1 Ge and Menendez (2017) and beyond

Morris (1991)

Saltelli et al. (2008)

Lemaire (2013)

Gentle (2006)

Ge and Menendez (2017)

Ge and Menendez (2014)

Campolongo et al. (2007)

Smith (2014)

1.1 Qualitative General Sensitivity Analysis

Qualitative Global Sensitivity Analysis (GSA) deals with computing measures that can rank random input parameters in terms of their importance on the function output and the variability thereof. If the measures for some input parameters are negligibly small, these parameters can be fixed so that the number of random input parameters decreases for a subsequent quantitative GSA. This pre-selection step is called Factor Fixing. The quantitative GSA then aims to determine the effect size. of the random input parameters on the function output. The most common measures in quantitative GSA are the so-called Sobol' sensitivtiy indices. Equation 1 shows the first order index. It is the share of the variance in the function output induced by exclusively one single input parameter X_i of the variance in the function output induced by all random input parameters $X_1, X_2, ..., X_k$.

$$S_i = \frac{\text{Var}_i[Y|X_i]}{\text{Var}[Y]} \tag{1}$$

Equation 2 show the total order index. This measure is equal to the first order index except of that it numerator includes the variance in the function output that is induced by changes in the other input parameters $X_{\sim i}$, caused by interactions with X_i.

$$S_i^T = \frac{\mathbb{E}_{\sim i}[\text{Var}_i[Y|\mathbf{X_{\sim i}}]]}{\text{Var}[Y]} \tag{2}$$

Computing these measures requires many function evaluations, even if estimators are used that can provide some shortcuts. The more time-intense one function evaluation is, the more appealing gets the aforementioned Factor Fixing. These can provide qualitative results with less function evaluations. The most commonly used measures in qualitative GSA is the Elementary Effect (EE), μ, the absolute Elementary Effects, μ^*, and the standard deviation of the Elementary Effect σ. The Elementary Effect is given by the mean of a number of function derivatives with respect to one input parameter. The "change in", or the "step of" the input parameter, denotes by Δ, has not to be infinitesimally small.

The derivation is denoted as

$$d^{(j)} = \frac{Y(\mathbf{X_{\sim i}^{(j)}}, X_i^{(j)} + \Delta^{(i,j)})}{\Delta^{(i,j)}}, \tag{3}$$

where j is an index for the number of parameter-specific argument observations for the function derivative. Then, the Elementary Effect is given by

$$\mu = \frac{1}{r} \sum_{j=1}^{r} d^{(j)}. \tag{4}$$

The absolute Elementary Effects, μ^* is used to prevent observations to cancel each other out.

$$\mu^* = \frac{1}{r} \sum_{j=1}^{r} \left| d^{(j)} \right|. \tag{5}$$

In Equation 4 and 5, r is the number of parameter draws with index (j). Step $\Delta^{(j)}$ may or may not vary depending on the sample design that is used to draw the input parameters. These measures (together) are used to proxy the total Sobol' indices that contains the parameter-specific interactions with all other parameter in Equation(2). If they are close to 0 (,and given there are parameters with measures substantially different from 0), these respective factors' variation can be rendered as irrelevant for the variation in the function output.

1.2 Sampling Schemes

According to several experiments by Campolongo et al. (2011) using common test functions, the best design is the radial design (Saltelli (2002)) and the most commonly used is the trajectory design (Morris (1991)). Both samples consist of a set of $(k+1) \times k$-dimensional matrices. The columns represent the input parameters and each row is a complete input parameter vector.

A subsample, or matrix, in radial design is generated the 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:

$$\mathbf{R} = \begin{pmatrix} a_1 & a_2 & ... & a_k \\ \mathbf{b_1} & a_2 & ... & a_k \\ a_1 & \mathbf{b_2} & ... & a_k \\ \vdots & \vdots & \vdots & \vdots \\ a_1 & a_2 & ... & \mathbf{b_k} \end{pmatrix}$$

Note here, that each column consists only of the first row element, except of one row. From this matrix, one individual EE can be obtained for each parameter $X_i \in X_1, X_2, ..., X_k$. This is achieved by using the $i+1$-th row as function argument for the minuend and the first row as subtrahend in the formula for the individual EE. Then, $\Delta^{(i,j)} = b_i^{(j)} - a_i^{(j)}$. This yields to the following re-formulation of the derivation in Equation (3).

$$d^{(j)} = \frac{Y(\mathbf{a}_{\sim\mathbf{i}}^{(\mathbf{j})}, b_i^{(j)}) - Y(\mathbf{a})}{b_i^{(j)} - a_i^{(j)}} = \frac{Y(\mathbf{R}_{\mathbf{i},*}) - Y(\mathbf{R}_{\mathbf{1},*})}{b_i^{(j)} - a_i^{(j)}}. \tag{6}$$

If the number of radial subsamples is high, the quasi-random sequence lead to a good coverage of the input space. The quasi-random sequence considered here is the Sobol' sequence. This sequence is comparably succesful in covering interval the unit hypercube but also conceptually more involved. Therefore, it's 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 leads to frequent repetitions of similar draws for higher number of draws. In this outline, I skip the exact equations that produces a trajectory and simply present the method verbally. There are multiple approaches to construct different forms of trajectory. Here, I focus on the version presented in Morris (1991) that yields to equiprobable elements. The first step is to decide the number p of 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 the lowest point in the lowest half results in the lowest point of the upper half of the grid points if Δ is added. The rest of the rows is constructed by, first, copying the upper row and, second, by adding Δ to the k-th element of the $k+1$-th row. The implied matrix scheme is depictet below.

$$\mathbf{T} = \begin{pmatrix} a_1 & a_2 & ... & a_k \\ \mathbf{b_1} & a_2 & ... & a_k \\ \mathbf{b_1} & \mathbf{b_2} & ... & a_k \\ \vdots & \vdots & \vdots & \vdots \\ \mathbf{b_1} & \mathbf{b_2} & ... & \mathbf{b_k} \end{pmatrix}$$

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. The first transformation is skipped as it does not add additional coverage and because we need the stairs-shape facilitate later transformations to account for correlation between input parameters. The second transformation is adapted because it is important to also have negative Δ and because it does also sustain the stairs-shape. Yet, this implies that Δ is also column and trajectory specific. Let f and h be additional index parameters. The derivation formula is adapted to the trajectory design as follows[1]:

$$d^{(j)} = \frac{Y(\mathbf{b^{(j)}_{f\leq i}}, \mathbf{a^{(j)}_{h>i}}) - Y(\mathbf{b^{(j)}_{f<i}}, \mathbf{a^{(j)}_{h\geq i}})}{b_i^{(j)} - a_i^{(j)}} = \frac{Y(\mathbf{T_{i,*}}) - Y(\mathbf{T_{i-1,*}})}{b_i^{(j)} - a_i^{(j)}}. \tag{7}$$

The trajectory design involves first, a fixed grid, and second and more importantly, a fixed step Δ. Hence the coverage of points is worse for larger samples. Additionally, $\{\Delta\} = \{\pm\Delta\}$ implies less variety vis-á-vis the radial design.

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

References

Campolongo, F., J. Cariboni, and A. Saltelli (2007). An effective screening design for sensitivity analysis of large models. *Environmental modelling & software 22*(10), 1509–1518.

Campolongo, F., A. Saltelli, and J. Cariboni (2011). From screening to quantitative sensitivity analysis. a unified approach. *Computer Physics Communications 182*(4), 978–988.

Ge, Q. and M. Menendez (2014). An efficient sensitivity analysis approach for computationally expensive microscopic traffic simulation models. *International Journal of Transportation 2*(2), 49–64.

Ge, Q. and M. Menendez (2017). Extending morris method for qualitative global sensitivity analysis of models with dependent inputs. *Reliability Engineering & System Safety 100*(162), 28–39.

Gentle, J. E. (2006). *Random number generation and Monte Carlo methods*. Springer Science & Business Media.

Lemaire, M. (2013). *Structural reliability*. John Wiley & Sons.

Morris, M. D. (1991). Factorial sampling plans for preliminary computational experiments. *Technometrics 33*(2), 161–174.

Saltelli, A. (2002). Making best use of model evaluations to compute sensitivity indices. *Computer physics communications 145*(2), 280–297.

Saltelli, A., M. Ratto, T. Andres, F. Campolongo, J. Cariboni, D. Gatelli, M. Saisana, and S. Tarantola (2008). *Global Sensitivity Analysis: The Primer*. John Wiley & Sons.

Smith, R. C. (2014). *Uncertainty Quantification: Theory, Implementation, and Applications*. Philadelphia: SIAM-Society for Industrial and Applied Mathematics.