# Chapter 3:
# Sensitivity Analysis

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## Contents



## 1 Introduction

The objective of sensitivity analysis can be broadly viewed as quantifying the relative contributions of individual input model parameters variation on model output responses. The sensitivity analyses can 1) determine whether the model can be simplified by fixing insensitive parameters; 2) specify regimes in the parameter space that optimally impact model output or QoI and their uncertainties; 3) guide experimental design to determine measurement regimes that have the most significant impact on parameters or output/QoI sensitivity. In general, there are two sensitivity analysis methods:

- *Local sensitivity analysis.* Local sensitivity analysis focuses on the variability of the model output $\mathbf{y}$ or QoI when model parameters $\boldsymbol{\theta}$ are perturbed about a nominal value. This is often defined as the derivative $\dfrac{\partial \mathbf{y}}{\partial \theta_i}$. Local sensitivity analysis is central to adjoint-based optimization methods.

- *Global sensitivity analysis.* Global sensitivity analysis is more statistical in nature, and its objective is to ascertain how uncertainty in model outputs can be apportioned to uncertainties in model parameters, taken either singly or in combination. Thus, global sensitivity analysis compliment UQ analyses of computational models.

Due to the importance in UQ analyses, we focus on the global sensitivity analysis in this course. Throughout this section, we use $\mathbf{Y} = \mathbf{F}(\boldsymbol{\theta}) = \mathbf{F}(\theta_1, \cdots, \theta_p)$ notation to represent a model with $\mathbf{F}$ being the response function that maps input parameters $\boldsymbol{\theta}$ to model output $\mathbf{Y}$. In this notation, we suppress the possible time and space dependencies to simplify notation. This model can be an algebraic representation or result from an ODE or PDE's finite element or finite difference solution or numerical solution of discrete simulations such as molecular dynamics, discrete dislocation dynamics, or agent-based models.

***Example I: Additive model.*** A model $\mathbf{Y} = \mathbf{F}(\boldsymbol{\theta})$ is called an additive model if it can be expressed as $\mathbf{Y} = \sum_{i=1}^{p} \mathbf{F}_i(\theta_i)$. Consider an additive model,

$$Y = c_1 X_1 + c_2 X_2 \tag{1}$$

which has only a single output variable $Y$, and known as linear portfolio model in computational finance. Let us assume that the $c_1 = 2$ and $c_2 = 1$ are fixed coefficient and thus the active model parameters (input factors) are $\boldsymbol{\theta} = [X_1, X_2]$. We also consider the parameters are characterized as independent and distributed normally with mean zero,

$$X_1 \sim \mathcal{N}(0, \sigma_1^2), \quad X_2 \sim \mathcal{N}(0, \sigma_2^2)$$

with $\sigma_1 = 1$ and $\sigma_2 = 3$. It is trivial to show that with the above assumption, the model output can be represented as $Y \sim \mathcal{N}(0, \sigma_Y^2)$, where

$$\sigma_Y^2 = c_1^2 \sigma_1^2 + c_2^2 \sigma_2^2 = 13.$$

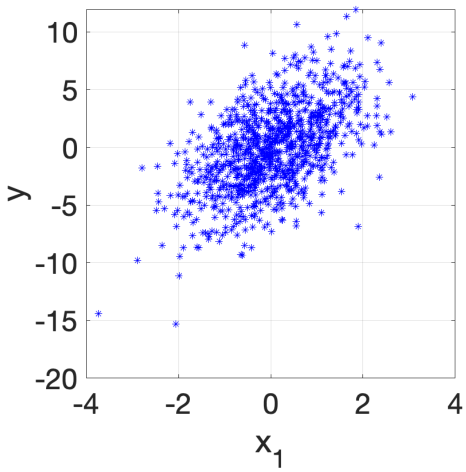
We now compare the scatter plots and derivatives of this model. The scatter plots are obtained by performing a Monte Carlo experiment with our model. Monte Carlo methods are based on sampling parameter values from their distribution. Drawing $N$ samples from the distributions of the two parameters, one can construct the matrix

$$\mathbf{M} = \begin{bmatrix} x_1^{(1)} & x_2^{(1)} \\ x_1^{(2)} & x_2^{(2)} \\ \vdots & \vdots \\ x_1^{(N)} & x_2^{(N)} \end{bmatrix}.$$

Computing $Y$ for each row of $\mathbf{M}$ using the model (1) produces the output vector,

$$\mathbf{Y} = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(N)} \end{bmatrix},$$

where $y^{(1)}$ is the value obtained by running (1) with the input parameters given by $x_1^{(1)}$ and $x_2^{(1)}$, and so on for the other rows of matrix. With this sample of model parameters and model output, one can produce two (i.e., number of parameters) scatterplots by projecting, in turn, the $N$ values of the selected output $Y$ (assumed to be a scalar here) against the $N$ values of each of the parameters. The scatterplots with $N = 1000$ joint realizations are plotted in Figure 1. These plots indicate that $X_2$ has more influence on $Y$ than $X_1$, since the realizations $(x_2, y)$ clearly reflect the trend of the model, whereas the realizations $(x_1, y)$ are nearly identical and there is no clear trend (shape) for the nearly uniform scatterplot. From a global perspective, $Y$ is thus considered more sensitive to $X_2$ than $X_1$.



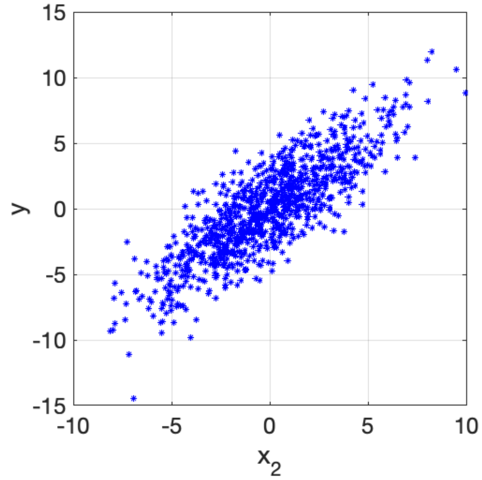




Figure 1: Scatterplots of $y$ versus $x_1$ and $x_2$ constructed using 1000 joint realization.

```
%% MATLAB script for
% scatterplots of the additive model
% Y = c1X1 + c2X2
clear all; close all; clc

%  coefficients
c1 = 2;
c2 = 1;
sigma1 = 1;
sigma2 = 3;

% number od samples
N = 1000;

% drawing samples from parameters and construct sample matrix M
x1 = normrnd(0,sigma1,[N,1]);
x2 = normrnd(0,sigma2,[N,1]);

M = [x1, x2];

% compute vector of model outputs
Y = c1*x1 + c2*x2;

%% scater plots
figure
plot(M(:,1), Y, '*b')
xlim([-4 4]), grid on
axis square,xlabel('x_1'),ylabel('y')
set(gca,'FontSize',24)
print('x1y','-dpng')

figure
plot(M(:,2), Y, '*b')
xlim([-10 10]), grid on
axis square,xlabel('x_2'),ylabel('y')
set(gca,'FontSize',24)
print('x2y','-dpng')
```

Now, let us look at the same problem from local sensitivity analyses. If we use the straightforward derivative of $Y$ versus $X_i$ to decide upon the relative importance of parameters,

$$S_i^p = \frac{\partial Y}{\partial X_i} \quad \Rightarrow \quad S_1^p = c_1,\ S_2^p = c_2,$$

we would conclude that $X_1$ is more important than $X_2$. This clearly not reasonable since $S_i^p$ ignores the values of $\sigma_i,\ i = 1, 2$. The superscript $p$ in $S_i^p$ indicates partial derivative and that the derivative is based on the raw values of both inputs and output. An improved measure is sigma-normalized derivatives,

$$S_i^\sigma = \frac{\sigma_{X_i} \partial Y}{\sigma_Y \partial X_i} \quad \Rightarrow \quad S_1^\sigma = c_1 \frac{\sigma_1}{\sigma_Y},\ S_2^\sigma = c_2 \frac{\sigma_2}{\sigma_Y},$$

which are hybrid local-global in nature since $\sigma_i$ incorporates variability over the range of input values. This relation constitutes one technique recommended by the 2001 Intergovernmental Panel for Climate Change (IPCC). In this example, $S_1^\sigma < S_2^\sigma$ which is consistent with the scatterplots. From the definition, it follows that

$$\sum_i S_i^\sigma = 1,$$

so that each $S_i^\sigma$ quantifies the contribution of that individual factor to the variance of model output or QoI. $\square$

# 2 Variance-based Global Sensitivity Analysis

## 2.1 Scatterplots

As shown in the previous example, the scatterplots are generally a straightforward and informative way of running global sensitivity analysis that provides an immediate visual depiction of the relative importance of parameters. What identifies an important parameter is the existence of “shape” or “pattern” in the points, while a uniform cloud of points in a scatterplot is a *symptom* (not a proof) of a non-influential parameter. We have a pattern when the distribution of $y$-points over the $x_i$ is nonuniform. In other words, if the $x_i$ axis is cut into slices, one can observe: (i) differences in the distribution of $y$-points over the slices; (ii) mean value of $y$ in each slice vary across the slices. The scatterplots of Figure 2, represent a model with four parameters. The ordering of parameters by importance is $Z_4 > Z_3 > Z_2 > Z_1$, according to how much the mean value of $Y$ varies from one slice to another. Thus the sensitivity measure is suggested as *variation over the slices of the expected value of $Y$ within each slice.*

For a model $Y = F(\boldsymbol{\theta}) = F(\theta_1, \cdots, \theta_p)$, the expected value of $Y$ over a very thin slice corresponds to keeping $\theta_i$ fixed while averaging over all-but-$\theta_i$, indicated as $\mathbb{E}_{\boldsymbol{\theta}_{\sim i}}(Y|\theta_i)$. Here we use the notation $\boldsymbol{\theta}_{\sim i} = [\theta_1, \cdots, \theta_{i-1}, \theta_{i+1}, \cdots, \theta_p]$. This, along with differences in the distribution of $y$-points over the slices, results in a measure $Var(\mathbb{E}_{\boldsymbol{\theta}_{\sim i}}(Y|\theta_i))$ in the limit of very thin slices.

## 2.2 Sobol method

Consider the scalar-value, nonlinear model,

$$Y = F(\boldsymbol{\theta}),$$

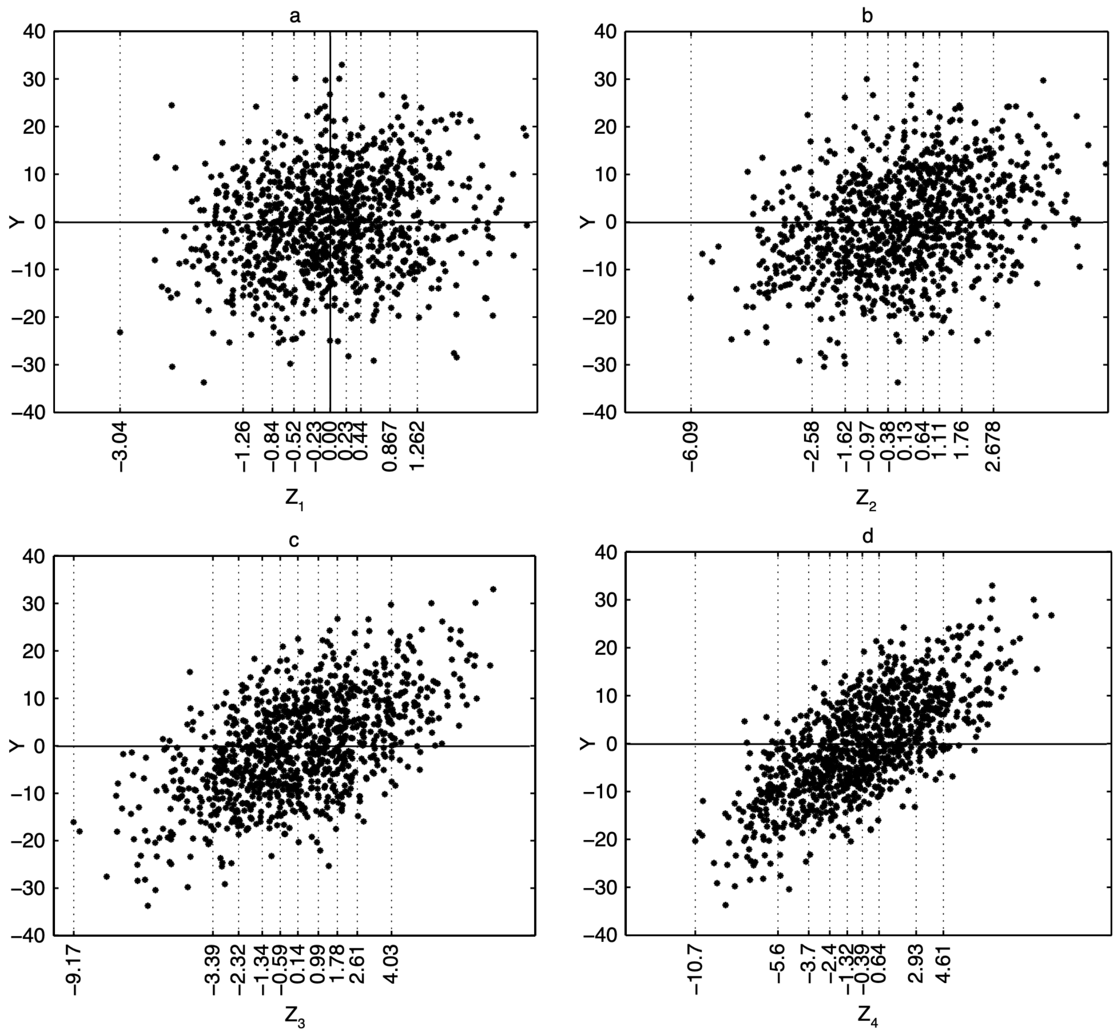



Figure 2: An example of scatterplots of an additive model $Y = F(Z_1, Z_2, Z_3, Z_4)$ cut into slices.

where $\boldsymbol{\theta} = (\theta_1, \cdots, \theta_p) \in \mathbb{R}$. We initially assume that the random variables are independent and uniformly distributed, $\theta_i \sim \mathcal{U}(0,1)$. In this setting, one can construct the Sobol representation for the response function $F(\boldsymbol{\theta})$, employing the finite and hierarchical expansion

$$\begin{aligned} F(\boldsymbol{\theta}) &= F_0 + \sum_{i=1}^{p} F_i(\theta_i) + \sum_{1 \le i < j \le p} F_{ij}(\theta_i, \theta_j) + \cdots \\ &+ \sum_{1 \le i_1 < \cdots < i_s \le p} F_{i_1, \cdots, i_s}(\theta_{i_1}, \cdots, \theta_{i_s}) + \cdots + F_{1,2,\cdots,p(\theta_1, \cdots, \theta_p)}. \end{aligned} \tag{2}$$

We will establish that the constant function $F_0$ is the mean response of $F$, whereas the first-order univariate functions $F_i(\theta_i)$ represent independent contributions due to the individual parameters. The bivariate functions $F_{ij}(\theta_i, \theta_j)$ quantifies the interactions of $\theta_i$ and $\theta_j$ on the response $Y$ with similar interpretations for higher-order interaction terms. The final term $F_{1,2,\cdots,p(\theta_1,\cdots,\theta_p)}$ quantifies unincorporated high-order residual effects, thus ensuring that the expansion (2) provide an exact representation for $F(\boldsymbol{\theta})$. In practice, one usually employs the approximate expansion,

$$F(\boldsymbol{\theta}) \approx F_0 + \sum_{i=1}^{p} F_i(\theta_i) + \sum_{1\le i<j\le p} F_{ij}(\theta_i, \theta_j).$$

In the context of projection-based reduced-order models, the terms $F_0$, $F_i$, and $F_{ij}$ constitute the reduced-order basis functions. As detailed in [6], the zeroth-, first-, and second-order terms can then be expressed as,

$$\begin{aligned} F_0 &= \int_{\Theta} F(\boldsymbol{\theta})\, d\boldsymbol{\theta} \\ F_i(\theta_i) &= \int_{\Theta^{p-1}} F(\boldsymbol{\theta})\, d\boldsymbol{\theta}_{\sim i} - F_0 \\ F_{ij}(\theta_i, \theta_j) &= \int_{\Theta^{p-2}} F(\boldsymbol{\theta})\, d\boldsymbol{\theta}_{\sim\{ij\}} - F_i(\theta_i) - F_j(\theta_j) - F_0, \end{aligned} \tag{3}$$

where $\Theta^{p-1} = [0,1]^{p-1}$. Recall that the notation $\boldsymbol{\theta}_{\sim i} = [\theta_1, \cdots, \theta_{i-1}, \theta_{i+1}, \cdots, \theta_p]$ denoting the vector with all components of $\boldsymbol{\theta}$ except $\theta_i$.

The total variance $V$ of output $Y$ is given by,

$$V = Var(Y) = \int_{\Theta} F^2(\boldsymbol{\theta})\, d\boldsymbol{\theta} - F_0^2,$$

since $F_0 = \mathbb{E}(Y)$. One can retrieve the following decomposition of the total variance $V$ [5],

$$V = \sum_{i=1}^{p} V_i + \sum_{1\le i<j\le p} V_{ij}, \tag{4}$$

where the partial variances are

$$\begin{aligned} V_i &= \int_0^1 F_i^2(\theta_i)\, d\theta_i, \\ V_{ij} &= \int_0^1 \int_0^1 F_{ij}^2(\theta_i, \theta_j)\, d\theta_i d\theta_j. \end{aligned} \tag{5}$$

The *Sobol indices* are defined to be

$$S_i = \frac{V_i}{V}, \quad S_{ij} = \frac{V_{ij}}{V}, \quad i, j = 1, \cdots, p,$$

so, by definition, they satisfy

$$\sum_{i=1}^{p} S_i + \sum_{1\le i<j\le p} S_{ij} = 1.$$

The term $S_i$ are often termed the *importance measure* or *first-order sensitivity indices*, and large value of $S_i$ indicate parameters that strongly influence the response variance. Similarly, $S_{ij}$ account for the influence of interaction terms. Because the number of first-and second-order Sobol indices increase with parameter dimensions, one considers *total sensitivity indices*

$$S_{T_i} = S_i + \sum_{j=1}^{p} S_{ij}, \tag{6}$$

which quantify the total effect of the parameter $\theta_i$ on the response $Y$. In general $\sum_{j=1}^{p} S_{T_i} \geq 1$, due to the fact that the interaction effect between $\theta_i$ and $\theta_j$ is counted in both $S_{T_i}$ and $S_{T_j}$.

**Mean and variance interpretation of Sobol indices.** Let,

$$\begin{aligned} \mathbb{E}(Y|\theta_i) &= \int_\Theta F(\boldsymbol{\theta}) d\boldsymbol{\theta}_{\sim i}, \\ \mathbb{E}(Y|\theta_i, \theta_j) &= \int_\Theta F(\boldsymbol{\theta}) d\boldsymbol{\theta}_{\sim \{ij\}}, \end{aligned} \tag{7}$$

denote the expected responses when the components $\theta_i$ and $\theta_i, \theta_j$ are fixed. From (3), it follows that

$$\begin{aligned} F_0 &= \mathbb{E}(Y), \\ F_i(\theta_i) &= \mathbb{E}(Y|\theta_i) - F_0, \\ F_{ij}(\theta_i, \theta_j) &= \mathbb{E}(Y|\theta_i, \theta_j) - F_i(\theta_i) - F_j(\theta_j) - F_0, \end{aligned} \tag{8}$$

Since

$$\mathbb{E}[\mathbb{E}(Y|\theta_i)] = \int_0^1 \left[ \int_\Theta F(\boldsymbol{\theta}) d\boldsymbol{\theta}_{\sim i} \right] d\theta_i = F_0,$$

it follows that

$$V_i = Var\left[\mathbb{E}(Y|\theta_i)\right] \tag{9}$$

and hence the *first order sensitivity index* is

$$\boxed{S_i = \frac{Var\left[\mathbb{E}(Y|\theta_i)\right]}{Var(Y)}.} \tag{10}$$

Similarly, one can show that

$$V_{ij} = Var[\mathbb{E}(Y|\theta_i, \theta_j)] - Var\left[\mathbb{E}(Y|\theta_i)\right] - Var\left[\mathbb{E}(Y|\theta_j)\right],$$

which yields a variance interpretation for $S_{ij}$. Finally, the *total sensitivity index* has the interpretation

$$\boxed{S_{T_i} = 1 - \frac{Var\left[\mathbb{E}(Y|\boldsymbol{\theta}_{\sim i})\right]}{Var(Y)} = \frac{\mathbb{E}\left[Var(Y|\boldsymbol{\theta}_{\sim i})\right]}{Var(Y)}.} \tag{11}$$

The interpretation of $\mathbb{E}(Y|\theta_i)$ and $Var[\mathbb{E}(Y|\theta_i)]$ is analogous to the scatterplots. The conditional expectations for fixed $\theta_i$ are the average value of $Y$ along vertical slices. The partial variances $V_i$ quantify the variability of these average values. Additionally, from (11), we note that if $S_{T_i} \approx 0$, then $\mathbb{E}\left[Var(Y|\boldsymbol{\theta}_{\sim i})\right] \approx 0$, which, by nonnegativity of the variance operator, implies that $Var(Y|\boldsymbol{\theta}_{\sim i}) \approx 0$ for any admissible value of $\boldsymbol{\theta}_{\sim i}$. The condition $S_{T_i} \approx 0$ thus implies that $\theta_i$ is noninfluential and can be fixed in subsequent model calibration and UQ. The application of the global sensitivity analysis to reduce model complexity will be discussed in the future chapters. According to (6), $S_{T_i}$ accounts for all higher-order effects due to the interaction and thus provides information on the non-additive feature of the model. Significant difference between $S_{T_i}$ and $S_i$ indicates important interaction involving $\theta_j$.

While the Sobol indices are derived based on uniformly distributed parameters, they can be extended for general densities, as shown in the following example.

***Example II:*** Consider the additive model

$$Y = \theta_1 + \theta_2 + \theta_3,$$

with uniformly distributed inputs $\theta_1 \sim \mathcal{U}(0.5, 1.5), \theta_2 \sim \mathcal{U}(1.5, 4.5)$, and $\theta_3 \sim \mathcal{U}(4.5, 13.5)$, and parameter vector $\boldsymbol{\theta} = [\theta_1, \theta_2, \theta_3]$. The sensitivity indices can be analytically computed as follow.

The expected value of model output is,

$$\mathbb{E}(Y) = \mathbb{E}(\theta_1) + \mathbb{E}(\theta_2) + \mathbb{E}(\theta_3) = 1 + 3 + 9 = 13,$$

and the output variance is

$$Var(Y) = V_1 + V_2 + V_3 = \frac{(1.5 - 0.5)^2}{12} + \frac{3}{4} + \frac{27}{4} = \frac{91}{12}.$$

The first-order sensitivity index for the parameter $\theta_1$ is evaluated as

$$S_1 = \frac{Var\left[\mathbb{E}(Y|\theta_1)\right]}{Var(Y)} = \frac{V_1}{V} = \frac{1/12}{91/12} = 0.011.$$

Similarly,

$$S_2 = \frac{3/4}{91/12} = 0.0989, \quad S_3 = \frac{27/4}{91/12} = 0.8901.$$

Now, the total sensitivity index for the parameter $\theta_1$ is computed by,

$$S_{T_1} = 1 - \frac{Var\left[\mathbb{E}(Y|\boldsymbol{\theta}_{\sim 1})\right]}{Var(Y)} = 1 - \frac{V_2 + V_3}{V} = 1 - \frac{3/4 + 27/4}{91/12} = 0.011.$$

Similarly,

$$S_{T_2} = 1 - \frac{1/12 + 27/4}{91/12} = 0.0989, \quad S_{T_3} = 1 - \frac{1/12 + 3/4}{91/12} = 0.8901.$$

We thus see that $S_i = S_{T_i}$ in additive models in which the interaction term $S_{ij} = 0$. $\square$

**Sobol decomposition for general densities.** Given the nonlinear model $Y = F(\boldsymbol{\theta})$ where $\boldsymbol{\theta} = [\theta_1, \cdots, \theta_p]$ are considered to be iid random variables with ranges $\Theta_k$ and densities $\pi(\theta_k)$. The range and joint density for $\boldsymbol{\theta}$ are then,

$$\Theta = \prod_{k=1}^{p} \Theta_k, \quad \pi(\boldsymbol{\theta}) = \prod_{k=1}^{p} \pi(\theta_k),$$

with $\int \pi(\boldsymbol{\theta}) d\boldsymbol{\theta} = 1$. The function mean can be defined as

$$\mathbb{E}(Y) = \int_{\Theta} F(\boldsymbol{\theta}) \pi(\boldsymbol{\theta}) \, d\boldsymbol{\theta},$$

and its variance as

$$\begin{aligned} Var(Y) &= \int_\Theta \left(F(\boldsymbol{\theta}) - \mathbb{E}(Y)\right)^2 \pi(\boldsymbol{\theta}) d\boldsymbol{\theta} \\ &= \int_\Theta F^2(\boldsymbol{\theta})\pi(\boldsymbol{\theta})d\boldsymbol{\theta} + \int_\Theta \mathbb{E}^2(Y)\pi(\boldsymbol{\theta})d\boldsymbol{\theta} - 2\int_\Theta \mathbb{E}(Y)F(\boldsymbol{\theta})\pi(\boldsymbol{\theta})d\boldsymbol{\theta} \\ &= \mathbb{E}(Y^2) + \mathbb{E}^2(Y) - 2\mathbb{E}^2(Y) \\ &= \mathbb{E}(Y^2) - \mathbb{E}^2(Y). \end{aligned}$$

The Sobol decomposition of the response function is given by

$$F(\boldsymbol{\theta}) = F_0 + \sum_{i=1}^{p} F_i(\theta_i) + \sum_{1\le i<j\le p} F_{ij}(\theta_i, \theta_j),$$

with

$$\begin{aligned} F_0 &= \mathbb{E}(Y) = \int_\Theta F(\boldsymbol{\theta})\pi(\boldsymbol{\theta})\, d\boldsymbol{\theta} \\ F_i(\theta_i) &= \int_{\Theta^{p-1}} F(\boldsymbol{\theta})\pi(\boldsymbol{\theta}_{\sim i})\, d\boldsymbol{\theta}_{\sim i} - F_0 && (12) \\ F_{ij}(\theta_i, \theta_j) &= \int_{\Theta^{p-2}} F(\boldsymbol{\theta})\pi(\boldsymbol{\theta}_{\sim\{ij\}})\, d\boldsymbol{\theta}_{\sim\{ij\}} - F_i(\theta_i) - F_j(\theta_j) - F_0. && (13) \end{aligned}$$

The total and partial variances are defined by,

$$\begin{aligned} V &= \int_\Theta F^2(\boldsymbol{\theta})\pi(\boldsymbol{\theta})\, d\boldsymbol{\theta} - F_0^2 = \sum_{i=1}^{p} V_i + \sum_{1\le i<j\le p} V_{ij}, \\ V_i &= \int_{\Theta_i} F_i^2(\theta_i)\pi(\theta_i)\, d\theta_i = Var[\mathbb{E}(Y|\theta_i)], \\ V_{ij} &= \int_{\Theta_j}\int_{\Theta_i} F_{ij}^2(\theta_i,\theta_j)\pi(\theta_i,\theta_j)\, d\theta_i d\theta_j = Var[\mathbb{E}(Y|\theta_i,\theta_j)] - V_i - V_j. && (14) \end{aligned}$$

The *Sobol indices* are then defined as before

$$S_i = \frac{V_i}{V}, \quad S_{ij} = \frac{V_{ij}}{V}, \quad i,j = 1, \cdots, p.$$

The total sensitivity indices

$$S_{T_i} = S_i + \sum_{j=1}^{p} S_{ij},$$

quantify the sensitivity of the variance of $Y$ with respect to the parameter $\theta_i$ and its interaction with all other inputs.

***Example III:*** We revisit the additive model in Example I,

$$Y = c_1\theta_1 + c_2\theta_2,$$

with normally distributed inputs $\theta_1 \sim \mathcal{N}(0, \sigma_1^2)$ and $\theta_2 \sim \mathcal{N}(0, \sigma_2^2)$ represented in PDFs,

$$\pi(\theta_1) = \frac{1}{\sigma_1\sqrt{2\pi}} e^{-\theta_1^2/2\sigma_1^2}, \quad \pi(\theta_2) = \frac{1}{\sigma_2\sqrt{2\pi}} e^{-\theta_2^2/2\sigma_2^2},$$

and $\pi(\boldsymbol{\theta}) = \pi(\theta_1)\pi(\theta_2)$, with $\boldsymbol{\theta} = [\theta_1, \theta_2]$.

In this example,

$$\begin{aligned} F_0 &= \mathbb{E}(Y) = 0, \\ F_1(\theta_1) &= \int_{-\infty}^{+\infty} \pi(\theta_2)[c_1\theta_1 + c_2\theta_2]d\theta_2 = c_1\theta_1, \\ F_2(\theta_2) &= c_2\theta_2, \end{aligned}$$

and $F_{ij}(\theta_i, \theta_j) = 0$. We leverage MATLAB symbolic integration to compute the integrals. The partial variances are

$$\begin{aligned} V_i &= \int_{-\infty}^{+\infty} c_i^2\theta_i^2\pi(\theta_i)d\theta_i = c_i^2\sigma_i^2, \\ V_{12} &= 0, \end{aligned}$$

and the total variance is

$$V = V_1 + V_2 + V_{12} = c_1^2\sigma_1^2 + c_2^2\sigma_2^2,$$

as noted in Example I. The Sobol indices are

$$S_i = \frac{c_i^2\sigma_i^2}{c_1^2\sigma_1^2 + c_2^2\sigma_2^2}, \quad S_{ij} = 0$$

so that $S_1 = \frac{4}{13}$ and $S_2 = \frac{9}{13}$ since $c_1 = 2, c_2 = 1, \sigma_1 = 1$, and $\sigma_2 = 3$. We thus see that $S_i = (S_i^\sigma)^2$, while this conclusion does not hold for non-additive models.

□

## 2.3 Algorithm to Estimate Sensitivity Indices

The analytical calculation of the sensitivity indices is impossible for nonlinear models of physical systems, and thus we would need to resort to numerical approximations. The computation of $S_i$ given by (10) requires the evaluation of $Var\left[\mathbb{E}(Y|\theta_i)\right]$. If one uses $M$ Monte Carlo evaluations to approximate the conditional mean $\mathbb{E}(Y|\theta_i)$ for fixed $\theta_i$ and repeat the procedure $M$ times to approximate the variance, a total of $M^2$ model evaluations will be required to evaluate a single sensitivity index. For large parameter dimensions $p$, this brute-force approach is clearly prohibitive. The following algorithm of Saltelli [4], which is based on Sobol's original approach [6], reduces the number of required function evaluations to $M(p+2)$. This Monte Carlo estimator is designed for the parameters with uniform distributions.

***Algorithm: estimators of Sobol indices.***

1. Create two $M \times p$ sample matrices, where each row is a sample point in the hyperspace of $p$ dimensions. $M$ is called a base sample with respect to the probability distributions of the input parameters.

$$\mathbf{A} = \begin{bmatrix} \theta_1^{(1)} & \cdots & \theta_i^{(1)} & \cdots & \theta_p^{(1)} \\ \vdots & & & & \vdots \\ \theta_1^{(M)} & \cdots & \theta_i^{(M)} & \cdots & \theta_p^{(M)} \end{bmatrix}, \quad \mathbf{B} = \begin{bmatrix} \hat{\theta}_1^{(1)} & \cdots & \hat{\theta}_i^{(1)} & \cdots & \hat{\theta}_p^{(1)} \\ \vdots & & & & \vdots \\ \hat{\theta}_1^{(M)} & \cdots & \hat{\theta}_i^{(M)} & \cdots & \hat{\theta}_p^{(M)} \end{bmatrix},$$

where $\theta_i^{(j)}$ and $\hat{\theta}_i^{(j)}$ are two samples drawn from the uniform density of $\theta_i$.

2. Create $M \times p$ matrices

$$\mathbf{C}_i = \begin{bmatrix} \hat{\theta}_1^{(1)} & \cdots & \theta_i^{(1)} & \cdots & \hat{\theta}_p^{(1)} \\ \vdots & & & & \vdots \\ \hat{\theta}_1^{(M)} & \cdots & \theta_i^{(M)} & \cdots & \hat{\theta}_p^{(M)} \end{bmatrix}, \quad i = 1, \cdots, p.$$

which are identical to $\mathbf{B}$ with the exception that the $i^{th}$ column is taken from $\mathbf{A}$.

3. Compute $M \times 1$ vectors of model outputs

$$\mathbf{y}_A = F(\mathbf{A}), \quad \mathbf{y}_B = F(\mathbf{B}), \quad \mathbf{y}_{C_i} = F(\mathbf{C}_i),\ i = 1, \cdots, p$$

by evaluating the model at the input values in $\mathbf{A}$, $\mathbf{B}$, and $\mathbf{C}_i$. The evaluation of $\mathbf{y}_A$ and $\mathbf{y}_B$ requires $2M$ model evaluations, whereas the evaluation of $\mathbf{y}_{C_i}, i = 1, \cdots, p$, requires $pM$ evaluations. Hence the total number of evaluations is $M(p+2)$.

4. The estimates for the first-order sensitivity indices are

$$S_i = \frac{Var[\mathbb{E}(Y|\theta_i)]}{Var(Y)} = \frac{\frac{1}{M}\mathbf{y}_A^T\mathbf{y}_{C_i} - F_0^2}{Var(Y)} = \frac{\frac{1}{M}\sum_{j=1}^M y_A^{(j)} y_{C_i}^{(j)} - F_0^2}{Var(Y)}, \tag{15}$$

and the estimates for the total effects indices are

$$S_{T_i} = 1 - \frac{Var[\mathbb{E}(Y|\boldsymbol{\theta}_{\sim i})]}{Var(Y)} = 1 - \frac{\frac{1}{M}\mathbf{y}_B^T\mathbf{y}_{C_i} - F_0^2}{Var(Y)} = 1 - \frac{\frac{1}{M}\sum_{j=1}^M y_B^{(j)} y_{C_i}^{(j)} - F_0^2}{Var(Y)}, \tag{16}$$

where the mean is approximated by

$$F_0^2 \approx \left(\frac{1}{M}\sum_{j=1}^M y_A^{(j)}\right)\left(\frac{1}{M}\sum_{j=1}^M y_B^{(j)}\right) \approx \left(\frac{1}{M}\sum_{j=1}^M y_A^{(j)}\right)^2,$$

and the variance is approximated by

$$Var(Y) = \frac{1}{M}\sum_{j=1}^M (y_A^{(j)})^2 - F_0^2$$

The relations (15) and (16) are obtained using the Monte Carlo estimators proposed by Sobol [6],

$$Var[\mathbb{E}(Y|\theta_i)] = \frac{1}{M}\sum_{j=1}^M y_A^{(j)} y_{C_i}^{(j)} - (\mathbb{E}(Y))^2$$

and Saltelli [4],

$$Var[\mathbb{E}(Y|\boldsymbol{\theta}_{\sim i})] = \frac{1}{M}\sum_{j=1}^M y_A^{(j)} y_{D_i}^{(j)} - (\mathbb{E}(Y))^2$$

along with

$$Var(Y) = \mathbb{E}(Y^2) - (\mathbb{E}(Y))^2 = \frac{1}{M}\sum_{j=1}^M y_A^{(j)} y_A^{(j)} - \left(\frac{1}{M}\sum_{j=1}^M y_A^{(j)}\right)^2,$$

where the $M \times p$ matrices $\mathbf{D}_i$ are identical to $\mathbf{A}$ with the exception that the $i^{th}$ column is taken from $\mathbf{B}$.

The intuition for the algorithm is that in the scalar product $\mathbf{y}_A^T\ \mathbf{y}_{C_i}$, the response computed from values in $\mathbf{A}$ is multiplied by values for which all parameters except $\theta_i$ have been samples. If $\theta_i$ is influential, then large (or small) values of $\mathbf{y}_A$ will be correspondingly multiplied by large (or small) values of $\mathbf{y}_{C_i}$, yielding a large value of $S_i$. If $\theta_i$ is not influential, large and small values of $\mathbf{y}_A$ and $\mathbf{y}_C$ will occur more randomly, and $S_i$ will be small. The number of parameter samples governs the accuracy of the estimated indices.

***Example IV:*** Let's again consider the additive model in Example II

$$Y = \theta_1 + \theta_2 + \theta_3,$$

with uniformly distributed inputs $\theta_1 \sim \mathcal{U}(0.5, 1.5), \theta_2 \sim \mathcal{U}(1.5, 4.5)$, and $\theta_3 \sim \mathcal{U}(4.5, 13.5)$, and parameter vector $\boldsymbol{\theta} = [\theta_1, \theta_2, \theta_3]$. We now use the Monte Carlo estimators to compute the sensitivity indices, as shown in Figure 3.

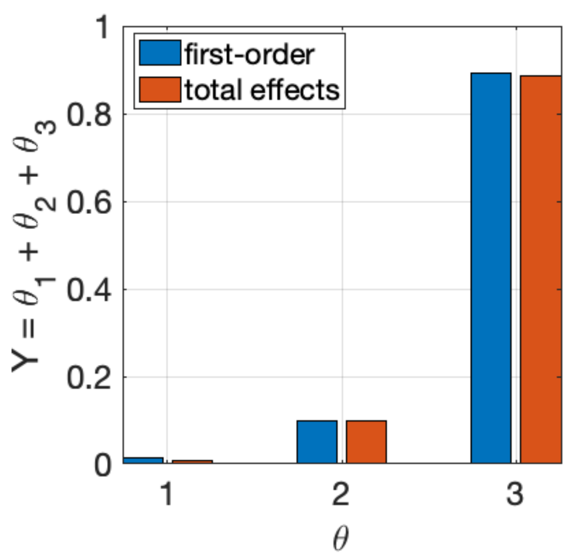



Figure 3: Estimations of first-order and total effects sensitivity indices of the $Y = \theta_1 + \theta_2 + \theta_3$ using (15) and (16).

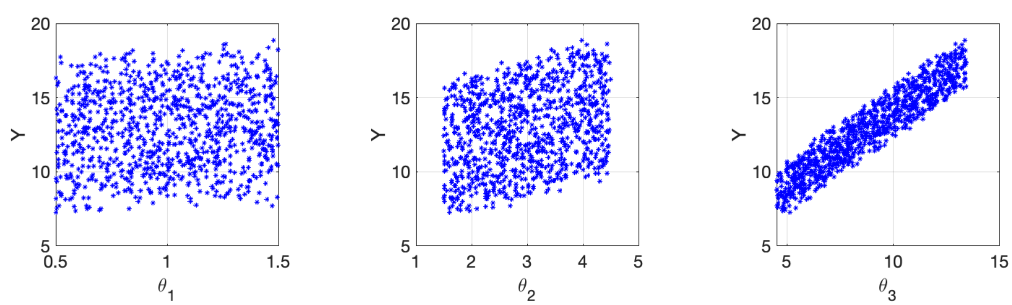



Figure 4: Scatterplots of the $Y = \theta_1 + \theta_2 + \theta_3$.

Matlab function for the additive model.

```
function [y] = additive_model(theta)
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% ADDITIVE FUNCTION
% Author: Danial Faghihi, University at Buffalo
%
% INPUTS:
% xx = [theta1, theta2, theta3]
%
% OUTPUTS:
% Y = theta1 + theta2 + theta3
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

theta1 = theta(1);
theta2 = theta(2);
theta3 = theta(3);
y = theta1 + theta2 + theta3;
end
```

Matlab function for the computing sensitivity indices using the Monte Carlo estimators.

```
%% Saltelli estimators of Sobol indices
%  This code illustrates the implementation of the Monte Carlo estimators
%  for computing the first first-order indices and total effects indices
%      Y = theta1 + theta2 + theta3
%  parameters theta = [theta1, theta2, theta3]
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
clear all; close all; clc
%% Setup the model and define input ranges
% number of parameters and parameter ranges
p = 3;
param1 =  [0.5  1.5];
param2 =  [1.5  4.5];
param3 =  [4.5  13.5];

%% Sample parameter space:
% number of samples
M = 10000;

%% Compute [A], [B] matrices and [C] as random variables
% Using random samples from the uniform distributions
% A(:,1) = param1(1) + (param1(2) - param1(1)).*rand(M,1);
% A(:,2) = param2(1) + (param2(2) - param2(1)).*rand(M,1);
% A(:,3) = param3(1) + (param3(2) - param3(1)).*rand(M,1);
%
% B(:,1) = param1(1) + (param1(2) - param1(1)).*rand(M,1);
% B(:,2) = param2(1) + (param2(2) - param2(1)).*rand(M,1);
% B(:,3) = param3(1) + (param3(2) - param3(1)).*rand(M,1);

% Using Latin hypercube samples (LHS) from the uniform distributions
% This approach converges with smaller M compared to random samples
% since LHS spreads the samples more evenly across the parameters space
A_lhs = lhsdesign(M,p);
B_lhs = lhsdesign(M,p);
params = [param1;param2;param3];
A = zeros(size(A_lhs));
B = zeros(size(B_lhs));
for i = 1:p
    A(:,i) = params(i,1) + (params(i,2) - params(i,1)).*A_lhs(:,i);
```

```
    B(:,i) = params(i,1) + (params(i,2) - params(i,1)).*B_lhs(:,i);
end

%% Compute [C] matrices
C = zeros(M,p,p);
for i = 1:p
    C(:,:,i) = B;
    C(:,i,i) = A(:,i);
end

%% Run the model and compute selected model output at sampled parameter
for  j = 1:M
    yA(j,1) = additive_model(A(j,:));
    yB(j,1) = additive_model(B(j,:));
    for i = 1:p
        yC(j,i) = additive_model(C(j,:,i));
    end
end

%% Compute sensitivity indices
f0  = mean(yA) ;
VARy = mean(yA.^2) - f0^2 ;

for i = 1:p
    yCi = yC(:,i);

  % fist order indices
    Si(i)  = ( 1/M*sum(yA.*yCi) - f0^2 ) / VARy ;
    % total effects indices
    STi(i) = 1 -  ( 1/M*sum(yB.*yCi) - f0^2 ) / VARy ;
end

%% Plot results
% sensitivity indices
indices = [Si' STi'];

figure
bar(indices)
axis square,xlabel('\theta'),ylabel('Y = \theta_1 + \theta_2 + \theta_3'),
    grid on
set(gca,'FontSize',24)
legend('first-order', 'total effects')

% scatter plots
figure
plot(A(:,1), yA, '*b')
axis square,xlabel('\theta_1'),ylabel('Y'), grid on
set(gca,'FontSize',24)

figure
plot(A(:,2), yA, '*b')
axis square,xlabel('\theta_2'),ylabel('Y'), grid on
set(gca,'FontSize',24)

figure
plot(A(:,3), yA, '*b')
axis square,xlabel('\theta_3'),ylabel('Y'), grid on
set(gca,'FontSize',24)
```

# 3 Elementary Effects Method: Morris Screening

Screening methods provide an alternative to variance-based methods for identifying critical inputs to high-dimensional input spaces or models whose computational expense prohibits the construction of Sobol indices. These methods generally provide the capability to rank parameters according to their importance, but, unlike variance-based methods, they typically do not quantify how much more important one parameter is than another. The goal of Morris screening is to identify parameters that are negligible, linear and additive, or nonlinear or comprised of interactions between inputs.

We again consider the model

$$Y = F(\boldsymbol{\theta}), \quad \boldsymbol{\theta} = [\theta_1, \cdots, \theta_p].$$

The concept of Morris screening is based on linearization of the model and consists of averaging coarse local sensitivity approximations, known as *elementary effect*, over the parameter space to provide a measure of global sensitivity. The principal ideas behind this method are listed as follows,

1. We rescale each parameter $\theta_i$ to the unit interval $[0, 1]$.

2. We consider an $p$-dimensional hypercube, $\Omega^p = [0, 1]^p$ which we partition into $l^p$ cells, $l$ being an integer number $> 2$, such that each parameter domain $[0, 1]$ is partitioned into bins $\theta_i \sim [0, 1] \sim [0, \frac{1}{l-1}, \frac{1}{l-2}, \ldots, 1]$. These bins contain sample points from which Monte Carlo samples of $\theta_i$ will be selected. The bins are called the *levels* of the cube.

3. We introduce a sampling distribution $\pi_i$ for each $\theta_i$, denoting parametric uncertainty (i.e., simply a uniform distribution) assigned to all $\theta_i,\ i = 1, 2, \ldots, n$.

4. We next choose a small number $\Delta$, for instance $\Delta = l/2(l-1)$, $l \geq 2$, and we compute the elementary effect $EE_i$ as the difference approximations,

$$EE_i = \frac{F(\theta_1, \cdots, \theta_{i-1}, \theta_i + \Delta, \theta_{i+1}, \cdots, \theta_p) - F(\boldsymbol{\theta})}{\Delta},$$

   The $EE_i$'s thus represent the change in the output due to a $\Delta$-perturbation in each parameter $\theta_i$.

5. We now compute $EE_i^{(j)}$ of the output for random (Monte Carlo) samples taken from each bin. To this end, we traverse through the hypercube doing sample paths, called *trajectories*, consisting of paths of $p + 1$ orthogonal steps through $\Omega^p$ as follows:

   (a) Select a random starting point $\boldsymbol{\theta}^{(1)}$

   (b) If $\boldsymbol{\theta}_i$ denotes a set of unit coordinate vectors on the axes of the hypercube, select a new vector $\boldsymbol{\theta}^{(2)}$ differing from $\boldsymbol{\theta}^{(1)}$ in its $i^{\text{th}}$ component by $\Delta$:

$$\boldsymbol{\theta}^{(2)} = \boldsymbol{\theta}^{(1)} \pm \boldsymbol{e}_i \Delta,$$

   where $\boldsymbol{e}_i$ is a vector pf zeros but with unit as its $i$th component and $+$ or $-$ taken such that $\boldsymbol{\theta}^{(2)} \in \Omega$ (the transformed point is still in $\Omega$).

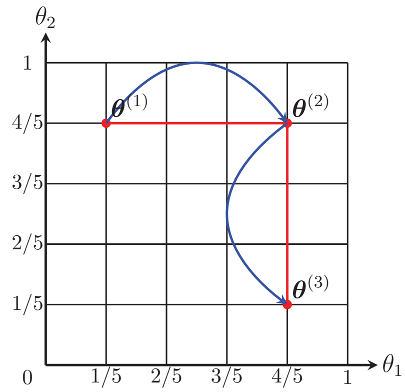



Figure 5: An illustration of a 2-dimensional hypercube ($p = 2$) with $l = 6$ levels, $\Delta = 3/5$, and a trajectory $r$ along $p + 1 = 3$ sampling points: $\boldsymbol{\theta}^{(1)}$, $\boldsymbol{\theta}^{(2)}$, $\boldsymbol{\theta}^{(3)}$.

(c) Continuing in this manner,

$$\boldsymbol{\theta}^{(3)} = \boldsymbol{\theta}^{(2)} \pm \boldsymbol{e}_j \Delta$$

we finally get,

$$\boldsymbol{\theta}^{(n+1)} = \boldsymbol{\theta}^{(n)} \pm \boldsymbol{e}_k \Delta.$$

This defines a trajectory $r$ through $\Omega^p$.

6. Next, we compute the elementary effects sensitivities and variances over $r$ trajectories,

$$\mu_i^* = \frac{1}{r} \sum_{j=1}^{r} |EE_i^{(j)}|, \tag{17}$$

$$\sigma_i^2 = \frac{1}{r-1} \sum_{j=1}^{r} (EE_i^{(j)} - \mu_i)^2. \tag{18}$$

with $\mu_i^*$ being a sample mean and $\sigma_i^2$ a variance at the $i$th parameter sensitivity (over $r$ trajectories). A common indication of the sensitivity assigned to parameter $i$ is $\mu_i^*$

By laying out the numbers $\mu_1^*, \mu_2^*, ..., \mu_p^*$, we can estimate the relative sensitivity of the output to changes in the parameters. When a measure $\mu_k^*$ is regarded as very "small" according to some preset tolerance, that parameter can be eliminated or set equal to a deterministic constant, this latter choice being sometimes made when sensitivities of other parameters are correlated with those of $\theta_i$. We note that the sensitivity measures $\sigma_i^2$ and $\mu_i^*$ depend on the number $r$ of trajectories. Presumably, these measures should converge to constants as $r \to \infty$. The details of efficient Morris sampling strategy can be found in [5]. Due to its semi-quantitative nature, this method can be considered a screening method, especially useful for investigating models with many (up to 100) uncertain parameters. It can also be used before applying a variance-based measure to *prune* the number of factors to be considered.

# 4 Time- or Space-Dependent Model Outputs

So far, we assumed that the nonlinear model $Y = F(\boldsymbol{\theta})$ is a scalar-value and a function only of parameters. However, several models of physical systems are also functions of time and space, such that

$$Y(t) = F(\boldsymbol{\theta}, t), \quad Y(\mathbf{x}) = F(\boldsymbol{\theta}, \mathbf{x}),$$

where $\mathbf{x} \in \mathbb{R}^3$ and $t \in [t_0, t_f]$ in general, where $t_0$ and $t_f$ are the initial and final times. For the time-dependent case, $Y(t)$, the most direct approach to the global sensitivity analysis is to construct a set of sensitivity indices $S_{T_i}(t_j),\ i = 1, \cdots, p$ at time points $t_j$ of interests to quantify the influence of parameters throughout the time interval. However, if the objective is to identify most influential parameters for the entire time interval, the time-dependent responses can be integrated to obtain a scalar-value response $\tilde{Y} = \int_{t_0}^{t_f} F(\boldsymbol{\theta}, t)dt$. Techniques for global sensitivity analysis for spatially varying model outputs $Y(\mathbf{x})$ are similar to those for time-varying responses. Advanced variance-based sensitivity analysis methods of the time-dependent model are presented in [1] and overview of the sensitivity analysis techniques of spatially-varying models provided in [3].

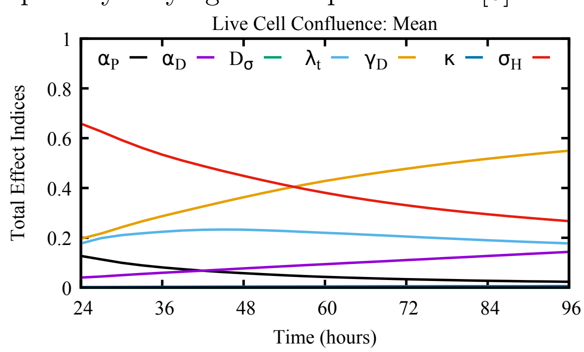



Figure 6: Time-dependent sensitivity analysis of an agent-based model of cancer consists of 7 model parameters and model output of live cell confluence [2].

# References

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