}) \end{array}\right\} F^{-1}(\Phi^c) \stackrel{\text{def}}{=} \mathcal{T}_2$$

Step 3 is specific to the normal sample space in which we are interested in. A mapping to other sample spaces can, for instance. be achieved by, first, applying Φ^c and, second, the inverse CDF of the desired distribution.
The procedure described in the three steps above is equivalent to an inverse Rosenblatt transformation, a linear inverse Nataf transformation[5] for parameters in normal sample space and connects to Gaussian copulas. These concepts can be used to transform deviates in [0,1] to the sample space of arbitrary distributions by using the properties sketched above under varying assumptions. Notes on this relation are provided in Appendix B.

The one most important point to understand is that the transformation comprised by the three steps listed above is not unique for correlated input parameters. Rather, the transformation changes with the order of parameters in vector $\mathbf{u}$[6]. This can be seen from the lower triangular matrix $\mathbf{Q^T}$. To prepare the next equation, let $\mathbf{R_k} = (\rho_{ij})_{ij=1}^{k}$ and sub-matrix $\mathbf{R_h} = (\rho_{ij})_{ij=1}^{h}$, $h \leq k$. Also let $\boldsymbol{\rho_i^{*,j}} = (\rho_{1,j}, \rho_{2,j}, ..., \rho_{i-1,j})$ for $j \geq i$ with the following abbreviation $\boldsymbol{\rho_i} \stackrel{\text{def}}{=} \boldsymbol{\rho_i^{*,i}}$. Following Madar (2015), the lower matrix can be written as

[5]For the first two transformations, see Lemaire (2013), page 78 - 113
[6]This point is more obvious in the formal definition of the Rosenblatt transformation.

$$\mathbf{Q^T} = \begin{pmatrix} 1 & 0 & 0 & \dots & 0 \\ \rho_{1,2} & \sqrt{1-\rho_{1,2}^2} & 0 & \dots & 0 \\ \rho_{1,3} & \frac{\rho_{2,3}-\rho_{1,2}\rho_{1,3}}{\sqrt{1-\rho_{1,2}^2}} & \sqrt{1-\boldsymbol{\rho_3}\mathbf{R_2^{-1}}\boldsymbol{\rho_3^T}} & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \rho_{1,k} & \frac{\rho_{2,k}-\rho_{1,2}\rho_{1,k}}{\sqrt{1-\rho_{1,2}^2}} & \frac{\boldsymbol{\rho_{3,k}}-\boldsymbol{\rho_3^{*,k}}\mathbf{R_2^{-1}}\boldsymbol{\rho_3^T}}{\sqrt{1-\boldsymbol{\rho_3}\mathbf{R_2^{-1}}\boldsymbol{\rho_3^T}}} & \dots & \sqrt{1-\boldsymbol{\rho_k}\mathbf{R_2^{-1}}\boldsymbol{\rho_k^T}} \end{pmatrix}. \tag{6}$$

Equation (11), together with Step 2, implies that the order of the uncorrelated standard normal deviates $\boldsymbol{z}$ constitute a hierarchy amongst the correlated deviates $\mathbf{z_c}$, in the following manner: The first parameter is not subject to any correlations, the second parameter is subject to the correlation with the first parameter, the third parameter is subject to the correlations with the parameters before, etc. Therefore, if parameters are correlated, typically $\mathbf{Q^T z^T} \neq \mathbf{Q^T}(\mathbf{z}')^\mathbf{T}$ and $F^{-1}(\Phi)(\mathbf{u}) \neq F^{-1}(\Phi)(\mathbf{u}')$, where $\mathbf{z}'$ and $\mathbf{u}'$ denote $\mathbf{z}$ and $\mathbf{u}$ in different orders. Metaphorically speaking, the correlations are transferred like the fall of dominoes.

Coming back to the EE-based measures for correlated inputs, Ge and Menendez (2017) attempt to construct two variations of EEs, d_i, in Equation (**??**). They name one derivative the independent Elementary Effects, d_i^{ind}, and the other the full Elementary Effects, d_i^{full}. For each of these two EEs, they derive the aggreate measures μ, μ^* and σ. The difference between the two EEs is that d^{ind} excludes and d^{full} includes the effect of the correlations from adding the step Δ^i to X_i on the other parameters $\mathbf{X_{\sim i}}$. Knowing d_i^{ind} is important because the correlations can decrease d_i^{full} (close to 0). However, if the independent-EE-based measures are not close to zero, X_i is still important. Additionally, fixing this parameter can potentially change d_i^{full} for $\mathbf{X_{\sim i}}$.

For the trajectory design, the formula for the full Elementary Effect, is given by

$$d_i^{full,T} = \frac{f\Big(\mathcal{T}(\mathbf{T_{i+1,*}}; i-1)\Big) - f\Big(\mathcal{T}(\mathbf{T_{i,*}}; i)\Big)}{\Delta}. \tag{7}$$

In Equation (12), $\mathcal{T}(\cdot; i) \overset{\text{def}}{=} \mathcal{T}_3\Bigg(\mathcal{T}_2\Big(\mathcal{T}_1(\cdot; i)\Big); i\Bigg)$. $\mathcal{T}_1(\cdot; i)$ orders the parameters, or the row elements, to establish the right correlation hierarchy. $\mathcal{T}_2$, or $F^{-1}(\Phi)$, correlates the draws in $[0, 1]$ and transforms them to the sample space. $\mathcal{T}_3(\cdot; i)$ reverses the element order back to the start, to be able to apply the subtraction in the numerator of the EEs row-by-row. Index i in $\mathcal{T}_1(\cdot; i)$ and $\mathcal{T}_3(\cdot; i)$ stands for the number of first row elements that is cut and moved to the back of the row in the same order. Applying $\mathcal{T}(\mathbf{T_{i+1,*}}; i-1)$ and $\mathcal{T}(\mathbf{T_{i+1,*}}; i)$ to all rows i of trajectory $\mathbf{T}$ as in Equation (12) gives the following two transformed trajectories:

$$\mathcal{T}_1(\mathbf{T_{i+1,*}}; i-1) = \begin{pmatrix} a_k & a_1 & \dots & \dots & a_{k-1} \\ \mathbf{b_1} & a_2 & \dots & \dots & a_k \\ \mathbf{b_2} & a_3 & \dots & \dots & \mathbf{b_1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \mathbf{b_k} & \mathbf{b_1} & \dots & \dots & \mathbf{b_{k-1}} \end{pmatrix} \tag{8}$$

$$\mathcal{T}_1(\mathbf{T_{i,*}}; i-1) = \begin{pmatrix} a_1 & a_2 & \dots & \dots & a_k \\ a_2 & \dots & \dots & a_k & \mathbf{b_1} \\ a_3 & \dots & \dots & \mathbf{b_1} & \mathbf{b_2} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \mathbf{b_1} & \mathbf{b_2} & \dots & \dots & \mathbf{b_k} \end{pmatrix} \tag{9}$$

Two points can be seen from Equation (8) and (9). First, $\mathcal{T}_1(\mathbf{T_{i+1,*}}; i-1)$ and $\mathcal{T}_1(\mathbf{T_{i,*}}; i)$, i.e. the $(i+1)$-th row in Eq. (13) and the (i)-th row in Eq. (14) only differ in the i-th element. The difference is $b_i - a_i$. Thus, these two rows can be used to compute the EEs like in the uncorrelated case in Equation (**??**). However, in this order, the parameters are in the wrong positions to be directly handed over to the function, as the i-th parameter is always in front. The second point is that in $\mathcal{T}_1(\mathbf{T_{i+1,*}}; i-1)$, b_i is in front of the i-th row. This order prepares the establishing of the right correlation hierarchy by $\mathcal{T}_2$, such that the Δ in $a_i + \Delta$ is included to transform all other elements that represent parameters $X_{\sim i}$. Importantly, to perform $\mathcal{T}_2$, the mean vector $\mathbf{x}$ and the covariance matrix $\mathbf{\Sigma}$ and its transformed representatives have always to be re-ordered according to each row. Then, $\mathcal{T}_3$ restores the original row order and d_i^{full} can comfortably be computed by comparing function evaluations of row $i+1$ in $\mathcal{T}(\mathbf{T_{i+1,*}}; i-1)$ with function evaluations of row i in $\mathcal{T}(\mathbf{T_{i,*}}; i-1)$. Now, the two transformed trajectories only differ in the i-th element in each row i.

The formula for the independent Elementary Effect for the trajectory design is given by

$$d_i^{ind,T} = \frac{f\Big(\mathcal{T}(\mathbf{T_{i+1,*}}; i)\Big) - f\Big(\mathcal{T}(\mathbf{T_{i,*}}; i)\Big)}{\Delta}. \tag{10}$$

Note that $\mathcal{T}(\mathbf{T_{i+1,*}}; i)$ equals $\mathcal{T}(\mathbf{T_{i,*}}; i-1)$ which is the funcion argument in the subtrahent in the definition of d^{full} in Equation (12). Therefore this transformation can be skipped for the trajectory design and the transformed trajectory in Equation (14) can be recycled. Here, the X_i that takes the step in the denominator of the Elementary Effect is moved to the back such that the step does not affect the other input parameters $\mathbf{X_{\sim i}}$ through the correlations. The left trajectory is constructed such that for each row i, a_i does take the step that b_i took in the aforementioned minuend trajectory. The argument of the subtrahend in the denominator in d_i^{ind} is given by the rows in

$$\mathcal{T}_1(\mathbf{T_{i,*}}; i-1) = \begin{pmatrix} a_2 & a_3 & ... & ... & a_1 \\ a_3 & ... & a_k & \mathbf{b_1} & a_2 \\ a_4 & ... & \mathbf{b_1} & \mathbf{b_2} & a_3 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \mathbf{b_2} & \mathbf{b_3} & ... & ... & \mathbf{b_1} \end{pmatrix} \tag{11}$$

The transformation for the samples in radial design work equally except of that the minuend samples are composed of the first row copied to each row below because the steps in the radial design are always taken from the draws in the first row. It is important to also reorder the minuend trajectories to account for the correlation hierarchy and the transformation to the sample space performed by $\mathcal{T}_2$. In fact, it is enough to compute one minuend trajectory if the order is regarded correctly. The forumalae of the Elementary Effects for the radial design are given by Equation (17) and (18).

$$d_i^{full,R} = \frac{f\Big(\mathcal{T}(\mathbf{R_{i+1,*}}; i-1)\Big) - f\Big(\mathcal{T}(\mathbf{R_{1,*}}; i)\Big)}{b_i - a_i}. \tag{12}$$

$$d_i^{ind,R} = \frac{f\Big(\mathcal{T}(\mathbf{R_{i+1,*}}; i)\Big) - f\Big(\mathcal{T}(\mathbf{R_{1,*}}; i)\Big)}{b_i - a_i}. \tag{13}$$

Each sample scheme requires $N(3k+1)$ function evaluations to compute both EEs. The first row of the minuend trajectories and the last row of the subtrahend can be skipped. If one transformed trajectory contains information for two EEs, then all rows are used.[7]

1.3 Implementation

I implemented the method by Ge and Menendez (2017) in Python 3. I wrote at least one test for each function. This is a coverage of 100 %. I am able to replicate their results for the normally distributed examples, i.e. Test Case 1 and Test Case 2 up to a reasonable degree given that they do not use a large number of samples. The replication can be found in the two notebooks at branch *replication_gm17*.

In the next section, I will present the shortcomings of the Elementary Effects in Ge and Menendez (2017). There, I will explain why it not possible to solve common tests function for uncorrelated, normally distributed parameters.

I will also present improved measures that I created. With these, I can solve all test functions for uncorrelated and correlated normalinput parameters and uncorrelated

[7]Ge and Menendez (2017) claim that the radial design requires only $3Nk$ evaluations.

parameters in [0,1]. Test functions that I solved exactly are, first, the large test function with six paramters in [0,1] based on the so-called g-function, presented in Saltelli et al. (2008), page 123 - 129. The second test function is the linear function with two normally distributed input parameters and non-unit variance in Smith (2014), page 335. This function is similar to Test Case 1 and 2 and provides intuition on what the results for well-defined Elementary Effects for correlated input parameters should be. I am able to generate these results with the implementation of my measures.

1.4 Drawbacks in Ge and Menendez (2017) and Corrected Elementary Effects.

The drawback in the definition of the Elementary Effects is that the step is transformed in the numerator multiple times but not in the denominator. Therefore, these measures are not Elementary Effects in the sense of a derivation. The transformation in the numerator is performed by applying $F^{-1}(\Phi)$ to $u_i^j = a_i^j + \Delta^{(i,j)}$. The corrected and slightly renamed measures are the correlated and the uncorrelated Elementary Effects d_i^c and d_i^u. They are given below for arbitrary input distributions and for samples in trajectory and radial design. Let ${Q^T}_{k,*k-1}$ be the last row except of the last element of the lower triangular Cholesky matrix of the correlation matrix in the respective order of $\mathcal{T}_1(\mathbf{T_{i+1,*}}; i-1)$ and $\mathcal{T}_1(\mathbf{T_{i+1,*}}; i-1)$. Let ${Q^T}_{k,k}$ be the last element of the same matrix. Let F^{-1} be a transformation that maps standard normal deviates to an arbitrary sample space. Index $*k-1$ represent all elements except of the last one of a vector of length k. Index j is used to indicate an element-wise multiplication. Then

$$d_i^{c,T} = \frac{f\Big(\mathcal{T}(\mathbf{T_{i+1,*}}; i-1)\Big) - f\Big(\mathcal{T}(\mathbf{T_{i-1,*}}; i)\Big)}{F^{-1}\Big(\Phi(b_i)\Big) - F^{-1}\Big(\Phi(a_i)\Big)} \tag{14}$$

$$d_i^{u,T} = \frac{f\Big(\mathcal{T}(\mathbf{T_{i+1,*}}; i)\Big) - f\Big(\mathcal{T}(\mathbf{T_{i,*}}; i)\Big)}{F^{-1}\Big({Q^T}_{k,*k-1}(j)T^T_{i+1,*k-1}(j) + {Q^T}_{k,k}\Phi(b_i)\Big) - F^{-1}\Big({Q^T}_{k,*k-1}(j)T^T_{i,*k-1}(j) + {Q^T}_{k,k}\Phi(a_i)\Big)} \tag{15}$$

$$d_i^{c,R} = \frac{f\Big(\mathcal{T}(\mathbf{R_{i+1,*}}; i-1)\Big) - f\Big(\mathcal{T}(\mathbf{R_{1,*}}; i-1)\Big)}{F^{-1}\Big(\Phi(b_i)\Big) - F^{-1}\Big(\Phi(a_i)\Big)} \tag{16}$$

$$d_i^{u,R} = \frac{f\Big(\mathcal{T}(\mathbf{R_{i+1,*}}; i)\Big) - f\Big(\mathcal{T}(\mathbf{R_{1,*}}; i)\Big)}{F^{-1}\Big({Q^T}_{k,*k-1}(j)R^T_{i+1,*k-1}(j) + {Q^T}_{k,k}\Phi(b_i)\Big) - F^{-1}\Big({Q^T}_{k,*k-1}(j)R^T_{i,*k-1}(j) + {Q^T}_{k,k}\Phi(a_i)\Big)}. \tag{17}$$

In Equation (22), ${Q^T}_{k,*k-1}(j)R^T_{i,*k-1}(j)$ refers to the transformed trajectory of the copied first rows, $\mathcal{T}(\mathbf{R_{i+1,*}}; i)$, as described in the previous section.

The denominator of the correlated Elementary Effect, d_i^c, consists of Φ and F^{-1}. These functions account for the transformation from uniform to arbitrary sample space. In d_i^c, the denominator must not account for a correlating transformation of a_i and b_i because ${Q^T}_{1,*} = (1, 0, 0, ..., 0)$. Therefore, b_i and a_i are multiplied by one in the correlation step of the standard normal deviates.

The last point is not true for the uncorrelated Elementary Effect d_i^c. One accounts for the correlation step by multiplying $\Phi(b_i)$ by ${Q^T}_{k,*k-1}(j)T^T_{i+1,*k-1}(j)/\Phi(b_i) + {Q^T}_{k,k}$. The respective operation is done for $\Phi(b_i)$. Not accounting for Q_t like Ge and Menendez (2017) leads to arbitrarily decreased independent Elementary Effects for input parameters with higher correlations. As d_i^{full} and d_i^{ind} are interpreted jointly, both measures are in fact useless.

For $X_1, ..., X_k \sim \mathcal{N}_k(\boldsymbol{\mu}, \boldsymbol{\Sigma})$, the denominator of $d_i^{\bullet,R}$ simplifies drastically to

$$\begin{aligned}
&\Big(\mu_i + \sigma_i\Big({Q^T}_{k,*k-1}(j)T^T_{i+1,*k-1}(j) + {Q^T}_{k,k}\Phi(b_i)\Big) \\
-&\Big(\mu_i + \sigma_i\Big({Q^T}_{k,*k-1}(j)T^T_{i+1,*k-1}(j) + {Q^T}_{k,k}\Phi(a_i)\Big) \\
&\qquad = \sigma_i {Q^T}_{k,k}\Big(\Phi(b_i) - \Phi(a_i)\Big).
\end{aligned} \tag{18}$$

1.5 Replication and Validation

Let $f(X_1, ..., X_k) = \sum_{i=1}^k c_i X_i$ be an arbitrary linear function. Let $\rho_{i,j}$ be the linear correlation between X_i and X_j. Then, for all $i \in 1, ..., k$,

$$d_i^{u,T} = d_i^{u,R} = c_i \tag{19}$$

$$d_i^{c,T} = d_i^{c,R} = \sum_{j=1}^k \rho_{i,j} c_j. \tag{20}$$

This implies that the mean and the mean absolute aggregate effects are equal to their respective (individual) uncrrelated and correated Elementary Effect and that the respective standard deviation for both Elementary Effects is 0. This corresponds to the uncorrelated example in Saltelli et al. (2008), page 123.

Table 1. Replication and validation for test case 1 - trajectory design

Measure	GM'17	Repl. μ^*	Repl. σ	S'20
	1.20	1.36	0.83	1.00
$\mu^{*,ind}$	1.30	1.48	0.91	1.00
	3.20	3.11	1.94	1.00
	0.55	0.00	0.56	0.00
σ^{ind}	0.60	0.00	0.62	0.00
	1.30	0.00	1.32	0.00
	14.90	16.20	9.97	2.30
$\mu^{*,full}$	12.50	13.45	8.31	1.91
	10.00	9.93	6.18	1.41
	6.50	0.00	6.74	0.00
σ^{full}	5.50	0.00	5.63	0.00
	4.00	0.00	4.20	0.00

Table 2. Replication and validation for test case 1 - radial design

Measure	GM'17	Replication	S'20
	0.60	0.57	1.00
$\mu^{*,ind}$	0.75	0.85	1.00
	1.50	1.31	1.00
	0.20	0.10	0.00
σ^{ind}	0.30	0.41	0.00
	0.85	0.22	0.00
	7.50	6.84	2.30
$\mu^{*,full}$	6.80	7.77	1.91
	4.75	4.19	1.41
	2.90	1.15	0.00
σ^{full}	2.65	3.68	0.00
	2.50	0.70	0.00

Figure 1. Grid points for trajectory design in Ge and Menendez (2017)

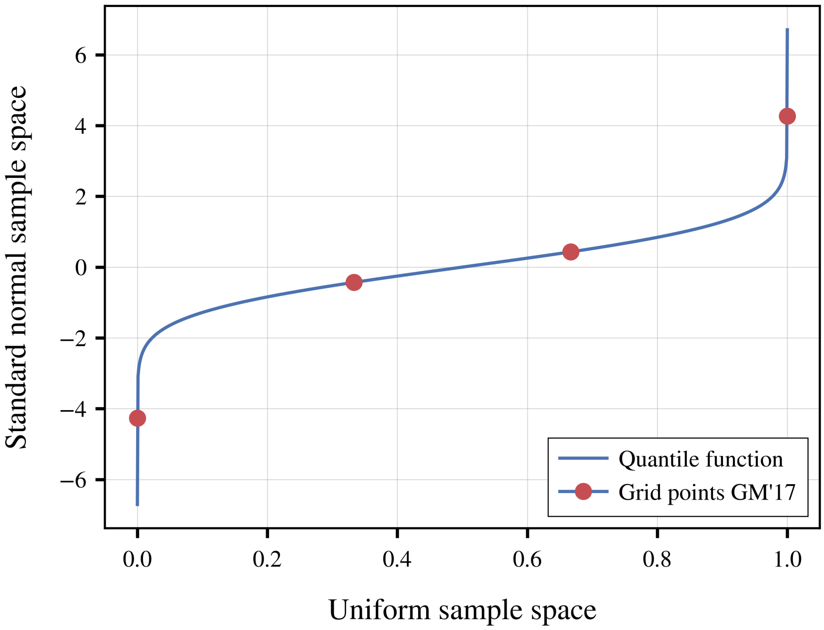


Figure 2. Sigma-normalized mean absolute Elementary Effects for trajectory design

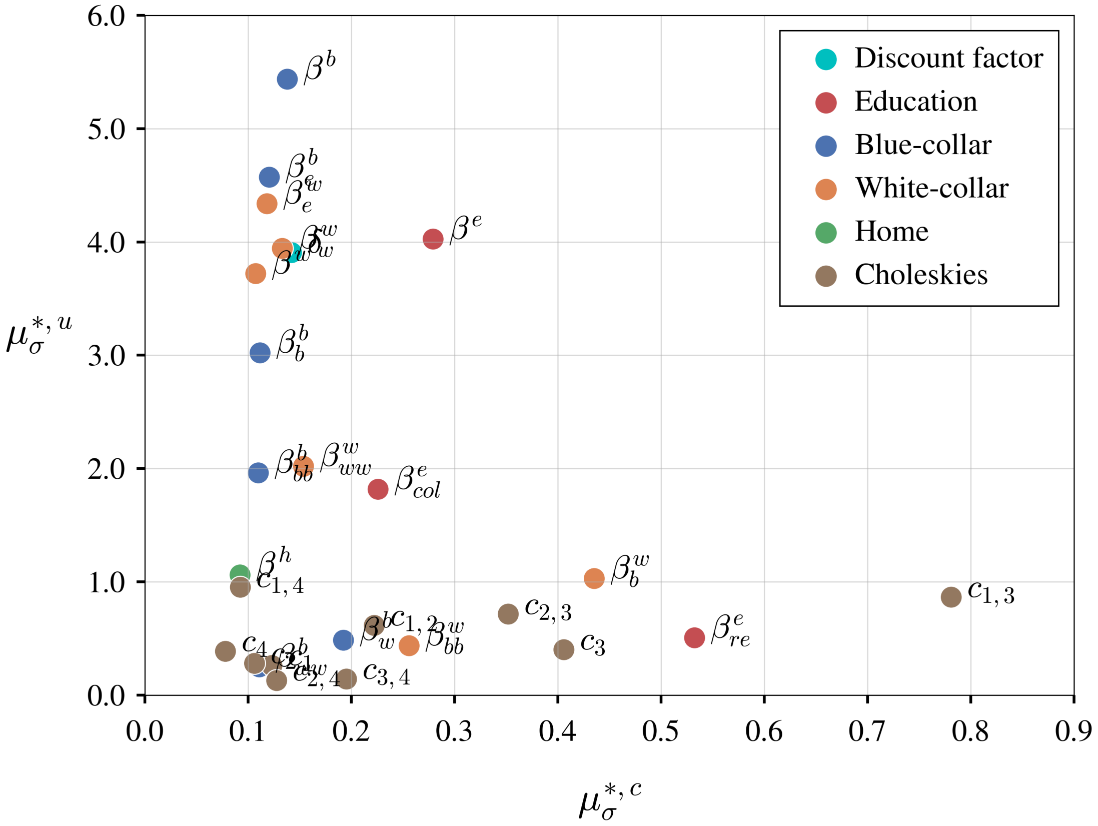
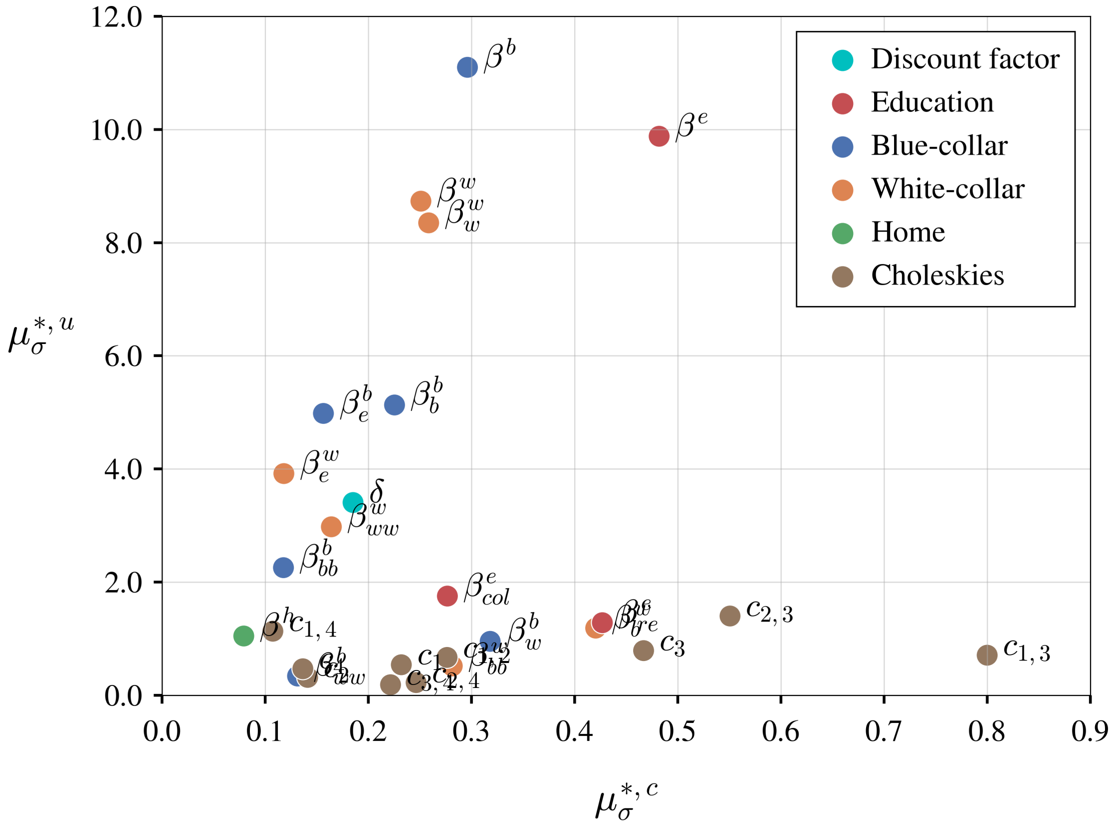


Figure 3. Sigma-normalized mean absolute Elementary Effects for radial design



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