

Chapter 6

Global Sensitivity Analysis

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Global sensitivity analysis (GSA) aims at quantifying the contribution of individual random variables $\mathbf{X}$ to a quantity of interest. Sensitivity analysis can be used to screen out unimportant variables before main analysis and to gain engineering insights about the model at hand. Let us consider a function

$$Y = g(\mathbf{X}) \quad (6.0.1)$$

We would like to identify the fraction of the uncertainty (variance) of Y that can be attributed to each random variable.*

For example, consider a multi-story building with random property subjected to random ground motion excitation. The structural responses of interest can be peak displacement, peak velocity, peak acceleration etc. Below are some of the engineering questions that may arise.

- To reduce the peak acceleration response, which factor should be changed? In other words, which factor affects the peak displacement the most?
- Are all of the variables actually affecting the peak acceleration? Can we set some of the variables to be deterministic to simplify the analysis? (Model simplification)
- Is the randomness in the structural property so significant that we need to consider it in our reliability analysis, or is it very trivial compared to the randomness in the excitation?
- We want to optimize the importance sampling density for reliability analysis but the input dimension is too high. Can we optimize the sampling density only for selected variables instead of considering all the variables?
- Is this model overly dependent on fragile assumptions? (Model corroboration)

On the other hand, GSA can also be used to assist resource allocation decision.

- If we have some resources to collect more information, should we plan a field investigation to identify soil property or should we focus more on structural deterioration inspection? In which variables should we reduce the uncertainty?

These are some of the questions that can be answered by sensitivity analysis[†].

*Main reference: Saltelli, A., Ratto, M., Andres, T., Campolongo, F., Cariboni, J., Gatelli, D., Saisana, M. and Tarantola, S., 2008. Global sensitivity analysis: the primer. John Wiley & Sons.

[†]Razavi, S., Jakeman, A., Saltelli, A., Prieur, C., Iooss, B., Borgonovo, E., Plischke, E., Piano, S.L., Iwanaga, T., Becker, W. and Tarantola, S., 2021. The future of sensitivity analysis: An essential discipline for systems modelling and policy support. Environmental Modelling & Software, 137, p.104954.

6.1 Local versus Global

6.1.1 Local Sensitivity Analysis

The local sensitivity can simply be defined as a ‘rate of change’ or ‘slope’ of the response surface, i.e.

$$S_i^D(\mathbf{X}) = \frac{\partial g(\mathbf{X})}{\partial X_i} \quad (6.1.1)$$

The local sensitivity is therefore defined at a certain reference point $\mathbf{X}$ and it is obtained by changing one factor at a time (OAT). It does not depend on the distribution of $\mathbf{X}$ nor its range of interest. If one is interested in identifying influence of each variable throughout the whole domain of interest, it requires selection of multiple reference points and gradient evaluations in each direction per each point.

6.1.2 Sigma-normalized Derivative

Still, the derivative measure can miss the whole picture. For example, consider a model

$$Y = X_1 + X_2 \quad (6.1.2)$$

where X_1 and X_2 each follow a Gaussian distribution with standard deviations $\sigma_1 = 1$ and $\sigma_2 = 5$. Figure 6.1.1 shows scatter plots obtained by performing Monte Carlo simulation. The plots indicates that Y is more sensitive to X_2 than X_1 , because we can observe a clearer pattern on the right-hand side plot. However, if we decide the relative importance based on the gradient measure, this behavior will not be captured and sensitivity to both variables will be deemed to be equal. A modified of local sensitivity index consistent with this intuition is called sigma-normalized derivatives:

$$S_i^{SD} = \frac{\sigma_{X_i}}{\sigma_Y} \frac{\partial g(\mathbf{X})}{\partial X_i} \quad (6.1.3)$$

This can be applied only when input variables are independent to each other.

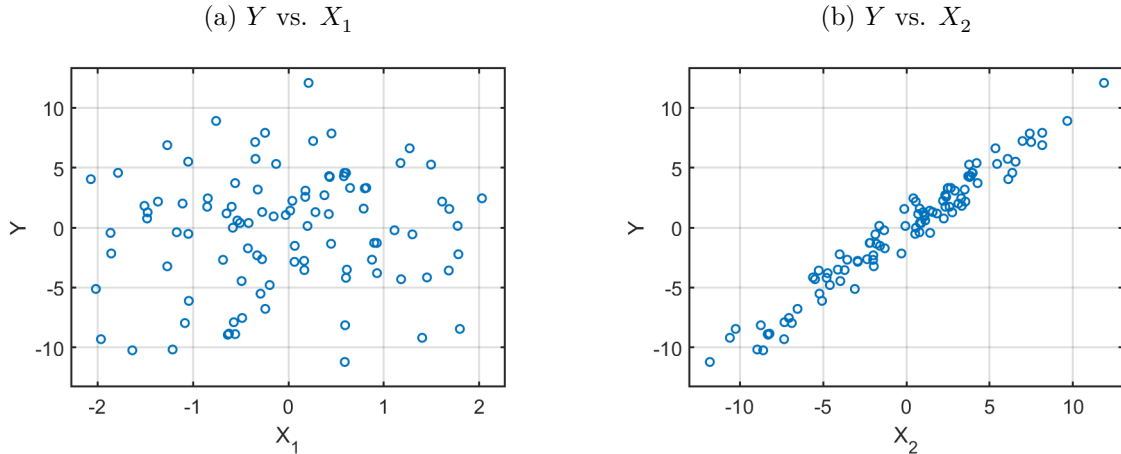


Figure 6.1.1: Realizations of $Y = X_1 + X_2$.

Alternative approach to account for the input randomness in the local sensitivity analysis is to transform each variables x_i into standard normal space $z_i = T(x_i)$ and get partial derivatives using $G(\mathbf{u})$. Again this is appropriate only when input random variables are independent to each other. For example, recall the variable transform introduced in Eq.(4.1.1) introduced for

FORM analysis. In fact, FORM analysis approximates the limit state using the gradient (local sensitivity index) at design point value. Often the vector of normalized gradient is denoted as α :

$$\alpha = -\frac{\nabla G(\mathbf{z}^*)}{\|\nabla G(\mathbf{z}^*)\|} \quad (6.1.4)$$

and α is called importance vector, as it represents the importance of each random variable around the design point. Further α is the directional cosines of the design point (See Figure 6.1.2).

$$\alpha = -\frac{\mathbf{z}^*}{\beta} \quad (6.1.5)$$

The $(-)$ sign is attached indicating that α is directed towards the failure domain.

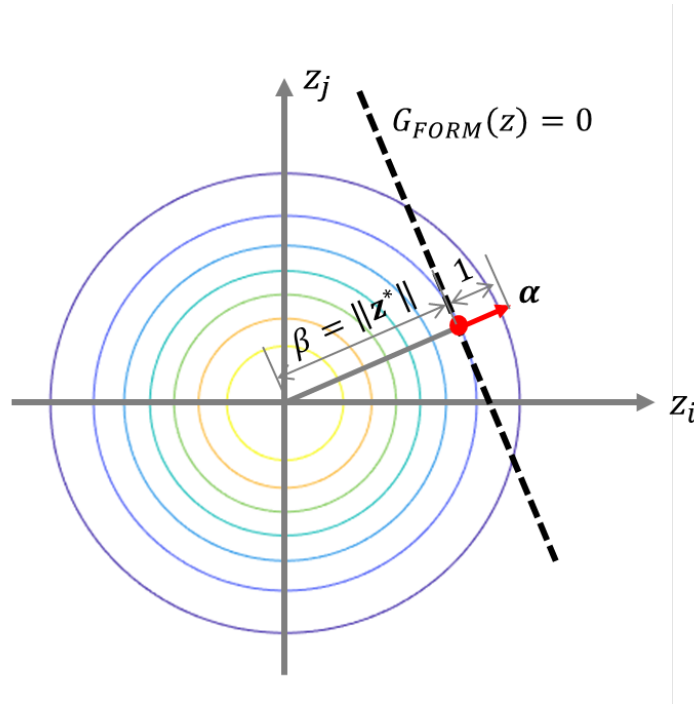


Figure 6.1.2: Geometric interpretation of α .

However, when input random variables are not independent, α_i can not represent the local sensitivity of original variable, X_i , because transformation of dependent random variables, i.e. Eq.(4.1.5), no longer establishes one-on-one relationship between X_i and Z_i . Therefore, effect of more than one original variable can be mixed up in a single transformed variable, i.e. transformation into Z_i may involve X_j .

Alternatively one can perform linear regression to assess sensitivity - when the slope is larger for a variable, the variable is more influential. However, it does not capture the nonlinear dependencies between $\mathbf{X}$ and Y .

On the other hand, global sensitivity analysis (GSA) considers the sensitivity across the 'whole range' of input space and considers also nonlinear dependencies. There are different global sensitivity measures available in literature, e.g. Pearson correlation, Morris method, cross-entropy-based method, and one of the most widely accepted concept is variance-based sensitivity index, also called as Sobol index.

6.2 Intuition Behind Variance-based Sensitivity Analysis

6.2.1 Scatter Plots

Let us consider the following model with d -input variables.

$$Y = g(X_1, X_2, \dots, X_d) \quad (6.2.1)$$

where $\mathbf{X} = (X_1, X_2, \dots, X_d)$ follows some probability distribution. Suppose Monte Carlo simulation is performed to collect the samples of $\mathbf{X}$ and Y . Figure 6.2.1 illustrates the pair-wise scatter plots of (Y, X_i) and (Y, X_j) . These scatter plots can be used to investigate the influence of each variable to the model response. For instance, the first plot does not have a trend of increasing or decreasing, implying that Y is likely to be not sensitive to the change in X_i . On the other hand, Y rapidly drops with a clear trend when X_j increases, having more influence compared to X_i .

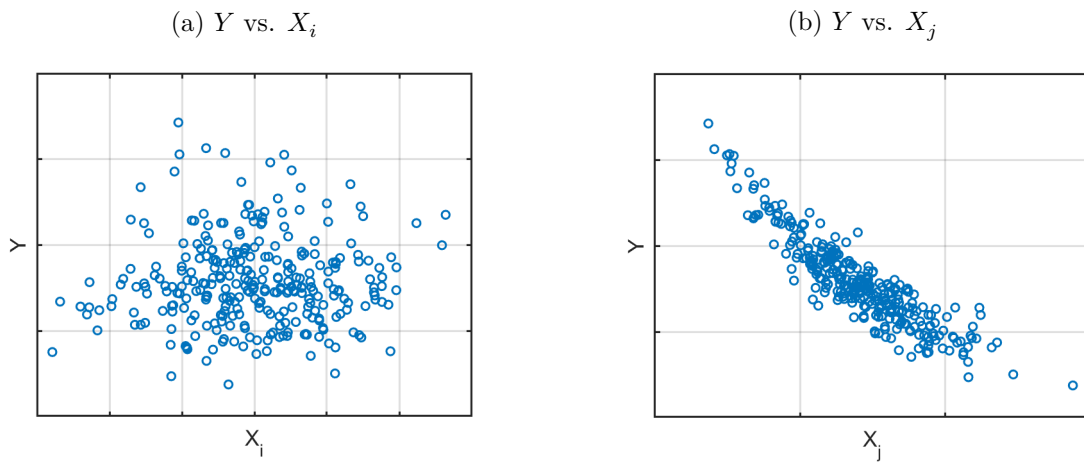


Figure 6.2.1: Realizations of $Y = g(X_1, X_2, \dots, X_d)$.

Using the statistical term, the ‘trend’ corresponds to the conditional mean of Y given different X values and whether the **conditional mean** is variant or invariant to different X values becomes the key question when evaluating the sensitivity index. The variability is measured by the **variance** operation. To summarize, the following two statements support the assumption that the ‘variance of conditional mean’, i.e. $\text{Var}_{X_i} [\mathbb{E}_{\mathbf{X}_i} [Y|X_i]]$ is a good measure of sensitivity.

- In Figure 6.2.1(a)
 - $\mathbb{E}_{\mathbf{X}_i} [Y|X_i]$ is near constant.
 - $\text{Var}_{X_i} [\mathbb{E}_{\mathbf{X}_i} [Y|X_i]]$ is near zero.
 - Y is **not sensitive** to the change of X_i
- In Figure 6.2.1(b)
 - $\mathbb{E}_{\mathbf{X}_j} [Y|X_j]$ drops as X_j increase.
 - $\text{Var}_{X_j} [\mathbb{E}_{\mathbf{X}_j} [Y|X_j]]$ is larger.
 - Y is **sensitive** to the change of X_j

where $\mathbf{X}_{\bar{i}}$ represents the $d - 1$ dimensional vector containing all the components of $\mathbf{X}$ except X_i .

On the other hand, the *Law of Total Variance* states that the variance of output can always be decomposed into two parts.

Law of Total Variance

$$\mathbb{V}ar[Y] = \mathbb{V}ar_{X_i} [\mathbb{E}_{\mathbf{X}_{\bar{i}}} [Y|X_i]] + \mathbb{E}_{X_i} [\mathbb{V}ar_{\mathbf{X}_{\bar{i}}} [Y|X_i]] \quad (6.2.2)$$

In this equation, the total variance is decomposed to ‘explained’ and ‘unexplained’ parts, i.e. ‘explained’ part means the portion of variance that can be explained from the regression model of X_i and Y , and ‘unexplained’ represents the portion of variance that cannot be reduced by adding knowledge on X_i . The proof is as follows.

$$\begin{aligned} \mathbb{V}ar[Y] &= \mathbb{E}[Y^2] - \mathbb{E}[Y]^2 \\ &= \mathbb{E}_{X_i} [\mathbb{E}_{\mathbf{X}_{\bar{i}}} [Y^2|X_i]] - \mathbb{E}_{X_i} [\mathbb{E}_{\mathbf{X}_{\bar{i}}} [Y|X_i]]^2 \\ &\quad (\text{law of iterated expectation, law of total probability}) \\ &= \mathbb{E}_{X_i} [\mathbb{V}ar_{\mathbf{X}_{\bar{i}}} [Y|X_i] + \mathbb{E}_{\mathbf{X}_{\bar{i}}} [Y|X_i]^2] - \mathbb{E}_{X_i} [\mathbb{E}_{\mathbf{X}_{\bar{i}}} [Y|X_i]]^2 \\ &\quad (\text{definition of variance for } Y|X) \\ &= \mathbb{E}_{X_i} [\mathbb{V}ar_{\mathbf{X}_{\bar{i}}} [Y|X_i]] + \mathbb{E}_{X_i} [\mathbb{E}_{\mathbf{X}_{\bar{i}}} [Y|X_i]^2] - \mathbb{E}_{X_i} [\mathbb{E}_{\mathbf{X}_{\bar{i}}} [Y|X_i]]^2 \\ &= \mathbb{E}_{X_i} [\mathbb{V}ar_{\mathbf{X}_{\bar{i}}} [Y|X_i]] + \mathbb{V}ar_{X_i} [\mathbb{E}_{\mathbf{X}_{\bar{i}}} [Y|X_i]] \\ &\quad (\text{definition of variance for } \mathbb{E}[Y|X]) \end{aligned} \quad (6.2.3)$$

Note that the first term of Eq.(6.2.2) correspond to our intuitive definition of the measure of sensitivity. By dividing both sides of the equation by $\mathbb{V}ar[Y]$, we get

$$1 = \underbrace{\frac{\mathbb{V}ar_{X_i} [\mathbb{E}_{\mathbf{X}_{\bar{i}}} [Y|X_i]]}{\mathbb{V}ar[Y]}}_{\text{measure of sensitivity}} + \frac{\mathbb{E}_{X_i} [\mathbb{V}ar_{\mathbf{X}_{\bar{i}}} [Y|X_i]]}{\mathbb{V}ar[Y]} \quad (6.2.4)$$

Finally, the sensitivity index is defined as

Sobol Main Sensitivity Index

$$S_i = \frac{\mathbb{V}ar_{X_i} [\mathbb{E}_{\mathbf{X}_{\bar{i}}} [Y|X_i]]}{\mathbb{V}ar[Y]} \quad (6.2.5)$$

Note that because of Eq.(6.2.4), $S_i \in [0, 1]$ always hold. Also by re-arranging Eq.(6.2.4), we get an alternative expression of the Sobol index

Sobol Main Sensitivity Index (2)

$$S_i = 1 - \frac{\mathbb{E}_{X_i} [\mathbb{V}ar_{\mathbf{X}_{\bar{i}}} [Y|X_i]]}{\mathbb{V}ar[Y]} \quad (6.2.6)$$

This definition of Sobol index is referred to as the *main-effect index* or *first-order index*.

6.3 Interaction Effects

6.3.1 Higher-order Sensitivity Indices

The concept of sensitivity analysis can be extended to more than one random variable. For example, to estimate the joint contribution of two variables, the following second order measure can be introduced

Second-order Sensitivity Index

$$S_{ij} = \frac{\text{Var}_{X_i, X_j} [\mathbb{E}_{\mathbf{X}_{\bar{ij}}} [Y|X_i, X_j]]}{\text{Var}[Y]} - S_i - S_j \quad (6.3.1)$$

In this case, we are conditioning over two variables X_i and X_j . The inner mean operator must be taken over all variables but X_i and X_j , while the outer variance operator is taken over the two conditioned variables. Since we have subtracted individual contributions from the joint contribution, the remaining term quantifies the pure *interaction effect* of the two variables, i.e. the part of contribution from X_i and X_j that cannot be captured by simple summation of S_i and S_j . The interaction effect is present when the model is nonadditive.

6.3.2 Nonadditive Models

When the model is an additive function, the terms only containing each variable can be separated by the plus operators. For example, consider two functions

$$g_A(X_1, X_2) = 3X_1^3 + \log(X_2) \quad (6.3.2)$$

$$g_B(X_1, X_2) = 3X_1^3 + \log(X_2) + X_1X_2 \quad (6.3.3)$$

In function A, the two variables X_1 and X_2 are additive. On the other hand, in function B, two variables are nonadditive because of the third term. Similarly, $Y = \sum_i X_i^2$ is an additive function, but $Y = \prod_i X_i^2$ is nonadditive. If a model is additive, it is possible to separate the effects of individual input variables. That means in case of function A,

$$\text{Var}_{X_1, X_2} [\mathbb{E}_{\mathbf{X}_{12}} [Y|X_1, X_2]] = \text{Var}_{X_1} [\mathbb{E}_{\mathbf{X}_1} [Y|X_1]] + \text{Var}_{X_2} [\mathbb{E}_{\mathbf{X}_2} [Y|X_2]] \quad (6.3.4)$$

holds, and therefore, their interaction effect is zero, i.e. $S_{12}^A = 0$. On the other hand, for nonadditive models, presence of the interaction term produces additional variance

$$\text{Var}_{X_1, X_2} [\mathbb{E}_{\mathbf{X}_{12}} [Y|X_1, X_2]] \geq \text{Var}_{X_1} [\mathbb{E}_{\mathbf{X}_1} [Y|X_1]] + \text{Var}_{X_2} [\mathbb{E}_{\mathbf{X}_2} [Y|X_2]] \quad (6.3.5)$$

resulting in $S_{12}^B > 0$. Similarly to the second-order index, the third-order sensitivity index is defined as

Third-order Sensitivity Index

$$S_{ijk} = \frac{\text{Var}_{X_i, X_j, X_k} [\mathbb{E}_{\mathbf{X}_{\bar{ijk}}} [Y|X_i, X_j, X_k]]}{\text{Var}[Y]} - S_i - S_j - S_k - S_{ij} - S_{jk} - S_{ik} \quad (6.3.6)$$

that will have non-zero values when there exists a nonadditive term of X_i, X_j and X_k . However it is important to note that in real-world applications, the presence of interaction terms is often unknown in advance, therefore sensitivity results can be a useful indication of the presence of the interaction effect.

The most general expression of Sobol index is

Higher-order Sensitivity Index

$$S_u = \frac{\text{Var}_{\mathbf{X}_u} [\mathbb{E}_{\mathbf{X}_u} [Y|\mathbf{X}_u]] - \sum_{v \subset u} (-1)^{|u|-|v|} \text{Var}_{\mathbf{X}_v} [\mathbb{E}_{\mathbf{X}_v} [Y|\mathbf{X}_v]]}{\text{Var}[Y]} \quad (6.3.7)$$

further, higher-order Sobol indices collectively have below property

Property of Sobol Indices

When input variables are independent,

$$1 = \sum_i S_i + \sum_{i < j} S_{ij} + \dots + S_{12\dots d} \quad (6.3.8)$$

The proof will be provided in the next section. Because of the property, for additive models, the first-order Sobol indices add up to one, i.e. $\sum_i S_i = 1$. For nonadditive models, sum of the first-order Sobol indices is always smaller than one, i.e. $\sum_i S_i < 1$. This holds only when the input variables are independent of each other.

6.3.3 Total-effect Index

Another useful sensitivity measure is so called total-effect index. Total-effect index is used to account for all the interaction effects associated with a variable X_i .

Sobol Total-effect Index

$$S_i^\top = 1 - \frac{\text{Var}_{\mathbf{X}_i} [\mathbb{E}_{\mathbf{X}_i} [Y|\mathbf{X}_i]]}{\text{Var}[Y]} \quad (6.3.9)$$

equivalently from the *Law of Total Variance*,

Sobol Total-effect Index (2)

$$S_i^\top = \frac{\mathbb{E}_{\mathbf{X}_i} [\text{Var}_{\mathbf{X}_i} [Y|\mathbf{X}_i]]}{\text{Var}[Y]} \quad (6.3.10)$$

For example, when the model gets total of three variables, the total-effect index for X_1 is calculated by

$$S_1^\top = 1 - S_{23} - S_2 - S_3 \quad (6.3.11)$$

When the variables are uncorrelated, the following also holds

$$S_1^\top = S_1 + S_{12} + S_{13} + S_{123} \quad (6.3.12)$$

from the property in Eq.(6.3.8).

6.4 Analysis of Variance (ANOVA) Decomposition

An alternative way of understanding (deriving) the Sobol indices is by introducing Sobol-Hoeffding decomposition, also known as ANOVA(analysis of variance) decomposition*.

*Saltelli, A. and Sobol', I.Y.M., 1995. Sensitivity analysis for nonlinear mathematical models: numerical experience. *Matematicheskoe Modelirovanie*, 7(11), pp.16-28.

ANOVA Decomposition

Consider a function with uncorrelated input $\mathbf{X}$ uniformly distributed within a unit hypercube.

$$Y = g(\mathbf{X}) \quad (6.4.1)$$

The model can be decomposed into summands of increasing dimension.

$$Y = g_0 + \sum_i g_i(X_i) + \sum_{i < j} g_{ij}(X_i, X_j) + \dots + g_{12\dots d}(X_1, \dots, X_d) \quad (6.4.2)$$

or using more compact ensemble notation,

$$Y = \sum_{\mathbf{u} \subseteq \{1,2,\dots,d\}} g_{\mathbf{u}}(\mathbf{X}_{\mathbf{u}}) \quad (6.4.3)$$

The decomposition always exists and is unique when the below holds

$$\int g_{\mathbf{u}}(\mathbf{X}_{\mathbf{u}}) dX_k = 0 \quad (6.4.4)$$

where $X_k \in \mathbf{X}_{\mathbf{u}}$, i.e. integration of the each component function with respect to any of their “own” variables are zero. The expansion is called ANOVA-representation.

Variance of these summands divided by total variance is defined as global sensitivity analysis.

Sobol Indices - ANOVA Definition

Given that $g(\mathbf{X})$ is square-integrate, global importance measure is

$$S_{\mathbf{u}} = \frac{\mathbb{V}ar[g_{\mathbf{u}}(\mathbf{X}_{\mathbf{u}})]}{\mathbb{V}ar[Y]} \quad (6.4.5)$$

where $g_{\mathbf{u}}(\mathbf{X}_{\mathbf{u}})$ is a ANOVA summand.

Eq.(6.4.5) represent the contribution of partial variances, associated with each combination of random variables. That is the reduction in the total variance of the system, induced by freezing the associated random variables. Because of the independent assumption, it can be shown that variance values of each component function sums up to the total variance of Y (i.e, variance sum law).

$$\mathbb{V}ar[Y] = \sum_i \mathbb{V}ar[g_i(X_i)] + \sum_{i < j} \mathbb{V}ar[g_{ij}(X_i, X_j)] + \dots + \mathbb{V}ar[g_{12\dots d}(X_1, X_2, \dots, X_d)] \quad (6.4.6)$$

Therefore,

$$1 = \sum_i S_i + \sum_{i < j} S_{ij} + \dots + S_{12\dots d} \quad (6.4.7)$$

The equivalence of the previous Sobol index in Eq.(6.2.5) and the ANOVA partial variance Eq.(6.4.5) can be drawn as the follows. From the property Eq.(6.4.4). Below can be derived

$$\begin{aligned} \mathbb{E}[Y] &= g_0 \\ \mathbb{E}_{\mathbf{X}_i}[Y|X_i] &= g_0 + g_i(X_i) \\ \mathbb{E}_{\mathbf{X}_{ij}}[Y|X_i, X_j] &= g_0 + g_i(X_i) + g_j(X_j) + g_{ij}(X_i, X_j) \end{aligned} \quad (6.4.8)$$

On the other words,

$$\begin{aligned}
g_0 &= \mathbb{E}[Y] \\
g_i(X_i) &= \mathbb{E}_{\mathbf{X}_i}[Y|X_i] - g_0 \\
g_{ij}(X_i, X_j) &= \mathbb{E}_{\mathbf{X}_{ij}}[Y|X_i, X_j] - \mathbb{E}_{\mathbf{X}_i}[Y|X_i] - \mathbb{E}_{\mathbf{X}_j}[Y|X_j] + g_0
\end{aligned} \tag{6.4.9}$$

Further by taking variance operator on both sides and dividing them by $\text{Var}[Y]$,

$$\begin{aligned}
\frac{\text{Var}_{X_i}[g_i(X_i)]}{\text{Var}[Y]} &= \frac{\text{Var}_{X_i}[\mathbb{E}_{\mathbf{X}_i}[Y|X_i]]}{\text{Var}[Y]} \\
\frac{\text{Var}_{X_i, X_j}[g_{ij}(X_i, X_j)]}{\text{Var}[Y]} &= \frac{\text{Var}_{X_i, X_j}[\mathbb{E}_{\mathbf{X}_{ij}}[Y|X_i, X_j]]}{\text{Var}[Y]} \\
&\quad - \frac{\text{Var}_{X_i}[\mathbb{E}_{\mathbf{X}_i}[Y|X_i]]}{\text{Var}[Y]} - \frac{\text{Var}_{X_j}[\mathbb{E}_{\mathbf{X}_j}[Y|X_j]]}{\text{Var}[Y]}
\end{aligned} \tag{6.4.10}$$

In this way, starting from the ANOVA definition of partial variance (left) we arrived at the expression of Sobol index (right). Note that Eq.(6.4.7) is also equivalent to Eq.(6.2.4) obtained from the *Law of Total Variance*. This derivation using S-H decomposition clearly shows that Sobol index represents the fraction of total response variance, which can be attributed to each individual (sets) of input variables. Again, it is noted that this property Eq.(6.4.7) is acquired only because the variables are assumed to be independent to each other.

6.5 Correlated Random Variables and Transformation Invariancy

- When the variables X_i and X_j are correlated, main-effect Sobol index still indicates the relative importance of each variable to one another (Recall that the derivation based on the *Law of Total Variance* did not require independence assumption). However, the sum of the Sobol indices can be greater than one.
- **Input variable transform:** When $\mathbf{X}$ is independent random variables, given any one-on-one transformation $Z_i = T_i(X_i)$, and for corresponding model form $g_Z(\mathbf{Z}) = g(T^{-1}(\mathbf{Z}))$, the sensitivity index does not change, i.e.

$$S_i^{g_Z(\mathbf{Z})} = S_i^{g(\mathbf{X})} \tag{6.5.1}$$

- **Output quantity transform:** S_i is also invariant to the linear transform of output, $\tilde{Y} = aY + b$

6.6 Special case: Linear model

6.6.1 Equivalence Between Different Sensitivity Measures

For linear models, sigma-normalized derivative, linear regression coefficients, and variance-based first-order sensitivity indices are the same. Therefore, variance-based sensitivity can be viewed as a model-free extension of those to the models of unknown linearity.

6.6.2 GSA for the FORM Limit-state Surface

Recall FORM approximation where we approximate the limits-state with a linear hyperplane that passes through the design point,

$$G_{FORM}(z) = \nabla G(\mathbf{z}^*)(z - \mathbf{z}^*) \quad (6.6.1)$$

Given the linear limit-state expression, let us identify the sensitivity index of each random variable. Given the linear expression in Eq.(6.6.1) the variance of response is derived as

$$\text{Var}[Y_{FORM}] = \|\nabla G(\mathbf{z}^*)\|^2 \quad (6.6.2)$$

Because the variance of Z_i is one. Similarly, partial variance due to Z_i is

$$\text{Var}_{Z_i} [\mathbb{E}_{\mathbf{Z}_{\bar{i}}} [Y_{FORM}|Z_i]] = \left(\frac{\partial G(\mathbf{z}^*)}{\partial z_i} \right)^2 \quad (6.6.3)$$

Therefore,

$$S_i^{G_{FORM}(z)} = \frac{\text{Var}_{Z_i} [\mathbb{E}_{\mathbf{Z}_{\bar{i}}} [Y_{FORM}|Z_i]]}{\text{Var}[Y_{FORM}]} = \alpha_i^2 \quad (6.6.4)$$

from the definition of α in Eq.(6.1.4). Because the Sobol index is invariant to one-on-one transform of input variables, provided that the input variables are independent to each other, Eq.(6.6.4) can be directly used as the approximated importance measure of non-standardized variable X_i .

6.7 Algorithms to Estimate Sobol Indices

Global sensitivity analysis is an excellent way of understanding the model, and it is especially useful as a pre-analysis step before performing computationally expensive main analysis, e.g. reliability analysis or optimization. However, because of the two-fold integration associated with the numerator, i.e. $\text{Var}_{\mathbf{X}_u} [\mathbb{E}_{\mathbf{X}_{\bar{u}}} [Y|\mathbf{X}_u]]$, the analysis can be computationally demanding. Here we would like to algorithms for efficient global sensitivity analysis.

6.7.1 Monte Carlo Estimation

The most straightforward approach is to perform two-fold Monte Carlo integration. Let us first consider main Sobol index for variable X_i .

1. For $n = 1, 2, \dots, N$

- (a) Draw one sample of X_i , say $X_i^{(n)}$
- (b) Draw N -samples of $\mathbf{X}_{\bar{i}}$, say $\{\mathbf{X}_{\bar{i}}^{(m)}\}_{m=1, \dots, N}$
- (c) Compute N -sample responses with $\{X_i^{(n)}, \mathbf{X}_{\bar{i}}^{(m)}\}$, say $\{Y^{(n,m)}\}_{m=1, \dots, N}$.
- (d) Compute the sample mean of the response, let us call this $E_i^{(n)}$, i.e.

$$\mathbb{E}_{\mathbf{X}_{\bar{i}}} [Y|X_i^{(n)}] \simeq E_i^{(n)} = \frac{1}{N} \sum_{m=1}^N Y^{(n,m)} \quad (6.7.1)$$

2. Compute sample variance of $\{E_i^{(n)}\}_{n=1,2,\dots,N}$

$$\text{Var}_{X_i} [\mathbb{E}_{\mathbf{X}_{\bar{i}}} [Y|X_i]] \simeq \frac{1}{N} \sum_{n=1}^N (E_i^{(n)} - \bar{E}_i)^2 \quad (6.7.2)$$

where $\bar{E}_i$ is sample mean of $E_i^{(n)}$

3. Compute the variance of Y using $\{Y^{(n,m)}\}_{n,m=1,\dots,N}$ and compute the main Sobol index.

This algorithm requires $(d \times N^2)$ model evaluations to get main Sobol indices. Total-effect indices can be calculated similarly (by switching sampling order of X_i and $\mathbf{X}_{\bar{i}}$ and by subtracting the final results from 1) and it requires the same amount of calculations to the main-effect index.

6.7.2 Smart Monte Carlo

Sensitivity indices can be obtained much more efficiently by carefully designing the sampling sequence.*

1. Draw two independent N -sample sets, say set $\mathbf{A}$ and set $\mathbf{B}$ (i.e., total $2N$ sample points are randomly sampled). Let us denote the corresponding sample responses as $\mathbf{Y}_A$ and $\mathbf{Y}_B$, respectively.
2. Compute the response mean and variance, $\bar{Y} = \mathbb{E}[Y]$ and $\text{Var}[Y]$, using $\mathbf{Y}_A$ and $\mathbf{Y}_B$
3. For $i = 1, 2, \dots, d$
 - (a) Let us define a new sample set by combining sample set $\mathbf{A}$ and $\mathbf{B}$. By bringing the sample values of only i -th variable, X_i , from sample set $\mathbf{B}$ and bringing $\mathbf{X}_{\bar{i}}$ from $\mathbf{A}$, a new sample set can be defined, say $\mathbf{A}_B^i$, that has N sample points.
 - (b) Compute corresponding sample responses $\mathbf{Y}_{A_B^i}$
 - (c) Main- and total-effect indices can be estimated using

$$\begin{aligned} \text{Var}_{X_i} [\mathbb{E}_{\mathbf{X}_{\bar{i}}} [Y|X_i]] &= \frac{1}{N} \sum_{n=1}^N Y_{\mathbf{A}}^{(n)} Y_{\mathbf{A}_B^i}^{(n)} - \bar{Y}^2 \\ \text{Var}_{\mathbf{X}_{\bar{i}}} [\mathbb{E}_{X_i} [Y|\mathbf{X}_{\bar{i}}]] &= \frac{1}{N} \sum_{n=1}^N Y_{\mathbf{B}}^{(n)} Y_{\mathbf{A}_B^i}^{(n)} - \bar{Y}^2 \end{aligned} \quad (6.7.3)$$

This algorithm requires total $(d + 2) \times N$ model evaluations to get both main- and total-effect indices of all random variables. The derivation can be found in Saltelli *et al.* (2010)

6.7.3 Probability Model-based Global Sensitivity Analysis

This algorithm[†] first approximates the joint PDF of $f(\mathbf{X}_{\mathbf{u}}, Y)$ using the samples obtained by Monte Carlo simulation and computes $\text{Var}[\mathbb{E}[Y|\mathbf{X}_{\mathbf{u}}]]$ from the approximated distribution. Any parametric distributions with sufficient flexibility can be used to fit the distribution, but here we are introducing the Gaussian mixture-based approach.

*Saltelli, A., Annoni, P., Azzini, I., Campolongo, F., Ratto, M. and Tarantola, S., 2010. Variance based sensitivity analysis of model output. Design and estimator for the total sensitivity index. Computer physics communications, 181(2), pp.259-270.

[†]Hu, Z. and Mahadevan, S. (2019). Probability models for data-driven global sensitivity analysis. Reliability Engineering and System Safety, 187, 40-57.

1. Draw N -samples and compute $\mathbb{V}ar[Y]$ using the sample responses.
2. For $i = 1, 2, \dots, d$
 - (a) Collect samples of X_i and Y , say $\{X_i^{(n)}, Y^{(n)}\}_{n=1, \dots, N}$
 - (b) Approximate the joint distribution of $\{X_i, Y\}$ using the joint sample set. Fit bivariate Gaussian mixture distribution

$$f(X_i, Y) = \sum_{k=1}^m \alpha_k f_N([X_i, Y]; \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \quad (6.7.4)$$

where $f_N(\cdot; \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$ represents k -th Gaussian distribution and α_k is their weight:

$$\boldsymbol{\mu}_k = (\mu_{x,k} \quad \mu_{y,k}) \quad (6.7.5)$$

$$\boldsymbol{\Sigma}_k = \begin{pmatrix} \sigma_{x,k}^2 & \sigma_{x,k}\sigma_{y,k}\rho_{xy,k} \\ \sigma_{x,k}\sigma_{y,k}\rho_{xy,k} & \sigma_{y,k}^2 \end{pmatrix} \quad (6.7.6)$$

and

$$\sum_{k=1}^m \alpha_k = 1 \quad (6.7.7)$$

For example, expectation-maximization algorithm can be used to identify the parameters $\{\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k, \alpha_k\}$.

- (c) Calculate $E_i^{(n)} = \mathbb{E}_{\mathbf{X}_i} [Y|X_i^{(n)}]$ corresponding to each $X_i^{(n)}$ using the property of Gaussian mixture distribution, i.e., $E_i^{(n)}$ can be derived in analytic closed-form expression as

$$E_i^{(n)} = \sum_{k=1}^m \tilde{\alpha}_k^{(n)} \tilde{\mu}_k^{(n)} \quad (6.7.8)$$

where,

$$\begin{aligned} \tilde{\alpha}_k^{(n)} &= \frac{\alpha_k f_N(X_i^{(n)}; \mu_{x,k}, \sigma_{x,k}^2)}{\sum_{j=1}^m \alpha_j f_N(X_i^{(n)}; \mu_{x,j}, \sigma_{x,j}^2)} \\ \tilde{\mu}_k^{(n)} &= \mu_{y,k} + \frac{\sigma_{y,k}}{\sigma_{x,k}} \rho_{xy,k} (X_i^{(n)} - \mu_{x,k}) \end{aligned} \quad (6.7.9)$$

- (d) Compute sample variance of $\{E_i^{(n)}\}_{n=1,2,\dots,N}$

$$\mathbb{V}ar_{X_i} [\mathbb{E}_{\mathbf{X}_i} [Y|X_i]] \simeq \frac{1}{N} \sum_{n=1}^N (E_i^{(n)} - \bar{E}_i)^2 \quad (6.7.10)$$

where $\bar{E}_i$ is sample mean of $E_i^{(n)}$

- (e) Compute the main Sobol index.

Total-effect index can be obtained in a similar manner by replacing X_i with $\mathbf{X}_i$ and subtracting the final result from 1. For the total-effect index, the Gaussian mixture fitting is performed in the higher d -dimension space and Eq.(6.7.9) becomes

$$\begin{aligned} \tilde{\alpha}_k^{(n)} &= \frac{\alpha_k f_N(\mathbf{X}_i^{(n)}; \boldsymbol{\mu}_{x,k}, \boldsymbol{\Sigma}_{x,k})}{\sum_{j=1}^m \alpha_j f_N(\mathbf{X}_i^{(n)}; \boldsymbol{\mu}_{x,j}, \boldsymbol{\Sigma}_{x,j})} \\ \tilde{\mu}_k^{(n)} &= \mu_{y,k} + \boldsymbol{\Sigma}_{yx,k} \boldsymbol{\Sigma}_{xx,k}^{-1} (\mathbf{X}_i^{(n)} - \boldsymbol{\mu}_{x,k}) \end{aligned} \quad (6.7.11)$$

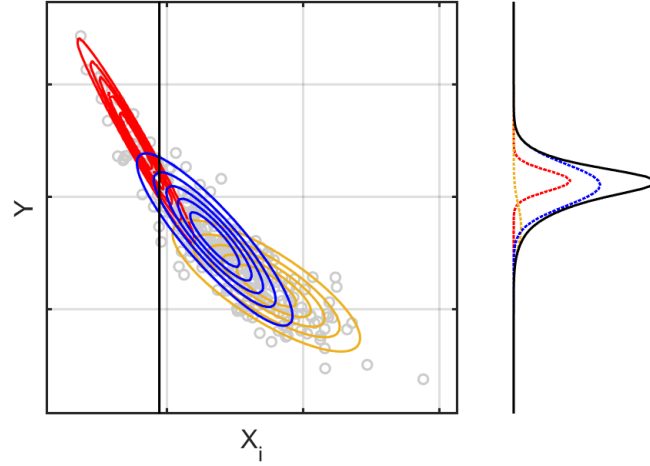


Figure 6.7.1: Estimation of $\mathbb{E}_{X_i}[Y|X_i]$ using Gaussian mixture model.

6.8 Reliability-oriented GSA

6.8.1 Reformulation of Sobol Index

Sensitivity analysis can be combined to reliability analysis to identify what are the most important variables in triggering the failure. In particular, instead of a continuous quantity of interest, now we are interested in Bernoulli output defined as

$$q = 1(G(\mathbf{x})) \quad (6.8.1)$$

In this case, the mean and variance of q is expressed in terms of its occurrence probability, i.e. the failure probability in the reliability problems.

$$\begin{aligned} \mathbb{E}[q] &= P_f \\ \text{Var}[q] &= P_f(1 - P_f) \end{aligned} \quad (6.8.2)$$

Similarly, the conditional variance can be written in terms of conditional probability.

$$\begin{aligned} \text{Var}_{\mathbf{X}_u}[\mathbb{E}_{\mathbf{X}_u}[q|\mathbf{X}_u]] &= \text{Var}_{\mathbf{X}_u}[P_{f|\mathbf{X}_u}] \\ &= \mathbb{E}_{\mathbf{X}_u}[P_{f|\mathbf{X}_u}^2] - \mathbb{E}_{\mathbf{X}_u}[P_{f|\mathbf{X}_u}]^2 \\ &= \mathbb{E}_{\mathbf{X}_u}[P_{f|\mathbf{X}_u}^2] - P_f^2 \end{aligned} \quad (6.8.3)$$

Thus Sobol index is reformulated as,

$$S_u = \frac{\text{Var}_{\mathbf{X}_u}[\mathbb{E}_{\mathbf{X}_u}[q|\mathbf{X}_u]]}{\text{Var}[q]} = \frac{\mathbb{E}_{\mathbf{X}_u}[P_{f|\mathbf{X}_u}^2] - P_f^2}{P_f(1 - P_f)} \quad (6.8.4)$$

In the following sections, we will show that the sensitivity index can be obtained as a by-product of reliability analysis, i.e. FORM and sampling-based methods. With the knowledge of design point or given the failure domain samples, Sobol indices can be calculated without additional model evaluations.

6.8.2 From FORM Design Point

FORM uses the information on design point to define linearized limit state. Using the information, one can approximate the conditional probability required in Eq.(6.8.4) in terms of reliability index β and the importance vector $\boldsymbol{\alpha}^*$. Let us first consider the first-order Sobol index. The conditional failure probability associated with Z_i is

$$\begin{aligned}
 P_{f|Z_i} &= \mathbb{P}(\boldsymbol{\alpha}_{\bar{i}} \mathbf{Z}_{\bar{i}} \geq \beta - \alpha_i Z_i) \\
 &\quad (\text{separating } Z_i \text{ term from } \{G(\mathbf{Z}) \leq 0\}, \text{ or equivalently, } \{\boldsymbol{\alpha} \mathbf{Z} \geq \beta\}) \\
 &= \mathbb{P}\left(\tilde{z} \leq \frac{\alpha_i Z_i - \beta}{\|\boldsymbol{\alpha}_{\bar{i}}\|}\right) \\
 &\quad (\text{where } \tilde{z} \text{ is standard normal distribution, because } \boldsymbol{\alpha}_{\bar{i}} \mathbf{Z}_{\bar{i}} \sim N(0, \|\boldsymbol{\alpha}_{\bar{i}}\|^2))
 \end{aligned} \tag{6.8.5}$$

Therefore,

$$\begin{aligned}
 \mathbb{E}_{Z_i} [P_{f|Z_i}^2] &= \mathbb{E}_{Z_i} \left[\mathbb{P}\left(\tilde{z} \leq \frac{\alpha_i Z_i - \beta}{\|\boldsymbol{\alpha}_{\bar{i}}\|}\right)^2 \right] \\
 &= \mathbb{E}_{Z_i} \left[\mathbb{P}\left(\tilde{z}_1 \leq \frac{\alpha_i Z_i - \beta}{\|\boldsymbol{\alpha}_{\bar{i}}\|}, \tilde{z}_2 \leq \frac{\alpha_i Z_i - \beta}{\|\boldsymbol{\alpha}_{\bar{i}}\|}\right) \right] \\
 &\quad (\tilde{z}_1 \text{ and } \tilde{z}_2 \text{ are independent standard normal}) \\
 &= \mathbb{P}\left(\tilde{z}_1 \leq \frac{\alpha_i Z_i - \beta}{\|\boldsymbol{\alpha}_{\bar{i}}\|}, \tilde{z}_2 \leq \frac{\alpha_i Z_i - \beta}{\|\boldsymbol{\alpha}_{\bar{i}}\|}\right) \\
 &\quad (\text{Total probability theorem}) \\
 &= \mathbb{P}(\tilde{y}_1 \leq -\beta, \tilde{y}_2 \leq -\beta) \\
 &\quad (\text{by letting } \tilde{y}_k = \tilde{z}_k \|\boldsymbol{\alpha}_{\bar{i}}\| - \alpha_i Z_i \text{ for } k = 1, 2) \\
 &= \Phi_2(-\beta, -\beta, \alpha_i^2) \\
 &\quad (\tilde{y}_k \text{ are standard normal with correlation } \alpha_i^2)
 \end{aligned} \tag{6.8.6}$$

Meanwhile, bivariate normal CDF can be expressed in terms of single-fold integral (Papaioannou and Straub, 2021)

$$\Phi_2(-\beta, -\beta, \alpha_i^2) = \underbrace{\Phi(-\beta)^2}_{P_f^2} + \int_0^{\alpha_i^2} \varphi_2(-\beta, -\beta, r) dr \tag{6.8.7}$$

By substituting above equations to Eq.(6.8.4), the formulation for the reliability-oriented sensitivity index is derived:

First-order Sobol Index for FORM Analysis

Given a linear limit state with design point $\mathbf{z}^*$, the main-effect Sobol index for output q is

$$S_i = \frac{1}{P_f(1 - P_f)} \int_0^{\alpha_i^2} \varphi_2(-\beta, -\beta, r) dr \tag{6.8.8}$$

where $\beta = \|\mathbf{z}^*\|$, $\alpha_i = z_i^*/\beta$, and $P_f = \Phi(-\beta)$.

In a similar way, the total-effect index can be derived as

*Papaioannou, I. and Straub, D., 2021. Variance-based reliability sensitivity analysis and the FORM a-factors. Reliability Engineering and System Safety, 210, p.107496.

Total-effect Sobol Index for FORM Analysis

$$S_i^\top = \frac{1}{P_f(1 - P_f)} \int_{1-\alpha_i^2}^1 \varphi_2(-\beta, -\beta, r) dr \quad (6.8.9)$$

Therefore, the first-order and total-effect indices can be completely determined given the design point (or α and β). Figure 6.8.1 shows the sensitivity indices for different α_i and β values. One thing to be noticed is that as the probability becomes smaller, the main-effect index approaches zero, while the total-effect index approaches one. It is because the rare events are often triggered by particular combinations of random variables rather than an extreme realization of just a single variable. Therefore, the interaction effect dominates the response.

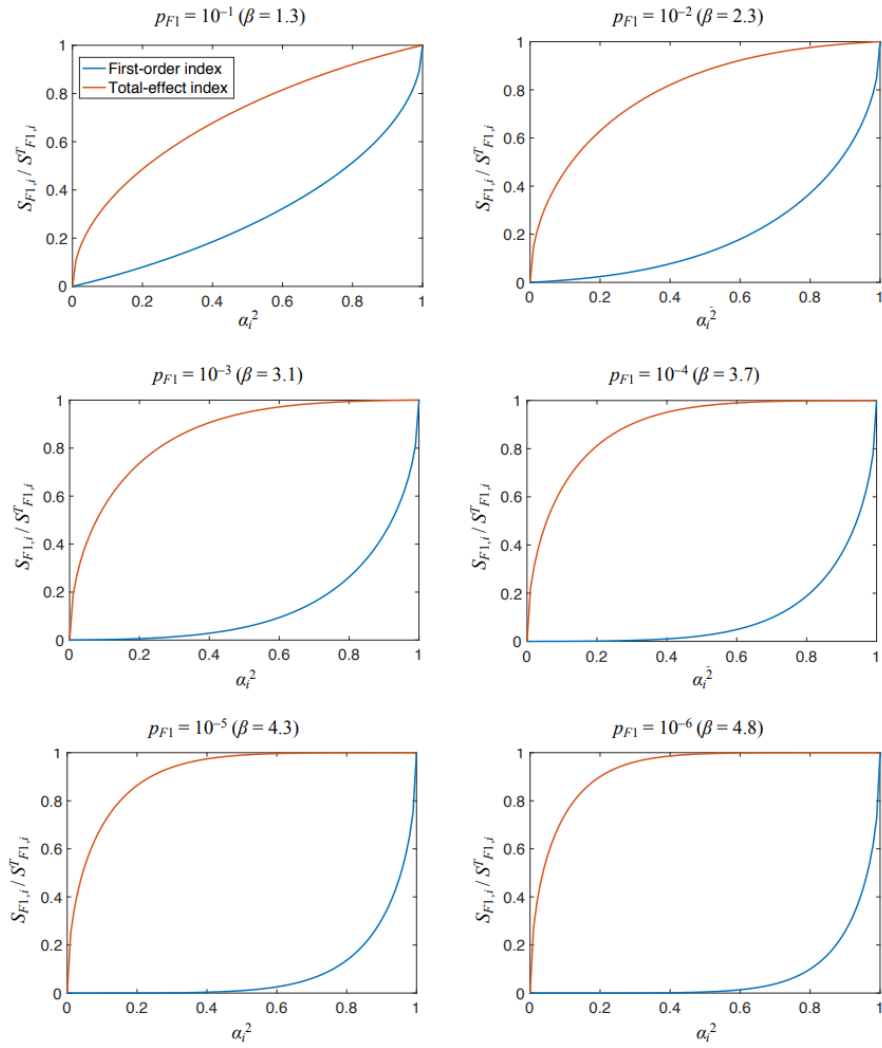


Figure 6.8.1: Example results of the first-order and total-effect indices for different failure probabilities (Papaioannou and Straub, 2021).

6.8.3 From Samples in the Failure Domain

In most sampling-based reliability methods, samples of the input random variables $\mathbf{X}$ in the failure domain are obtained. These samples provides an alternative means of computing $P_{f|X_i}$

in Eq.(6.8.4).^{*} In particular $P_{f|X_i}$ can be reformulated in terms of failure-conditional PDF.

$$\begin{aligned} P_{f|X_i} &= \mathbb{P}(\mathcal{F}|X_i) \quad (\mathcal{F} := \{\mathbf{X} : G(\mathbf{X}) \leq 0\}) \\ &= \frac{\mathbb{P}(X_i|\mathcal{F})\mathbb{P}(\mathcal{F})}{\mathbb{P}(X_i)} \quad (\text{Bayes' rule}) \\ &= \frac{f_{X_i|\mathcal{F}}(X_i)P_f}{f_{X_i}(X_i)} \end{aligned} \quad (6.8.10)$$

where $f_{X_i|\mathcal{F}}$ is conditional PDF of X_i given failure $\mathcal{F}$. Once the samples of X_i are obtained, the conditional PDF can be approximated by kernel density estimation or maximum entropy method.

Kernel Density Estimation

The probability distribution of given samples $\{\mathbf{x}^{(n)}\}, n = 1, \dots, N$, can be approximated as

$$k(\mathbf{x}) = \frac{1}{N} \sum_{n=1}^N \frac{1}{w^d} K\left(\frac{\mathbf{x} - \mathbf{x}^{(n)}}{w}\right) \quad (6.8.11)$$

where $K(\cdot)$ is called kernel PDF and w is a bandwidth parameter.

A popular choice for kernel PDF is standard normal PDF, i.e. $K(\cdot) = \varphi(\cdot)$ and the optimal bandwidth can be found by solving the following optimization problem.

$$w_{opt} = \arg \min_w \left(\mathbb{E}_{X_i} [\hat{P}_{f|X_i}(w)] - \hat{P}_f \right)^2 \quad (6.8.12)$$

By approximating $f_{X_i|\mathcal{F}}(X_i) \simeq k(X_i)$, $P_{f|X_i}$ can be computed and the sensitivity index is calculated using Eq.(6.8.4). The mean operation can be replaced by the sample mean of $P_{f|X_i}$ obtained using different X_i values.

6.8.4 Extrapolation of Sobol Indices

It is often helpful to know the importance of each variable before conducting the reliability analysis, for example, for variable screening. However, it is challenging to calculate the sensitivity beforehand because the values of P_f and $P_{f|X_i}$ required for computing the sensitivity index (Eq.(6.8.4)) are unknown. One approach to approximate the sensitivity index is via extrapolation. Consider the probability model-based approach GSA algorithm introduced in the previous section, which approximated the joint distribution of $f(X_i, Y)$ using the Gaussian mixture model (Eq.(6.8.14)) utilizing the samples obtained by a modest number of Monte Carlo simulations. Having such a parametric form of joint distribution allows us to estimate the reliability-oriented sensitivity index with small number of pre-simulations. Let us define Y as the limit-state function value.

$$Y = G(\mathbf{x}) \quad (6.8.13)$$

The failure event is defined as $\mathcal{F} = \{\mathbf{x} : G(\mathbf{x}) \leq 0\}$. Suppose, based on the Monte Carlo simulation samples, the joint PDF can be approximated as the following Gaussian mixture form.

$$f(X_i, Y) = \sum_{k=1}^m \alpha_k f_N([X_i, Y]; \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \quad (6.8.14)$$

^{*}Li, L., Papaioannou, I. and Straub, D., 2019. Global reliability sensitivity estimation based on failure samples. Structural Safety, 81, p.101871.

Meanwhile, the conditional probability of failure can be written as

$$P_{f|X_i} = \mathbb{P}(Y \leq 0|X_i) = \frac{\mathbb{P}(X_i, Y \leq 0)}{f(X_i)dX_i} \quad (6.8.15)$$

where

$$\begin{aligned} \mathbb{P}(X_i, Y \leq 0) &= \int_{-\infty}^0 f_{X_i, Y}(X_i, Y) dY dX_i \\ &\simeq \int_{-\infty}^0 \sum_{k=1}^m \alpha_k f_N([X_i, Y]; \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) dY dX_i \\ &= \sum_{k=1}^m \alpha_k F_N([X_i, Y = 0]; \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) dX_i \end{aligned} \quad (6.8.16)$$

in which $F_N(\cdot)$ is bivariate normal CDF. Given this $P_{f|X_i}$ formulation, the sensitivity index can be derived using Eq.(6.8.4). The mean operation can be replaced by the sample mean of $P_{f|X_i}$ obtained using different X_i samples.