Global Sensitivity

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1) Local Sensitivity

Most sensitivity analyses [1] are based on local estimates of sensitivity, typically by expanding the response in a Taylor series about some specific values of the parameters to give, for example for two parameters

\[
R(X + \delta X) = R(X) + \frac{\partial R}{\partial x_1} \delta x_1 + \frac{\partial R}{\partial x_2} \delta x_2 + \frac{\partial^2 R}{\partial x_1^2} \frac{\delta x_1^2}{2} + \frac{\partial^2 R}{\partial x_1 \partial x_2} \delta x_1 \delta x_2 + \frac{\partial^2 R}{\partial x_2^2} \frac{\delta x_2^2}{2} + \ldots |X^*.
\]  

Here \( R \) is the response, \( x_1 \) and \( x_2 \) are the parameters whose influences are sought, and \( |X^* \) represents the values of these parameters at which the terms are evaluated.

The local sensitivity is defined as the coefficients of the 1st order effects evaluated at \( X^* \) i.e.,

\[
S^*_x = \frac{\partial R}{\partial x} |X^*.
\]

Figure 1 depicts the response as a function of the two parameters, \( x_1 \) and \( x_2 \) at different locations, \( X^* \).

While local sensitivities are commonly used to investigate the properties of system responses, they suffer from several serious deficiencies:

1. the computation of 2nd and higher order terms is not a trivial undertaking.
2. they represent the behavior only at the specific values of the parameters, \( X^* \), at which the terms of the Taylor series are evaluated. For nonlinear problems they may vary substantially. Figure 1 illustrates how they may vary as \( X^* \) is varies. We see that at point \( X^* = (a) \), the slopes are very small and the system is insensitive to both \( x_1 \) and \( x_2 \). At point (b), it is sensitive primarily to \( x_1 \), while at point (c) it is sensitive to both \( x_1 \) and \( x_2 \). Clearly different conclusions about the sensitivity of the system would be drawn depending upon the point at which the sensitivities were evaluated.

3. the conclusions are also dependent upon the values of \( \delta x_1 \) and \( \delta x_2 \), i.e. upon the direction of interest. For some directions the contributions of some of the cross terms may vanish, while in other directions they may dominate.

4. the cross derivative terms represent interactions between the parameters and it is difficult to understand their effects.

**Additive Models** In regression and sensitivity analyses considerable importance is attached to additive models. These are models of system responses that are the sum of functions, each of which is a function of only one variable,

\[
\text{additive model : } R(x_1, x_2, \ldots, x_m) = f_0 + f_1(x_1) + f_2(x_2) + \cdots f_m(x_m)
\]

The constituent functions, \( f_i(x_i) \), may be complex nonlinear functions of the single parameter, \( x_i \). Additive models have several very desirable characteristics,

1. the behavior of the model with respect to any single parameter, \( x_j \), can be determined without specifying any of the other parameters
2. the maximum/minimum response is simply the sum of the maximum/minimum values of each of the constituent functions
3. when solving inverse problems for parameter values, the sum of the residuals squared is a \( m \) dimensional hyper ellipsoid and finding the minimum is achieved using standard minimization techniques.
4. confidence intervals for the parameters are easily determined
5. error analyses are simple to conduct.

Unfortunately, models of technical systems are rarely additive. Instead, the model is usually a function of several parameters that often occur in groups, e.g. Reynolds or Nusselt numbers. When this happens cross derivative terms appear in the Taylor series. As a result of these cross derivatives, parameter estimation problems may become much more complex, depending upon the magnitude and the character of the interactions. Because of the emphasis on additive models, much of the literature on sensitivity analysis and regression is not applicable to engineering models.

2) **Global Sensitivity**

Instead of using local sensitivities, Saltelli and colleagues [2] have suggested the use of 'global sensitivity' based upon variances. The idea is to evaluate the contribution of the different parameters to the variance over the range of the parameters. This is best done using Sobol’s [3] concept of 'total sensitivities.' Let the response be \( f(x_1, x_2, \ldots, x_m) \). Sobol showed that a function could be decomposed in the form

\[
f(X) = f_0 + \sum_{i}^{m} f_i(x_i) + \sum_{i}^{m} \sum_{j > i}^{m} f_{i,j}(x_i, x_j) \\
+ \sum_{i}^{m} \sum_{j > i}^{m} \sum_{k > j}^{m} f_{i,j,k}(x_i, x_j, x_k) \ldots
\]
$f_i(x_i)$ are termed 1st order effects (main effects) and $f_{i,j}(x_i, x_j)$ and higher order terms represent the interactions. The functions $f_i, f_{i,j}, f_{i,j,k}$ et seq. are of zero mean and orthogonal. Because of these properties, evaluating the variances is particularly easy.

Now it is not easy to decompose $f(X)$ in the form of Eq. 3. Fortunately Sobol also showed that the variances can be expanded in a similar way and suggested the use of 'total sensitivity' defined in terms of the 'total variance due to $x_i$'

$$S_{Ti} = \frac{\text{sum of first effect variance due to } x_i + \text{the sum of all interactions involving } x_i}{\text{Var}[f(X)]}$$

(4)

Although $X_i$ can represent several parameters of interest, we will restrict $X_i$ to be a single parameter $x_i$. $X_{-i}$ represents all parameters except $x_i$, i.e., the complementary set of parameters. $f(X|X_{-i})$ is the function evaluated with all parameters $X$ except $X_i$ considered as known, $E_i$ is the conditional expectation taken over $X_i$, and $\text{Var}_{-i}$ is the variance taken over the complementary set. The sensitivity of the first order effect is defined as

$$S_i = \frac{\text{Var}_{-i}[E_i[f(X|x_i)]]}{\text{Var}[f(X)]}$$

For a 3 parameter model $S_{T1} = S_1 + S_{1,2} + S_{1,3} + S_{1,2,3}$ If there are no interactions, $S_i = S_{Ti}$ for all i. While $S_{Ti}$ is easy to interpret, $S_i$ has no obvious direct meaning.

Haylock and O’Hagan [4] gave an interesting interpretation of these sensitivities by noting that from the fundamental theorem relating the variance and the conditional expectations and variances

$$\text{Var}[f(X)] = E_i[\text{Var}_{-i}[f(X|x_i)]] + \text{Var}_i[E_{-i}[f(X|x_i)]]$$

(5a)

so that

$$S_i = \frac{\text{Var}[f(X)] - E_i[\text{Var}_{-i}[f(X|x_i)]]}{\text{Var}(f(X))}$$

(5b)

In other words $S_i$ is the fractional reduction in the $\text{Var}[f(X)]$ observed when we know $x_i$. Likewise, $S_{T1}$ is the fraction of the variance due to $x_i$ and its interactions with all of the other parameters, i.e., over the range of these other parameters, $X_{-i}$ are known. The difference between $S_{Ti}$ and $S_i$ is a direct measure of the sum of the effects of $x_i$ interacting with the rest of the parameters. An especially important result is that

$$1 - \sum_i^M S_i = \sum_{\text{of all interactions}}$$

(6)

and thus $1 - \sum_i^M S_i$ is a direct measure of all of the interactions between the parameters. Upon decomposing $f(X)$, one could examine the behavior of these interaction terms to evaluate their effects.

We define the sensitivity to the interaction effects relative to the first order effects as

$$SIE = \frac{1 - \sum_i^M S_i}{\sum_i^M S_i}$$

(7)

which provides a direct measure of the combined interactions.
2.1) Example 1

Consider the simple function

\[ f(x_1, x_2) = x_1^2 + x_1 x_2 + x_2 \]  

defined over \( 0 \leq x_1 \leq 1, \ 0 \leq x_2 \leq 1 \). The decomposition is

\[ f(x_1, x_2) = \frac{13}{12} + (x_1^2 + \frac{x_1}{2} - \frac{7}{12}) + (\frac{3x_2}{2} - \frac{3}{4}) + (x_1 x_2 - \frac{x_1}{2} - \frac{x_2}{2} + \frac{1}{4}) \]  

Figure 2 depicts \( f(x_1, x_2) \) and \( f_{1,2}(x_1, x_2) \). From the figure it appears that there is a strong interaction but it is difficult to estimate the effects of the interaction. While it may be possible to analytically or numerically evaluate the interaction effects, there are a total of \( 2^M - 1 \) terms in the expansion, meaning a computationally intractable approach for a large number of parameters, and even unrealistic for \( M \) as small as 4.

Figure 2: left: Response Surface for \( f(x_1, x_2) = x_1^2 + x_1 x_2 + x_2 \) right: interaction

From Figure 2b it appears that there is considerable interaction. However, \( S_1 = 0.4982, \ S_2 = 0.4839, \) and \( S_{1,2} = 0.0179 \). Thus, contrary to the impression gained from Fig. 2b, the interaction is seen to be negligible.

2.2) Example 2

Consider the function shown in Figure 3a

\[ f(x_1, x_2) = x_1 x_2 \]  

From Eq.10 the function is nothing but an interaction and one might think that the first order effects would be zero. However, its expansion in the form of Eq.3 is

\[ f(x_1, x_2) = \frac{1}{4} - \frac{1}{2}(x_1 - \frac{1}{2}) - \frac{1}{2}(x_2 - \frac{1}{2}) + (x_1 x_2 + \frac{x_1}{2} + \frac{x_2}{2} - \frac{3}{4}) \]  

with the interaction shown in Figure 3b. From Eq.11, a direct evaluation of the variances gives

\[ \text{var}(f) = \frac{7}{144}, \quad \text{var}_{x_1} = \frac{3}{144}, \quad \text{var}_{x_2} = \frac{3}{144}, \quad \text{var}_{x_1 x_2} = \frac{1}{144} \]

and

\[ S_{x_1} = \frac{3}{7}, \quad S_{x_2} = \frac{3}{7}, \quad S_{x_1 x_2} = \frac{1}{7} \]  

(12)
It is not always easy or even possible to express a nonlinear function in terms of Sobol’s expansion, Eq. 3. However, one can always evaluate the sensitivities using Eq. 5b. For this function, assuming uniform and independent distributions for $0 \leq x_1 \leq 1, 0 \leq x_2 \leq 1$ we have

$$
\text{var}_{x_2}(f|x_2) = x_2^2 \frac{1}{12}, \quad E_{x_1} = \frac{1}{36}
$$

and using Eq.5b we easily obtain the sensitivities. Note that the total sensitivities are $S^{T}_{x_1} = 4/7, S^{T}_{x_2} = 4/7$ and that the interactions are $1/3$th of the first order sensitivities.

2.3) Example 3

In general, the response of engineering systems cannot be described by equations such as treated in Examples 1 and 2. Instead the response is commonly determined through the solution of partial differential equations or their discrete equivalents, finite elements or finite volumes. In these cases, it is not possible to represent them in the form of Eq.3 and the sensitivities can only be found using Eq.5b.

Consider one-dimensional heat transfer in a slab of thickness $L$. We examined the effect of the different thermal parameters on the temperature measured at $x = 0$ when a heat flux, $Q$, is prescribed at $x = L$. Since the time at which the thermal flux reaches $x = 0$ is a function of the diffusivity, $\kappa = k/\rho c$, we expected to see considerable interaction between these two properties. As shown on Figure 3a, we see a high sensitivity to $k$ and $\rho c$ with both parameters showing substantial interactions. The initial response at $x=0$ is a very weak function of $Q$ and $h_0$. As steady state is approached, the sensitivity to $k$ and $\rho c$ vanishes. With the steady state temperature given by

$$
T(x = 0) - T_\infty = \frac{Q}{h_0}
$$

It is clear that it will be difficult to accurately estimate $k$ and $\rho c$ simultaneously because of: a) the rapid reduction of sensitivities, b) the strong interaction between these two parameters. The cause of this interaction is obvious, but the evaluating its effect is not trivial. The estimation of $Q$ and $h_0$ at longer times is similarly affected. However, its magnitude is easily estimated since it occurs because of the existence of the second order derivative with respect to $Q$ and $h_0$. Note that the second derivative with respect to $Q$ vanishes while that to $h_0$ exists. Thus the sensitivity to $Q$ is linear while that to $h_0$ is nonlinear.
Quantifying the effect can only be done by examining the sum of the sensitivities, Eq. Figure 4b illustrates the total interaction involved in the model. At early times, the interactions are substantial, approximately 11%, at steady state they are reduced to the order of 2%. One precaution must be taken. Even though the interactions may be large, they are of little concern if the total variance is negligible. The star on Figure 4b marks the point where the variance first exceeds 5% of the steady state value; interactions prior to this time of little interest. The maximum sum of the interactions are less than 5% and show the same reduction as steady state is approached for the other two problems.

References


