PhD THESIS DECLARATION

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Abstract

Computer codes are widely used nowadays to support scientific investigation and also policy making. Sensitivity analysis is essential in understanding how a computer code responds to variations in its inputs. In this thesis, we study the sensitivity analysis of model output for both models with a deterministic response and models with a stochastic response. For models with a deterministic response, in several situations, not only the datasets of realizations of the model output are available, but also of the corresponding partial derivatives. Making the most out of this information can lead to increasing transparency in understanding the model results and allows for correctly communicating the decision making insights. Herein, aside a thorough investigation of methods available in the extant literature, we introduce a new method based on repeated model evaluations at random locations in the model input space. The corresponding sensitivity indicator does not require independence among model inputs and possesses the additivity property, which makes the calculation of joint sensitivities seamless. We study numerical estimation and obtain an expression for the convergence rate of $O(N^{-1}(log\ N)^n)$. Analytical examples help us illustrate asymptotic convergence. We carry out a thorough comparison of the method with other methods based on the randomization of partial derivatives such as the distributed evaluation of local sensitivity analysis (DELSA) and derivative based global sensitivity measures (DGSM).

In the second part of the thesis, we consider models whose response is stochastic with respect to the distributional parameters of model inputs. The sensitivity analysis with respect to the parameters is carried out on the expected value of the model output seen as a deterministic function of the parameters, hence integrating out the uncertainty induced by the inputs.

The last part of the thesis considers sensitivity analysis for stochastic models, when the output inherits a randomness not necessarily due to the uncertainty of the model inputs. We propose the use of density based sensitivity measures based on the family of Cziszár f-divergences to carry out the identification of the key-drivers of the model response.

Chapter 1

Introduction

This thesis is about sensitivity analysis and its implementation in deterministic and stochastic frameworks.

1.1 Introduction

Computer experiments play an important role in science related applications. Scientists and policy makers increasingly rely on the output of computer codes in applications ranging from policy making in climate change [Smith et al., 2009] to the risk assessment of complex technological systems [Borgonovo and Smith, 2012]. The increased computing power allows the simulation of complex physical processes and analysts cannot rely on intuition to appreciate the models' response to changes in their inputs. Thus, to gain insights about the relationship between the model and its inputs, we need a systematic approach. This approach has been recently made systematic in the field of sensitivity analysis (SA) of model output (see Saltelli et al. [2008] and Borgonovo et al. [2016]).

The scope of SA is vast. Sensitivity analysis questions can be specific and responding to a specific scientific quest. For instance, a scientist may be investigating the sensitivity of temperature in a given region of the ocean to changes in pressure in the same region. In this thesis, SA concerns sensitivity methods which are quantitative and model free, as per Saltelli [2002]. By quantitative and model free, one means that the method is producing objective numerical information and is applicable to a wide class of computer codes (in principle, with no restrictions to the type of mathematical equation involved in the model). Moreover, the use of SA methods have become broad. There are variety of problems that have been answered through SA methods, for instance Lefebvre et al. [2010] determine the most influential model input among thirty for an aircraft infra-red signature simulation model. Saltelli and Tarantola [2002a] deal with the LEVEL E model, a model for the transmigration of radioactive materials in the soil. Borgonovo et al. [2003] address the use of sensitivity analysis with uncertainty analysis of complex risk assessment

codes. Rabitz [1989] discusses the use of sensitivity analysis in the modelling of molecular systems.

SA techniques are traditionally grouped into the classes of local, global and screening methods [Saltelli et al., 2008]. In a local sensitivity analysis, the behaviour of the model around a reference value of the inputs is studied. Such reference value, usually called the base-case value, represents the central scenario of interest. In a global sensitivity analysis, the objective is to study the key drivers of the model response, while allowing the inputs to vary throughout the entire model input space. In particular, as Rakovec et al. [2014] state, "global methods provide stable results because they produce measures of parameter importance that are averaged over the range of the parameter space from which samples are obtained "(page 2). The class of global sensitivity methods comprises regression-based [Kleijnen and Helton, 1999, Storlie et al., 2009], variance-based [Saltelli and Tarantola, 2002a, Oakley and O'Hagan, 2004], and moment-independent methods [Borgonovo et al., 2013, Rahman, 2016]. These methods find their rationale in the so-called *factor prioritization setting*. On the other hand, screening methods are concerned with the computationally frugal identification of model inputs that do not impact the model output, in the *factor fixing setting*. The methods of Morris [Morris, 1991] and derivative-based sensitivity methods [Sobol' and Kucherenko, 2009] are among the most widely used.

1.2 Objectives

The thesis has three main objectives. When not only the values of the output of the computer code, but also of the corresponding derivatives are available, we first propose a method that complements extant derivative-based approaches by relying on a convenient transformation of partial derivatives. The objective is to gain maximum information out of the available partial derivatives by conveniently rearranging them to form the differential importance of a model input ([Borgonovo and Apostolakis, 2001]). Then, we could potentially obtain a derivative-based sensitivity measure which is additive, thanks to the additivity of the differential importance measure (DIM). We prove that this is indeed the case if we consider the average of the differential importance measures evaluated at different points in the model input space. We call the resulting sensitivity indicator *Randomized Differential Importance Measure (RDIM)*. Aside additivity, RDIM has the advantage of not requiring the assumption of independence among the model inputs.

The second objective of this thesis is to define a differential based sensitivity measure on the expectation of the output of a deterministic model with respect to distributional parameters when the provided model is analytically intractable. In this case the model is deterministic with respect to model inputs. The model inputs are not observable directly.

Only their probability distributions are known which depends on some parameters. Hence the randomness of the model output with respect to the parameters of the model input distributions is considered. In this case the necessity of evaluating the differential based sensitivity measure numerically is crucial. Thus, we propose the use of a likelihood ratio method also known as the score function method. Likelihood ratio methods have been widely used to estimate derivatives of expectations of random variables with respect to the parameters of the model input distributions through simulations.

The third objective of this thesis is the identification of the key-uncertainty drivers of computer codes with a purely stochastic response. Towards this goal, we study the application of density-based sensitivity measures associated with Csiszár f-divergences on stochastic models. The model in this case is purely stochastic in the sense that for a fixed set of inputs, the model produces different output values each time it is run. However, when the original model being studied is costly in terms of computer time, a meaningful analysis of the sensitivity measure is cumbersome. Instead, we propose to use an emulator constructed using original data in place of the original model and perform sensitivity analysis with data generated from the emulator. This part of the thesis is explorative and opens the avenue for future research.

1.3 Outline of thesis

The rest of the work is organized as follows. Differential based and distance based sensitivity analyses are the main focuses of this thesis, and we begin with a thorough review of sensitivity methods of this type in chapter 2. We also discuss other types of sensitivity methods providing a unifying framework for the methods of interest, since choosing among the numerous competing methodologies requires a detailed understanding of their properties.

Chapter 3 introduces a new bridge between local and global sensitivity analysis. We define a new measure based on randomizing the model inputs through the use of a probability measure on the input space.

Chapter 4 presents a generalized differential sensitivity measure that can be applied to evaluate the sensitivity of the expectation of the model output with respect to the parameters of the model input distributions.

Chapter 5 details the application of Csiszár's f-divergences in stochastic models using a toy example.

Finally, in Chapter 6, we provide a brief discussion on the topics covered and potential directions for future work.

Chapter 2

Literature Review

Several SA methods have been discussed in the literature by grouping them into local and global methods. This chapter is devoted to providing an overview , in a complete methodological framework, of various local and global sensitivity analysis methods.

2.1 Introduction

Computer experiments play a significant role in many areas of science and engineering. Decision makers tend to rely on the output of computer codes in several applications. The increase in computing power of the recent years allows analysts to encode scientific models of increasing complexity. This then makes it impossible to appreciate the response of the quantities of interest (model outputs) to variations in the model inputs. Thus, one considers the computer code as a black box that processes a set of inputs and produces a set of outputs of interest. Sensitivity analysis then makes systematic the inference performed on the computer code, towards gaining several insights about the input-output relationship. Several international institutions including the Florida Commission on Hurricane Loss Projection Methodology [Iman et al., 2005] , NICE (2013) and the US Nuclear Regulatory Commission recommend the use of SA methods in gaining insights of the complex model.

There are numerous ways in which an SA can be performed. Experience shows that a poor definition of the objective of the sensitivity analysis can lead to confused or inconclusive results. Thus, to minimize the risk of making incorrect inferences, it is in the analyst's best interests to define beforehand what definition of an objective is relevant for the problem at hand. Saltelli et al. [2008] name these objectives as *settings*, where "a setting is a way of framing the sensitivity quest in such a way that the answer can be confidently entrusted to a well defined measure "(page 24). In general, each sensitivity measure produces its own results by factor importance.

We present a summary of existing *settings* in the literature. We consider this as im-

portant because we will be using these *settings* in following chapters. Saltelli's *Factor Prioritization setting* describes the problem of identifying the most important model inputs. The questions *which inputs contribute most to the output uncertainty?* and *which inputs require additional research to reduce the uncertainty of the output?* are approached with it. The identification of model inputs that almost do not influence the output variability is associated with the settings *Factor Fixing* and *Factor Screening*. The detected model inputs can be fixed to any value within their range and thereby allowing a simplification in the analysis. Moreover, *direction of change setting* provides information to assess the monotonic behaviour of the model at each point in the model input space. These settings are "old "and refer solely to a variance based view of sensitivity analysis.

2.1.1 Notation and terminology

We introduce some relevant notation that will be used throughout this study. Let n denote the number of model inputs, $\mathcal{X} \subseteq \mathbb{R}^n$ denote the possible values that the model inputs can assume called the *model input space*, and $g : \mathcal{X} \longrightarrow \mathcal{Y}$ denote the model, an input-output mapping,

$$y = g(\boldsymbol{x}) \tag{2.1}$$

where, $\mathcal{Y} \subseteq \mathbb{R}$ is the set of values that the model output can assume and $\boldsymbol{x} = \{x_1, x_2, ..., x_n\}$. Alternative names are assigned to the model inputs ($\boldsymbol{x}$) and output (y) depending on the field of application. For instance, in statistics $\boldsymbol{x}$ are called variables. In engineering $\boldsymbol{x}$ are called parameters and in economics exogenous variables. Henceforth, we will call $\boldsymbol{x}$ *model inputs* through out this thesis. Let $\boldsymbol{\alpha} = \{i_1, i_2, ..., i_k\}$ denote a subset of indices of a group of k model inputs with $k \leqslant n$ and $\boldsymbol{x}_{\boldsymbol{\alpha}} = \{x_{i_1}, x_{i_2}, ..., x_{i_k}\}$. To denote the complimentary set of $\boldsymbol{x}_{\boldsymbol{\alpha}}$, we shall use $\boldsymbol{x}_{\sim\boldsymbol{\alpha}}$. A sensitivity measure of x_i is a number which denotes the sensitivity of a model output with respect to a model input x_i. When a *sensitivity measure* is used to rank model inputs based on their influence on the model output, it is called an *importance measure*.

2.2 Local sensitivity analysis methods

The first approach to SA we are to discuss is known as the *local approach*. In this framework one is interested in studying the response of the computer model around a point of interest in the model input space. The point of interest can be a point of reference for a policy maker or base case for a decision maker. We denote, this point as $\boldsymbol{x}^0$. The following subsections discuss briefly local sensitivity analysis methods widely used in applications.

2.2.1 Sensitivity analysis with finite differences: one at a time approach

The simplest way of studying the behaviour of a model is to use the one at a time approach (OAT). The method consists on changing one model input at a time to evaluate the corresponding model output changes. We let $\boldsymbol{x}^0$ denote the base case and $\boldsymbol{x}^+$ denote the sensitivity case [Borgonovo and Plischke, 2015] of the model inputs. Then, the corresponding vector of model input changes is $\triangle^+\boldsymbol{x} = \boldsymbol{x}^+ - \boldsymbol{x}^0 = (\triangle^+x_1, \triangle^+x_2, ..., \triangle^+x_n)$. We evaluate the model by varying model inputs one at a time from the base case to the sensitivity case and define the sensitivity measure as the change occurred due to the variation of a corresponding model input:

$$\triangle_i^+ y = g(x_i + \triangle x_i^+, \boldsymbol{x}_{\sim i}^0) - g(\boldsymbol{x}^0) \tag{2.2}$$

where $(x_i + \triangle x_i^+, \boldsymbol{x}_{\sim i}^0)$ is the point of $\mathcal{X}$ obtained moving x_i alone to the sensitivity case. Thus, intuitively we call $\triangle_i^+ y$ the finite change in y provoked by individual change in model input x_i. The insights obtained from this sensitivity measure concern both the magnitude of the impact and the direction of change. The most used graphical representation of the OAT approach is the so called *Tornado diagram* introduced by Howard [1988]. The sensitivity measures given in equation (2.2) are represented by horizontal bars sorted from the largest to smallest (see figure (2.1)). For a detailed description of their implementation we refer to the work of Eschenbach [1992]. An example of a Tornado diagram is given in figure (2.1) which illustrates the impact of each factor's uncertainty on value . As the diagram illustrates, the variation in market share and technology penetration have the bigger impact on profit. Tornado Diagrams are widely used in a business context, due to their computational convenience and ease in interpretation. Nonetheless, some limitations associated to their use emerge, such as the inability to account for simultaneous model input changes and the inability to detect the relevance of interactions. These limitations have been widely underlined in the literature (see for instance, Saltelli and D'Hombres [2010]).

2.2.2 Spider plots and one way sensitivity functions

The method of one way sensitivity functions is concerned with the evaluation of the model output following model input variations over an entire predetermined range. The sensitivity measure in this case is defined as the function [Borgonovo and Plischke, 2016]

$$h_i(x_i) = g(x_i; \boldsymbol{x}_{\sim i}^0). \tag{2.3}$$

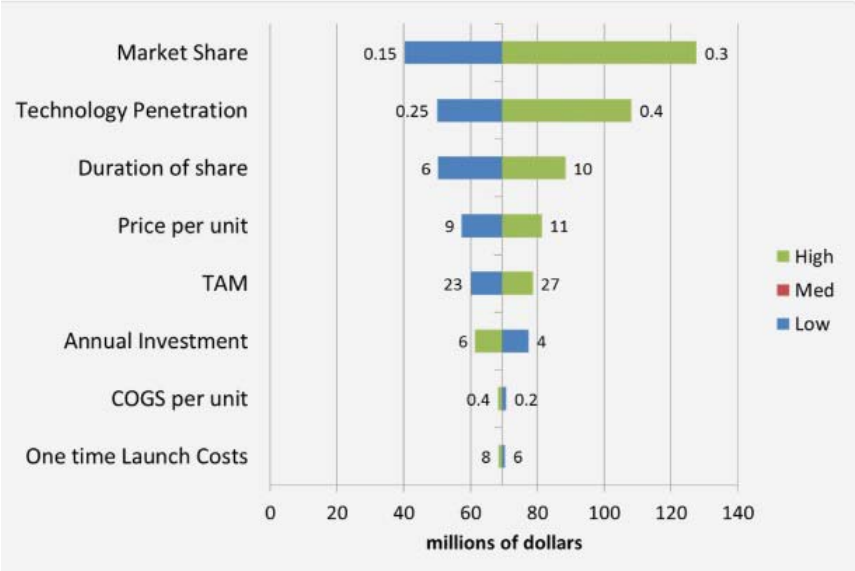


Figure 2.1: An example of a Tornado diagram showing the impact of each factor's uncertainty on value (http://smartorg.com/tornado-diagram-resolving-conflict-and-confusion-with-objectivity-and-evidence/).

One is interested in the graphical representation of $h_i(x_i)$. The sensitivity functions can be plotted either individually or in the same plot. If the sensitivity functions are condensed in the same graph, we obtain the so called *spiderplot graph* [Eschenbach, 1992]. Here one usually displays the deviation of the model output from a base case , i.e., the quantity

$$h_i^*(x_i) = g(x_i; \boldsymbol{x}^0_{\sim i}) - g(\boldsymbol{x}^0), \tag{2.4}$$

for all i over the ranges of the model inputs. We observe that the sensitivity functions of the spider plots are the sensitivity measures of tornado diagrams evaluated at alternative values of x_i.

While one way sensitivity functions are applied in several fields, they are particularly popular in the study of Bayesian networks, where they deal with *systematically varying one of the network's parameter probabilities while keeping all other parameters fixed* [van der Gaag et al. [2007], p.104]. The idea of one-way sensitivity functions can be generalized to the multidimensional case, leading to n-way sensitivity plots. For an overview of n-way sensitivity plots, we refer to Kjaerulff and van der Gaag [2000].

2.2.3 Differentiation based sensitivity methods

An important class of sensitivity analysis methods is represented by differentiation methods. Partial derivatives are the most frequently used measures of local sensitivity. Thanks to the increasing computer power, researchers have been able to obtain partial derivatives numerically. Consequently, many differentiation based sensitivity measures have been

proposed during the last decade. We start with the formalization of Helton [1993] based on Tailor Series expansion of the model output. Assuming that g is differentiable, we can write:

$$\triangle y = g(\boldsymbol{x}^+) - g(\boldsymbol{x}^0) = \sum_{i=1}^{n} \frac{\partial g(\boldsymbol{x}^0)}{\partial x_i}(x_i^+ - x_i^0) + \frac{1}{2}\sum_{i=1}^{n}\sum_{k=1}^{n} \frac{\partial^2 g(\boldsymbol{x}^0)}{\partial x_i \partial x_k}(x_i^+ - x_i^0)(x_k^+ - x_k^0) + o(||\boldsymbol{x}^+ - \boldsymbol{x}^0||^2) \tag{2.5}$$

If the changes $(x_i^+ - x_i^0)$ can be considered small, the second order terms can be neglected. Hence, $\triangle y \approx \sum_{i=1}^{n} \frac{\partial g(\boldsymbol{x}^0)}{\partial x_i}(x_i - x_i^0)$, and as a result, partial derivatives turn out to be a natural sensitivity measure. This use of partial derivatives as sensitivity measures is also common to Samuelson [1941] seminal work on comparative statics in economics.

Moreover, partial derivatives play an extremely important role in reliability analysis where they are given the name of importance measures. Partial derivatives are a crucial tool in *direction of change* setting, i.e., an increase (decrease) in a model input provokes an increase (decrease) in model output. Hence, if infinitesimal perturbations are of concern, as in the original work of Samuelson, the sign of partial derivatives provides the desired answer.

Using partial derivatives, however, is not free from shortcomings. For instance, consider that the goal of the analyst is to rank model inputs based on the magnitudes of the corresponding partial derivatives. We would be in a *factor prioritization* setting. To over come the difficulty in f*factor prioritization* setting, a new differential based sensitivity measure was introduced by Borgonovo and Apostolakis [2001] named *differential importance measure (DIM)* which is a normalization version of partial derivatives. The DIM plays a fundamental role in the next chapter of this thesis. Therefore, we shall devote a separate section in the next chapter to discuss in greater detail by skipping the details of DIM in this section.

2.3 Global sensitivity analysis methods

The methods we have discussed so far consider a deterministic model evaluated at one individual point of the model input space. If an analyst wishes to explore the model behaviour across the entire model input space, then he/she needs to apply a global sensitivity method. Thus, the underlying mindset of this method allows the assignment of a probability distribution to the model inputs. In this respect, one often refers to this type of sensitivity analysis as to a *probabilistic sensitivity analysis* [Oakley and O'Hagan, 2004]. In this section, we shall present concisely the most used global sensitivity methods: regression based methods, variance based methods, density based and transformation invariant methods.

2.3.1 Statistical setup of global sensitivity analysis

As mentioned in Saltelli and Tarantola [2002a], the fundamental assumption of a probabilistic sensitivity analysis is that "we assume to have information about the model inputs' probability distributions, either jointly or marginal, with or without correlation "(page 704). We define the probability space $(\mathcal{X}, \mathcal{B}(\mathcal{X}), \mathbb{P}_X)$, where $\mathbb{P}_X$ is a probability distribution on the model input space. Thus, the model inputs become a random vector and we denote it as $\boldsymbol{X} = (X_1, X_2, ..., X_n)$. A realization of $\boldsymbol{X}$ is then denoted by $\boldsymbol{x} = (x_1, x_2, ..., x_n)$. We let $F_{\boldsymbol{X}}$ and $f_{\boldsymbol{x}}$ denote the joint cumulative distribution and the joint probability density associated to $\mathbb{P}_X$, respectively. It is clear that the uncertainty in the model inputs makes y in equation (2.1) a random variable and therefore we re-write equation (2.1) as $Y = g(\boldsymbol{X})$.

In most practical situations, $g(\cdot)$ is not available in a closed form expression. Thus, the uncertainty propagation is performed numerically through Monte Carlo simulation. We generate a random sample of size N for each model input from the predefined probability distribution ($F_{\boldsymbol{X}}$) and then we obtain the corresponding model output for all N realizations of the model input vector.

2.3.2 Regression based methods

These methods were the first class of global sensitivity methods that have been thoroughly investigated (Saltelli and Marivoet [1990]: Helton [1993]). Regression based methods have become considerably successful due to various reasons. One is that its corresponding sensitivity measures can be directly estimated from a given Monte Carlo sample and secondly, no particular design is required in the estimation of the input-output sample. The computational cost is equal to $c = N$ model evaluations, where N is the Monte Carlo sample size. Here, we recall that, in computer experiments, one measures the cost of a technique by the required number of model runs.

In this framework, we assume that the input-output sample is well fitted by a multiple linear regression model. That is, from a sample of inputs and output $\{(x_{j1}, x_{j2}, ..., x_{jn}, y_j)|j = 1, 2, ..., N\}$, it is possible to fit a regression model provided that the sample size N is sufficiently large ($N > n$). Thus, $g(\cdot)$ is approximated by the response surface $Y = \beta_0 + \sum_{i=1}^{n} \beta_i X_i + \varepsilon$ with its estimation $g(\boldsymbol{X}) \approx b_0 + \sum_{i=1}^{n} b_i X_i$.

We now refer to some global sensitivity measures associated with this regression model. First, we recall the *standardized regression coefficient (SRC)* [Saltelli and Marivoet, 1990]:

$$SRC_j = b_j \frac{s_j}{s_Y} \tag{2.6}$$

where, s_j and s_Y are the sample standard deviations of model input X_j and the model

output Y, respectively. Secondly, we recall the *Pearson's correlation coefficient*

$$\rho_j = \frac{Cov(Y, X_j)}{s_j s_Y} \tag{2.7}$$

If we assume that the model inputs are independent, it is clear that SRC_j and ρ_j coincides for the linear models.

Another measure which is used to check the regression fit is the coefficient of determination (R^2), where it explains the proportion of the variance in Y that is predictable from the model inputs. If a low value of R^2 is identified, it concludes that the model fit is poor. In this situation, Campolongo and Saltelli [1997] claim that it might become *unrealistic to assess influence of the input variables based on SRC's.* However, in general, when the input-output mapping is characterized by the presence of non-linearities and interactions, the regression fit tends to be weak [Saltelli and Marivoet, 1990].

2.3.3 Functional decomposition of the output variance: variance-based sensitivity methods

Variance-based sensitivity methods evaluate the importance of a model input based on the expected reduction in the model output variance when we are able to fix such model input [Sobol', 1993]. The functional ANOVA expansion is at the basis of variance-based sensitivity methods. Suppose our model $g(\cdot)$ is square integrable and without loss of generality suppose that the model input space is I^n, n-dimensional unit hyper cube, i.e., model inputs follow a uniform distribution between zero and one. The motivation of assuming uniform distribution on model inputs is to be consistent with the notations in the work of Sobol' [1993]. Given the model inputs are independent, $g(\cdot)$ can be decomposed in to 2^n terms [Efron and Stein, 1981] :

$$g(\boldsymbol{X}) = g_0 + \sum_{i=1}^{n} g_i(X_i) + \sum_{i<j} g_{i,j}(X_i, X_j) + ... + g_{1,2,...,n}(X_1, X_2, \cdots, X_n) \tag{2.8}$$

and this decomposition is called ANOVA representation of $g(\boldsymbol{X})$ if for $1 \leq i_1 < \cdots < i_n \leq n$

$$\int_0^1 \cdots \int_0^1 g_{i_1,i_2,...,i_n}(X_{i_1}, X_{i_2}, ..., X_{i_n}) \ \mathrm{d}x_k \ = 0 \ \text{ for } \ k = i_1, ..., i_n. \tag{2.9}$$

It follows from equation (2.9), that the terms in equation (2.8) are orthogonal and can be expressed as the integrals of $g(\boldsymbol{X})$. Indeed,

$$g_0 = \mathbb{E}(Y) = \int_0^1 \cdots \int_0^1 g(\boldsymbol{X}) \ \mathrm{d}\boldsymbol{x}$$

$$g_i(X_i) = \mathbb{E}(Y|X_i) - g_0 = \int_0^1 \cdots \int_0^1 g(\boldsymbol{X}) \prod_{k \neq i} \mathrm{d}x_k - g_0$$

$$g_{i,j}(X_i, X_j) = \mathbb{E}(Y|X_i, X_j) - g_i(X_i) - g_j(X_j) - g_0 = \int_0^1 \cdots \int_0^1 g(\boldsymbol{X}) \prod_{k \neq i,j} \mathrm{d}x_k$$

$$-g_i(X_i) - g_j(X_j) - g_0$$

and so on. Since $g(\boldsymbol{X})$ is square integrable, then all the $g_{i_1,i_2,\ldots,i_n}$ in equation (2.8) are square integrable also. If we square equation (2.8) and integrate over I^n, we get

$$\int \cdots \int g^2(\boldsymbol{X}) \, \mathrm{d}x - g_0^2 = \sum_{k=1}^{n} \sum_{i_1 < \cdots < i_k}^{n} \int \cdots \int g^2_{i_1,\cdots,i_k} \, \mathrm{d}x_{i_1} \cdots \mathrm{d}x_{i_k}. \tag{2.10}$$

Thus, due to orthogonality we obtain the complete decomposition of the variance of Y in $2^n - 1$ terms as [Sobol', 1993]

$$\mathbb{V}(Y) = \sum_{i=1}^{n} V_i + \sum_{i<j} V_{i,j} + \sum_{i<j<k} V_{i,j,k} + \ldots + V_{1,2,\ldots,n} \tag{2.11}$$

where, $V_{\boldsymbol{\alpha}} = \mathbb{V}[g_{\boldsymbol{\alpha}}(\boldsymbol{X}_{\boldsymbol{\alpha}})]$, i.e., each $V_{\boldsymbol{\alpha}}$ is equal to the variance of the corresponding ANOVA effect $g_{\boldsymbol{\alpha}}(\boldsymbol{X}_{\boldsymbol{\alpha}})$. It is clear that the ANOVA decomposition of the model input-output mapping, $g(\cdot)$ is in one-to-one correspondence with the decomposition of its variance, i.e.,

$$V_{\boldsymbol{\alpha}} = \int \cdots \int g^2_{\boldsymbol{\alpha}}(\boldsymbol{X}_{\boldsymbol{\alpha}}) \, \mathrm{d}x_{\boldsymbol{\alpha}} \tag{2.12}$$

In summary, we can state the main assumptions of functional ANOVA as the square integrability of $g(\cdot)$, the independence among model inputs and a single parametric distribution of $\boldsymbol{X}$. Next, we explore two standard measures of sensitivity of Y to an input X_i associated with the above variance decomposition. In particular, by the total law of variance, we can write

$$V_i = \mathbb{V}(Y) - \mathbb{E}[\mathbb{V}(Y|X_i)] = \mathbb{V}[\mathbb{E}(Y|X_i)]$$

The motivation of V_i is the expected amount by which the variance of Y will be reduced if we learn the true value of X_i. Then, note that V_i is the numerator of Pearson's

Correlation ratio,

$$\eta_i^2 := \frac{\mathbb{V}[\mathbb{E}(Y|X_i)]}{\mathbb{V}(Y)}, \tag{2.13}$$

the first index associated with V_i [Homma and Saltelli, 1996].

The second index, proposed by Homma and Saltelli [1996], is

$$V_i^T = \mathbb{V}(Y) - \mathbb{V}[\mathbb{E}(Y|\boldsymbol{X}_{\sim i})].$$

Then, V_i^T is the remaining uncertainty in Y that is unexplained after we have learnt all model inputs but X_i. In particular, V_i^T is equal to the sum of all terms in the variance decomposition that contain X_i.

By normalizing the terms in the variance decomposition, we obtain the so-called Sobol' (or variance-based) sensitivity indices:

$$S_i = V_i/\mathbb{V}(Y) = \eta_i^2, \tag{2.14}$$

$$S_i^T = V_i^T/\mathbb{V}(Y) = 1 - S_{\sim i} \tag{2.15}$$

S_i is called the first order sensitivity index of X_i and S_i^T is called the total sensitivity index of X_i. The total Sobol' sensitivity index can then be written as the summation of component wise sensitivity indices that contains i^{th} terms :

$$S_i^T = S_i + \sum_{j \neq i} S_{ij} + \sum_{j \neq i, k \neq i, j<k} S_{ijk} + ... \tag{2.16}$$

Variance-based sensitivity measures are introduced in Saltelli and Tarantola [2002b] in association with the *factor prioritization* setting. The rationale in Saltelli and Tarantola [2002b] is as follows. In *factor prioritization* setting , we assume that each factor has a true value which is unknown in practise and these values can be determined by the appropriate experiments. If we assume that these experiments have the same cost, then we would be interested to detect the model inputs which reduce the output variance the most, once they are fixed to its true value. Hence, Saltelli and Tarantola [2002b] suggested to use $\mathbb{E}[\mathbb{V}(Y|X_i)]$ or $\mathbb{V}[\mathbb{E}(Y|X_i)]$ to detect these input variables. The lower the value of $\mathbb{E}[\mathbb{V}(Y|X_i)]$, and thus the higher the value of $\mathbb{V}[\mathbb{E}(Y|X_i)]$ the most likely it is X_i that one should measure first since it reduces the model output variance the most.

From historical point of view, variance based methods have come across with alternative definitions. As it was seen above the fist order sensitivity index is same as the Pearson correlation ratio. Moreover, in risk analysis, Iman and Hora [1990] define a variance-based sensitivity measure $IH_i = \mathbb{V}[\mathbb{E}(Y|X_i)]$, which is the same as V_i. Sobol' [1993] defines the so called variance-based sensitivity indices in the context of high dimensional integration.

Note that the definition of Sobol' assumes the independence among the model inputs, i.e., assumes a product measure. However, later on, Wagner [1995] introduces first and total variance-based sensitivity indices particularly in the case where the model inputs are not probabilistically independent. Overall, Wagner [1995] defines the sensitivity measures independently of the work of Sobol'. In particular [Borgonovo and Plischke, 2016] "We observe that Sobol' [1993], Iman and Hora [1990] and Wagner [1995] arrive at similar definitions almost simultaneously but independently, as there are no cross-citations and, moreover these works do not cite Pearson's original work. Nonetheless, if we wish to be more historically accurate, all these works are preceded by the seminal work of Cukier, Fortuin, Shuler, Pet schek, and Schaibly(1973), where variance-based sensitivity measures are used in the context of scientific modelling for the first time"(page 8).

Oakley and O'Hagan [2004] state that, under independence, variance decomposition "reflects the structure of the model itself". However, under model input correlations, the correspondence between the functional ANOVA and variance decomposition is lost. Mathematically, if the measure used in the integration is not a product measure, orthogonality can not be achieved to eliminate the cross products (see equation (2.10)). Thus, the variance decomposition can not be obtained from the functional ANOVA decomposition under correlation. Moreover. it is noted that the existence of functional ANOVA under mixture of model input distributions is still an open question and thus the variance based sensitivity measures are yet to be defined.

Variance based methods are based on the intuition of summarizing the overall model output variability through the model output variance. However, these methods do not reassure the analyst that a null value of the sensitivity measure implies independence of Y and X_i. Thus, it is not sufficient to assess the impact of input uncertainty only on the output variance. A solution to this problem was provided by subsequent literature giving rise to the concept of moment independent methods [Borgonovo, 2007]. These methods are concerned at looking into the influence of input uncertainty on the entire output distribution without relying on a specific moment of the output. The next subsection is devoted to review this concept.

2.3.4 Density based sensitivity measures

First, we shall introduce some relevant notations. We call any operator $\eta(\cdot,\cdot)$ an inner operator if it satisfies $\eta(\mathbb{P},\mathbb{P}) = 0$ for all distributions. Further, we denote $\gamma_i(x_i) = \eta(\mathbb{P}_Y, \mathbb{P}_{Y|X_i=x_i})$ and name $\gamma_i(x_i)$ the inner statistic [Borgonovo et al., 2016]. Evidently, $\gamma_i(x_i)$ is a function of x_i, i.e. , $\gamma_i : \mathcal{X}_i \longrightarrow \mathbb{R}$, where $\mathcal{X}_i$ is the space of the model input X_i. Thus, $\gamma_i(x_i)$ represents the effect on the distribution of Y fixing X_i at x_i. Under probabilistic framework, X_i can assume any value in its support according to its marginal distribution. Therefore, the need of a sensitivity measure which evaluates the overall

effect of X_i on the output distribution is essential. This can be obtained by taking the expectation over all possible values of X_i. Formally, we can write the following definition.

Definition 1 (Borgonovo et al. [2016])**.** If $\eta(\cdot,\cdot)$ is an inner operator with corresponding inner statistic $\gamma_i(x_i)$, then we call

$$\rho_i = \mathbb{E}[\gamma_i(X_i)] = \mathbb{E}_{X_i}[\eta(\mathbb{P}_Y, \mathbb{P}_{Y|X_i})]$$

the global sensitvity measure of X_i based on $\eta(\cdot,\cdot)$.

If $\mathbb{P}$ represents a probability density function, we call ρ_i, a density based sensitivity measure. The first such density based sensitivity measure is the δ-sensitivity measure of Borgonovo [2007] defined as:

$$\delta_i = \frac{1}{2}\mathbb{E}\Big[\int_{\mathcal{Y}} \big|f_Y(y) - f_{Y|X_i=x_i}(y)\big|\,\mathrm{d}y\Big] \tag{2.17}$$

where δ_i was given the name of *moment independent sensitivity measure*. Intuitively, this measure represents the normalized expected shift in the probability distribution of Y provoked by X_i.

Further, it can be re-written as

$$\delta_i = \frac{1}{2}\int_{\mathcal{X}_i}\int_{\mathcal{Y}} \big|f_Y(y) - f_{Y|X_i=x_i}(y)\big|\, f_{X_i}(x_i)\,\mathrm{d}y\,\mathrm{d}x_i$$

In this case, the inner statistic is

$$\gamma_i(x_i) = \int_{\mathcal{Y}} \big|f_Y(y) - f_{Y|X_i=x_i}(y)\big|\,\mathrm{d}y \tag{2.18}$$

By the definition of the conditional probability, δ_i can also be expressed in terms of joint density between Y and X_i and marginal densities of X_i and Y:

$$\begin{aligned}\delta_i &= \frac{1}{2}\int_{\mathcal{X}_i}\int_{\mathcal{Y}} \left|f_Y(y) - \frac{f_{Y,X_i}(y,x_i)}{f_{X_i}(x_i)}\right| f_{X_i}(x_i)\,\mathrm{d}y\,\mathrm{d}x_i \\ &= \frac{1}{2}\int_{\mathcal{X}_i}\int_{\mathcal{Y}} |f_Y(y)f_{X_i}(x_i) - f_{Y,X_i}(y,x_i)|\;\mathrm{d}y\,\mathrm{d}x_i.\end{aligned}$$

It is clear from the definition of δ_i that it is non-negative and normalized between zero and unity. Hence, the higher the value of δ_i, the stronger the statistical dependence between Y and X_i.

In fact, one can prove that $\delta_i = 0$ if and only if Y and X_i are statistically independent. In terms of estimation of δ_i, several investigations have been conducted in the literature. We recall the works of Castaings et al. [2012]; Luo et al. [2014]; Liu and Homma [2010];

Zhang et al. [2014].

A generalization of the definition of δ_i is to consider as inner statistic any member of the family of Csiszár's $f-$divergences (see Borgonovo and Plischke [2015] and Rahman [2016]) :

$$\eta_\phi(X_i, Y) = \int_{\mathcal{Y}} f_{Y|X_i}(y)\phi\left[\frac{f_Y(y)}{f_{Y|X_i}(y)}\right] \mathrm{d}y \tag{2.19}$$

where, ϕ is a convex function such that $\phi(0) = 1$. If we chose $\phi(x) = |x - 1|$, the total variation distance, it leads to the exact definition of δ_i. Specifying alternative forms for the convex function $\phi(x)$, one obtains alternative metrics which are all monotonic transformation invariant (see Borgonovo and Plischke [2015]). A detailed study of the sensitivity measures associated with Csizár $f-$divergences is offered in Chapter 5.

2.3.5 Transformation invariant methods

It is a well known fact in the literature of statistic and data analysis that experts widely use variety of transformations such as logarithmic , power and rank to accelerate the rate of numerical convergence in practical applications. However, one might find it difficult in interpreting the results that are obtained on the transformed data, which might not directly be transferred back to the scale of the original data. Moreover, it is not always guaranteed that the ranking of a model input is the same on the original and transformed scales produced by a global sensitivity measure. Indeed, numerical experiments seen in the work of Borgonovo and Tonoli [2014] illustrates these facts.

A function $T = t(Y)$ is a monotonic transformation of the model output Y if $t(\cdot)$ is monotonically increasing (or decreasing) function. From an SA point of view, performing calculations on the transformed model output leads to the problem of interpreting results back to the original scale [Iman and Hora, 1990]. However, a monotonic transformation changes the model structure. For instance, we refer to the simple example in Borgonovo and Plischke [2016], where they consider a product model:

$$Y = X_1.X_2 \cdots X_n \tag{2.20}$$

Clearly, the model is not additive. Then, if we apply the logarithmic transformation to the model, we have

$$T = \log(Y) = \log(X_1) + \log(X_2) + \cdots + \log(X_n) \tag{2.21}$$

which is now additive and also no interactions are present. So, it is clear that the sensitivity insights obtained on the transformed model output are not directly transferable to the original model. But, if we adopt a monotonic transformation invariant sensitivity

measure, the result it produces is independent on the transformation [Borgonovo and Tonoli, 2014]. Hence, the analyst can benefit from accelerating numerical convergence while avoiding the difficulties of transferring results back to the original scale.

Let $\beta_i(Y)$ ($\beta_i(T)$) denote the generic sensitivity measure of model input X_i of the model output Y (T). We recall Baucells and Borgonovo [2013] and say that a sensitivity measure is monotonic transformation invariant if

$$\beta_i(Y) = \beta_i(T) \tag{2.22}$$

for all monotonic transformations, $T = t(Y)$.

To obtain transformation invariant global sensitivity measure, one needs to impose a transformation invariant inner statistic (γ_i). In this work, we consider mainly two global sensitivity measures based on invariant inner statistics. The statistics are Kolomogorov-Smirnov (KS) and Kuiper (Ku) distances [Baucells and Borgonovo, 2013] between cumulative distribution functions, defined as

$$\begin{aligned}
\beta_i^{KS}(X_i) &= \mathbb{E}\big[\sup_{y\in\mathbb{R}} \big|F_Y(y) - F_{Y|X_i}(y)\big|\big] \\
\beta_i^{Ku}(X_i) &= \mathbb{E}\big[\sup_{y\in\mathbb{R}} \big\{F_Y(y) - F_{Y|X_i}(y)\big\} + \sup_{y\in\mathbb{R}} \big\{F_{Y|X_i}(y) - F_Y(y)\big\}\big].
\end{aligned} \tag{2.23}$$

Note that δ_i discussed in the previous subsection is also monotonic transformation invariant. In summary, if we employ a monotonic transformation invariant sensitivity measure, the obtained results hold identical for Y and $t(Y)$ provided that $t(\cdot)$ is a monotonic function. This transformation has a notable implications for, example in decision science. i.e., the decision maker's preference is often expressed not through Y, but through a utility function of Y.

Up to now we have discussed various sensitivity measures by grouping them into local and global. Further, we split global sensitivity methods to sub-categories and we investigate them chronologically. However, to estimate all these measures require thousands of model runs. If the given model is computationally very slow, estimating the sensitivity indices becomes cumbersome. In this situation, one of the solutions is to replace the original model with a surrogate model (emulator) which is computationally fast with respect to the original model. This concept is known as metamodelling. The next section discusses briefly about metamodels.

2.4 Review of metamodels in sensitivity analysis

We close this section with a brief overview on metamodelling. By "metamodel "or "emulator "one means a surrogate model (or response surface) which is used to approximate

the deterministic response of a computer code. The starting point for the construction of a metamodel is a dataset which is output of the original computer code. This dataset is then used to fit a response surface. The key-premise is that, if the response surface actually fits well the original model output, then it can be used to replace the model output. In case the computational time of the model output is significant, then the emulator can be used instead of the original model, thus reducing the computational time.

First, let us illustrate alternative metamodelling types. The metamodel can be any linear regression model, non-linear parametric model, non-parametric model or even Bayesian non-parametric model. The most widely used metamodels include polynomials, splines, generalized linear models, generalized additive models, kriging, neural networks, boosting regression trees [Simpson et al., 2001]. In statistics, for example, a regression model refers to a probabilistic setup with unknown quantities (parameters or functions) which can then be estimated in different ways (Bayesian or frequentist), from the information contained in the initial sample, from the original deterministic model. The metamodel, in the SA context, is then the probabilistic model obtained after estimating the unknowns. However, these kinds of models are not always efficient, especially in simulation of complex and non-linear phenomena. In this case, modern statistical learning algorithms can show much better ability to build accurate surrogate models with strong predictive capabilities [Marrel et al., 2008].

Secondly, the design of numerical experiments i.e., the way in which the model input space is explored. It is desirable to use an experimental design that possesses good space filling properties and allows for the construction of a metamodel with a few model runs. Simpson et al. [2001] has offered a comparison of the performance of alternative experimental designs in the process of building a metamodel.

Finally, the issue of the validation of the metamodel is considered. In the field of classical experimental design, a proper validation of the response surface is a crucial step and is considered with care. However, in numerical experiments, this issue has not been studied deeply in the literature. The usual way is to estimate global criteria such as root mean square error, absolute error on a test basis, via cross validation and bootstrap [Kleijnen and Sargent, 2000]. In addition, some metamodels have the ability to produce sensitvity indices. For instance, Sudret [2008] showed that Sobol' indinces can be computed analytically once the coefficients of a polynomial chaos expansion are determined. Also, Sudret and Mai [2015] proposed a method to compute derivative-based global sensitivity measures (DGSM) using polynomial chaos expansions. DGSM are another class of sensitivity measures which we will introduce in the next chapter.

Chapter 3

Randomized Differential Importance Measure (RDIM)

The differential importance measure is a local importance measure that possesses two convenient properties such as additivity and sensitivity to relative changes. This chapter consists in the study of the properties of the randomized evaluation of the differential importance measures that is a bridge between local and global sensitivity methods. This has led to establishing a new sensitivity indicator, called Randomized Differential Importance Measure, that generalizes the derivative-based global sensitivity measures in previous works.

3.1 Motivation and Outline

The availability of numerical differentiation techniques and the increase in computing power allows analysts to have available not only the dataset of the model output but also the dataset of its partial derivatives with respect to the model inputs. This information, if available, should be used in order to produce insights for the analyst and the decision maker that would otherwise be lost.

The direct application of global sensitivity indices for high-dimensional models can be extremely time consuming (Sobol' and Kucherenko [2009]) since it often requires 10,000 or more model runs (Rakovec et al. [2014]). Thus, it can be computationally demanding. Thus, an efficient alternative would be to use sensitivity measures based on partial derivatives. Given that the model is differentiable, partial derivatives can be computed efficiently by using automatic differentiation algorithms available in mathematical softwares.

As we have discussed in Chapter 1, comparative static of Samuelson [1941] and DIM [Borgonovo and Apostolakis, 2001] (differential based sensitivity measures) are computationally efficient yet these are local measures. However, one can obtain a global measure

by averaging local measures after running the model at iterative locations of the model input space using Monte Carlo or Quasi Monte Carlo sampling methods. Such similar approaches have been discussed in existing literature: Distribution Evaluation of Local Sensitivity Analysis (DELSA) by Rakovec et al. [2014], screening method by Morris [1991], derivative based global sensitivity measures (DGSM) by Sobol' and Kucherenko [2009] , Iooss and Kucherenko [2015] and Lamboni et al. [2013a] (Some of these methods will be discussed later in this chapter). DELSA computes partial derivatives across the model input space by using quasi-random Sobol' sequence and produces the sensitivity index by averaging the local measure. Moreover, Rakovec et al. [2014] discuss how it relates to some existing SA methods, i.e., the Sobol' method. However, the above discussed sensitivity methods have some limitations. For instance, the sensitivity measure of Sobol' and Kucherenko [2009] does not allow to obtain insights on direction of change because it condenses the differential information into a square average. Further, the relative importance is also not efficient to evaluate in these methods. Another drawback of these methods is that it is computationally complex especially when it computes the joint sensitivity of a subset of model inputs for high dimensional data.

To overcome these problems and since partial derivatives are computationally efficient and less time consuming, we propose a useful class of a differential based sensitivity measure called *Randomized Differential Importance Measure (RDIM)* based on averaging DIM (Borgonovo and Apostolakis [2001]) using Monte Carlo or Quasi Monte Carlo sampling methods and it is a bridge between local and global sensitivity methods. In order to randomize the model inputs, we define a probability measure over the model input space. Then, DIM are evaluated at random points in the whole range of uncertainty. We carry out a thorough comparison of the method with other methods based on the randomization of partial derivatives such as DELSA and DGSM. Application to the sensitivity analysis of the large loss of coolant accident sequence of the advanced test reactor concludes the chapter.

3.2 RDIM- A new global sensitivity measure

In this section we give the definition of DIM and its properties. Then, we take a step forward to define RDIM and its properties. Next, we provide an estimator of RDIM and a theorem for its convergence.

3.2.1 The DIM

We start with a deterministic framework and consider the value assumed by the model at $\boldsymbol{x}^0$, i.e., we set $y = g(\boldsymbol{x}^0)$ for the present section. The DIM (Borgonovo and Apostolakis [2001]) is defined as the fraction of the total differential of g that is due to a change in

input x_i. DIM can be possibly define on a single model input or on multiple model inputs. However, DIM of multiple model inputs is simply the sum of individual DIMs which reveals the additive property of it. According to Borgonovo and Apostolakis [2001], this importance measure is the only additive local importance measure based on normalized partial derivatives.

The total variation of a differentiable function due to an infinitesimal perturbation of its inputs is expressed by the differential

$$\mathrm{d}y = \frac{\partial y}{\partial x_1}\mathrm{d}x_1 + \frac{\partial y}{\partial x_2}\mathrm{d}x_2 + ... + \frac{\partial y}{\partial x_n}\mathrm{d}x_n. \tag{3.1}$$

Then, the differential importance of the j^{th} model input at $\boldsymbol{x}^0$ is defined as

$$\mathrm{DIM}_j(\boldsymbol{x}^0) \equiv \frac{\mathrm{d}y_{x_j}}{\mathrm{d}y} = \frac{\left.\frac{\partial y}{\partial x_j}\right|_{\boldsymbol{x}^0}\mathrm{d}x_j}{\sum_{i=1}^{n}\left.\frac{\partial y}{\partial x_i}\right|_{\boldsymbol{x}^0}\mathrm{d}x_i}. \tag{3.2}$$

The change in y depends on how model inputs are varied and this is reflected in the value of DIM. Consider two specific situations: a) the analyst assumes that all model inputs undergo the same changes (uniform perturbations); b) the analyst assumed that the model inputs vary by the same percentage (proportional perturbations). Clearly, the two situations are not equivalent. More formally, these cases can be expressed as follows.

H_1: Uniform perturbations: $\mathrm{d}x_i = \mathrm{d}x_j \ \forall i, j$

$$\mathrm{DIM}_j(\boldsymbol{x}^0) = \frac{\left.\frac{\partial y}{\partial x_j}\right|_{\boldsymbol{x}^0}}{\sum_{i=1}^{n}\left.\frac{\partial y}{\partial x_i}\right|_{\boldsymbol{x}^0}} \tag{3.3}$$

H_2: Proportional perturbations: $\dfrac{\mathrm{d}x_i}{x_i^0} = \dfrac{\mathrm{d}x_j}{x_j^0} = \omega \quad \forall i, j$

$$\mathrm{DIM}_j(\boldsymbol{x}^0) = \frac{\left.\frac{\partial y}{\partial x_j}\right|_{\boldsymbol{x}^0} x_j^0}{\sum_{i=1}^{n}\left.\frac{\partial y}{\partial x_i}\right|_{\boldsymbol{x}^0} x_i^0} \tag{3.4}$$

The conditions under which one should apply H_1 or H_2 depends on the model and the problem at hand.

For instance, DIM_js are not comparable under H_1 when the model inputs have different

units. Instead, in this situation it is possible to apply proportional perturbations (H_2). Moreover, if one uses H_1, the rankings of the model inputs are equivalent to the rankings produce by partial derivatives whereas, if one uses H_2, the rankings of the model inputs are equivalent to the rankings produce by elasticity (ξ) [Borgonovo and Peccati, 2004]. The elasticity of y with respect to x_j at $\boldsymbol{x}^0$ is defined as

$$\xi_j = \left.\frac{\partial y}{\partial x_j}\right|_{\boldsymbol{x}^0} \frac{x_j^0}{g(\boldsymbol{x}^0)}.$$

Then, if we assume proportional model input perturbations, we have $\dfrac{\mathrm{d}x_i}{x_i^0} = \dfrac{\mathrm{d}x_j}{x_j^0}$ for all i and j. Multiplying and dividing each term of the equation (3.2) by x_j^0 and x_i^0, respectively, we obtain

$$\mathrm{DIM}_j(\boldsymbol{x}^0) = \frac{\left.\dfrac{\partial y}{\partial x_j}\right|_{\boldsymbol{x}^0} \dfrac{\mathrm{d}x_j}{x_j^0} x_j^0}{\sum_{i=1}^n \left.\dfrac{\partial y}{\partial x_i}\right|_{\boldsymbol{x}^0} \dfrac{\mathrm{d}x_i}{x_i^0} x_i^0} = \frac{\left.\dfrac{\partial y}{\partial x_j}\right|_{\boldsymbol{x}^0} \dfrac{x_j^0}{g(\boldsymbol{x}^0)}}{\sum_{i=1}^n \left.\dfrac{\partial y}{\partial x_i}\right|_{\boldsymbol{x}^0} \dfrac{x_i^0}{g(\boldsymbol{x}^0)}} = \frac{\xi_j}{\sum_{i=1}^n \xi_i}. \tag{3.5}$$

It is easy to prove that DIM is additive [Borgonovo and Apostolakis, 2001]. Suppose that we are interested in evaluating the joint sensitivity of a set of model inputs $x_{i_1}, x_{i_2}, ..., x_{i_k}$. Then

$$\begin{aligned}\mathrm{DIM}_{i_1,i_2,...,i_k}(\boldsymbol{x}^0) &= \frac{\left.\dfrac{\partial y}{\partial x_{i_1}}\right|_{\boldsymbol{x}^0} \mathrm{d}x_{i_1} + \left.\dfrac{\partial y}{\partial x_{i_2}}\right|_{\boldsymbol{x}^0} \mathrm{d}x_{i_2} + ... + \left.\dfrac{\partial y}{\partial x_{i_k}}\right|_{\boldsymbol{x}^0} \mathrm{d}x_{i_k}}{\mathrm{d}y} \\ &= \mathrm{DIM}_{i_1}(\boldsymbol{x}^0) + \mathrm{DIM}_{i_2}(\boldsymbol{x}^0) + ... + \mathrm{DIM}_{i_k}(\boldsymbol{x}^0).\end{aligned} \tag{3.6}$$

Thus, one can retrieve the importance of any group of variables as sum of the individual sensitivity measures of the variables in the group. From a numerical viewpoint, this has the advantage of allowing the evaluation of joint sensitivities without additional model runs with respect to the ones necessary to find individual sensitivities.

As for numerical calculation, differentiation can be either performed through brute force algorithms or through automated procedures (Bischof and Bücker [2000], see also www.autodiff.org). In this respect, the availability of automatic differentiation codes allows us to obtain partial derivatives at a relatively low computational cost, making the analysis feasible in most practical applications for which the model output is smooth. Yet, DIM addresses only the variation of a model around one point in the model input space ($\mathcal{X}$). Therefore, it does not permit a thorough exploration of the model behaviour as the inputs vary at several locations in $\mathcal{X}$. In the next subsection we introduce a new measure based on repeated evaluations of DIM in $\mathcal{X}$.

3.2.2 The RDIM

We now consider a framework in which the model inputs are uncertain. Let $\mathrm{DIM}_j : (\mathcal{X}, \mathcal{B}(\mathcal{X})) \to (\mathcal{D}, \mathcal{B}(\mathcal{D}))$, where $\mathcal{X} \subseteq \mathbb{R}^n$ and $\mathcal{D} \subseteq \mathbb{R}$ is a measurable function and let $\mu_{\boldsymbol{X}}$ be the probability measure on $(\mathcal{X}, \mathcal{B}(\mathcal{X}))$ assigned by the analyst. $\mu_{\boldsymbol{X}}$ does not need to be a product measure. Then, we define

$$\mathrm{RDIM}_j := \mathbb{E}_{\boldsymbol{X}}\big[\mathrm{DIM}_j(\boldsymbol{X})\big] = \int_{\mathcal{X}} \mathrm{DIM}_j(\boldsymbol{x})\, \mathrm{d}\mu_{\boldsymbol{X}}(\boldsymbol{x}).$$

RDIM is a derivative based global sensitivity measure since it is associated with derivatives and it considers not only a reference point in the model input space but many. A convenient property of RDIM is additivity. Let us state the following proposition.

Proposition 1. *Let $\boldsymbol{\alpha} = \{i_1, i_2, ..., i_k\}$ denote a generic set of indices. Then, let $RDIM_{\boldsymbol{\alpha}}$ denote the joint RDIM of the model inputs with indexes in $\boldsymbol{\alpha}$. Then, we have:*

$$RDIM_{\boldsymbol{\alpha}} = RDIM_{i_1} + RDIM_{i_2} + ... + RDIM_{i_k} \tag{3.7}$$

Proof. Follows by additivity of DIM and the linearity of the expectation

$$\begin{aligned} RDIM_{\boldsymbol{\alpha}} &= \mathbb{E}_{\boldsymbol{X}}[DIM_{\boldsymbol{\alpha}}] = \mathbb{E}_{\boldsymbol{X}}[DIM_{i_1,i_2,...,i_k}] \\ &= \mathbb{E}_{\boldsymbol{X}}[DIM_{i_1}] + \mathbb{E}_{\boldsymbol{X}}[DIM_{i_2}] + ... + \mathbb{E}_{\boldsymbol{X}}[DIM_{i_k}] \\ &= RDIM_{i_1} + RDIM_{i_2} + ... + RDIM_{i_k} \end{aligned}$$

□

We would like to observe that the definition of RDIM remains well posed also when the analyst assigns $\mu_{\boldsymbol{X}}$ as a finite mixture distribution which avoids the analyst to rely only on a single input distribution [Chick, 2001]. Specifically, let $\mathcal{M} = \left\{\mu^1_{\boldsymbol{X}}, \mu^2_{\boldsymbol{X}}, ..., \mu^m_{\boldsymbol{X}}, ...\right\}$ be a set of probability distributions on $(\mathcal{X}, \mathcal{B}(\mathcal{X}))$. Let $\mu_{\mathbf{X}}$ be assigned by the analyst in the form

$$\mu_{\boldsymbol{X}} = p_1\mu^1_{\boldsymbol{X}} + p_2\mu^2_{\boldsymbol{X}} + ... + p_M\mu^M_{\boldsymbol{X}}, \tag{3.8}$$

where $p_1, p_2, ..., p_M$ are appropriate weights such that $\sum_{m=1}^{M} p_m = 1$ and $p_m \geq 0$. Then we have the following result.

Proposition 2. *Let $\mu_{\boldsymbol{X}}$ be a mixture of probability measures as in eq. (3.8). Then we have:*

$$RDIM_i^{\mu_{\boldsymbol{X}}} = \sum_{m=1}^{M} p_m \cdot RDIM_i^{\mu^m_{\boldsymbol{X}}} \tag{3.9}$$

where further, suppose $RDIM_i^{\mu_{\boldsymbol{X}}}$ denote the RDIM evaluated with respect to $\mu_{\boldsymbol{X}}$ and $RDIM_i^{\mu^m_{\boldsymbol{X}}}$ denote the RDIM evaluated with respect to $\mu^m_{\boldsymbol{X}}$, a probability probability measure.

Proof.

$$\begin{aligned} RDIM_i^{\mu_{\boldsymbol{X}}} &= \int_{\mathcal{X}} DIM_i(\boldsymbol{x}) d\mu_{\boldsymbol{X}}(\boldsymbol{x}) \\ &= \int_{\mathcal{X}} DIM_i(\boldsymbol{x}) \sum_{m=1}^{M} p_m \, d\mu_{\boldsymbol{X}}^m(\boldsymbol{x}) = \sum_{m=1}^{M} p_m \int_{\mathcal{X}} DIM_i(\boldsymbol{x}) \, d\mu_{\boldsymbol{X}}^m(\boldsymbol{x}) \\ &= p_1 \cdot RDIM_i^{\mu_{\boldsymbol{X}}^1} + p_2 \cdot RDIM_i^{\mu_{\boldsymbol{X}}^2} + ... + p_M \cdot RDIM_i^{\mu_{\boldsymbol{X}}^M} \end{aligned}$$

□

Performing global sensitivity analysis by assigning a single probability distribution with a specific parameter vector (we are referring to a single parametric distribution of $\boldsymbol{X}$), the most commonly used approach, might tend to *underestimate the uncertainty about the underlying nature of the random process generating the data* [Chick, 2001]. To be more specific, there are many applications in which lack of data or experts disagreements do not allow the analyst to specify a unique model input distribution. For example, a typical situation reported in global sensitivity analysis is of climate change models where Meinshausen et al. [2009] claim that over 20 alternative probability distributions have been assigned in scientific studies during past 10 years. Therefore, instead of assigning a single input distribution, the result reported in the above proposition, allows the analyst to accommodate his degree of belief about the true distribution on the model inputs by assigning a mixture of appropriate probability distributions. However, in contrast to RDIM, this assignment raises some non-trivial methodological issues for other sensitivity measures, e.g., the existence of functional ANOVA expansion for the mixture is still an open question and thus variance based sensitivity measures are not defined under mixture of probability distributions (as we mentioned in Chapter 2).

3.2.3 Estimation and Error Analysis of RDIM

In this section, we give a detailed procedure of the approximation of RDIM via the Monte Carlo method (stochastic integration) together with a proof of its error bound. Under uncertainty, the differential importance of model input j is a random variable. Then, the Monte Carlo estimate of RDIM_j is obtained using N independent samples $\boldsymbol{X}^1, ..., \boldsymbol{X}^N \in \mathcal{X}$ from $\mu_{\boldsymbol{X}}$ and letting

$$\widehat{\text{RDIM}_j} \approx \frac{1}{N} \sum_{i=1}^{N} \text{DIM}_j(\boldsymbol{X}^i). \tag{3.10}$$

The strong law of large numbers guarantees that $\lim_{N \longrightarrow \infty} \frac{1}{N} \sum_{i=1}^{N} \text{DIM}_j(\boldsymbol{X}^i) = \mathbb{E}_{\boldsymbol{X}}\big[\text{DIM}_j(\boldsymbol{X})\big]$ $= \text{RDIM}_j$ almost surely. Thus, the estimator in equation (3.10) is asymptotically unbi-

ased. Further, the standard error of $\widehat{\text{RDIM}}_j$ is $\sigma_{\text{DIM}_j} N^{-0.5}$ (σ_{DIM_j} is the standard deviation of DIM_j) which is the classical error of a Monte Carlo estimator. This confirms that the crude Monte Carlo method yields a probabilistic error bound of order $\text{O}(N^{-0.5})$. This convergence rate is quit slow. This may be challenging for computation, if the running time of the computer code is large, because the number of model runs required to achieve a given precision may be high.

Latest improvements of Monte Carlo methods have become considerable impact of the efficiency and range of applicability of its computations. Indeed, a variety of methods have been in construction, for instance, such as variance reduction methods and quasi Monte Carlo method. Variance reduction methods accelerate the convergence rate by reducing the coefficient that appears in front of the $\text{O}(N^{-0.5})$ term. On the other hand quasi-Monte Carlo methods use low discrepancy sequences (also called quasi-random sequence or sub random sequence). Two notable examples are Halton sequence and Sobol sequence (Owen [2006]; Niederreiter [1992]). Using these sequences leads to relatively faster convergence rate [Caflisch, 1998] of the Monte Carlo estimates, a rate which is close to $\text{O}(1/N)$. Particularly, although we introduced a simulation based consistent estimate of RDIM, we are also interested in finding a theoretical error bound of this estimate which is $\epsilon = |\widehat{\text{RDIM}}_j - \text{RDIM}_j|$. The following theorem formalizes the error bound of RDIM.

Theorem 3.2.1. *If DIM_j has bounded variation V(DIM_j) on [0,1], then the error bound ϵ is $O(N^{-1}(log\ N)^n)$ where*

$$\epsilon = \left| \frac{1}{N} \sum_{i=1}^{N} DIM_j(\boldsymbol{X}^i) - \int_{[0,1]^n} DIM_j(\mathbf{u}) d\mathbf{u} \right|,$$

$\boldsymbol{X}^i$ is random point in the model input space $\mathcal{X}$ and $RDIM_j = \int_{[0,1]^n} DIM_j(\boldsymbol{u})\text{d}\boldsymbol{u}$ is the true value of $RDIM_j$ when the model inputs are transformed to a n-dimensional unit hypercude.

To prove theorem (3.2.1), we define the following quantities through this steps.

1. The discrepancy of the set $\{\boldsymbol{X}^1, ..., \boldsymbol{X}^N\}$.
2. The variance of DIM.
3. Koksma-Hlawka inequality.
4. Construction of the Halton sequence.

Step 1: Let H be a set of points $\{\boldsymbol{X}^1, \cdots, \boldsymbol{X}^N\}$ where we want these points to be evenly distributed within a n-dimensional unit cube. The discrepancy of the set H , $\text{D}_N(H)$, is

defined as

$$\mathrm{D}_N(H) = \sup_{Q \subset \mathfrak{Q}} \left| \frac{\text{number of points in } (H \cap Q)}{N} - \text{volume}(Q) \right| \tag{3.11}$$

where $\mathfrak{Q}$ is the set of n-dimensional intervals or rectangular solids in $[0,1]^n$ with sides parallel to the coordinate axes of the form

$$\prod_{i=1}^{n} [a_i, b_i) = \{ \boldsymbol{X} \in \mathbb{R}^n : a_i \leq X_i < b_i \}$$

More formally, let the counting function be defined as

$$Z(Q; H) = \sum_{i=1}^{N} c_Q(\boldsymbol{X}^i) \tag{3.12}$$

where c_Q is the indicator function of Q. Thus, $\mathrm{D}_N(H)$ is defined as [Niederreiter, 1992]

$$\mathrm{D}_N(H) = \sup_{Q \subset \mathfrak{Q}} \left| \frac{Z(Q; H)}{N} - \lambda_n(Q) \right| \tag{3.13}$$

where λ_n is the n-dimensional Lebesgue measure. We shall concentrate on the most widely studied discrepancy that is "star discrepancy."

Definition 2. The star discrepancy, D_N^*, is defined as [Niederreiter [1992]] $\mathrm{D}_N^*(H) = \mathrm{D}_N(H)$, where $\mathfrak{Q}$ is the family of all subintervals of $[0,1]^n$ of the type $\prod_{i=1}^{n} [0, u_i)$ where u_i is in the half-open interval $[0,1)$.

Step 2: We start with Vitali total variation concept. For DIM_j on $[0,1]^n$ and a n-dimensional subinterval Q of $[0,1]^n$, let $\nabla^{(n)}(\mathrm{DIM}_j; Q)$ be an alternating sum of the values of DIM_j at the vertices of Q and is defined as [Aistleitner and Dick, 2015]

$$\nabla^{(n)}(\mathrm{DIM}_j; Q) = \sum_{j_1=0}^{1} \dots \sum_{j_n=0}^{1} (-1)^{j_1 + \dots + j_n} \mathrm{DIM}_j(u_1 - j_1 u_1, \dots, u_n - j_n u_n). \tag{3.14}$$

Then the variation of DIM_j on $[0,1]^n$ according to Vitali is defined as

$$V^{Vitali_{(n)}}(\mathrm{DIM}_j) = \sup_{\mathfrak{Q}} \sum_{Q \in \mathfrak{Q}} \left| \nabla^n(\mathrm{DIM}_j; Q) \right|. \tag{3.15}$$

Further, it can be proven that, provided that $\mathrm{DIM}_j(\boldsymbol{x})$ is differentiable, $V^{Vitali_{(n)}}(\mathrm{DIM}_j)$ is

$$V^{Vitali_{(n)}}(\mathrm{DIM}_j) = \int_0^1 \dots \int_0^1 \left| \frac{\partial^n \mathrm{DIM}_j}{\partial x_1 \dots \partial x_n} \right| \mathrm{d}x_1 \dots \mathrm{d}x_n. \tag{3.16}$$

Let us now define the variation according to Hardy and Krause. For $1\leq k \leq n$ and $1\leq i_1 < i_2 < ... < i_k \leq n$, let $V^{Vitali_{(n)}}(\mathrm{DIM}_j;i_1,...,i_k)$ denote the $n-$dimensional variation in the sense of Vitali of the restriction of DIM_j to the face

$$T_n^{(i_1,i_2,...,i_k)} = \{(X_1,...,X_n) \ \in [0,1]^n : X_j = 1 \ for \ all \ j \neq i_1,...,i_k\}$$

of $[0,1]^n$. Then the variation in term of Hardy and Krause is defined as

$$V(\mathrm{DIM}_j) = \sum_{k=1}^{n} \sum_{1\leq i_1<i_2<...<i_k\leq n} V^{Vitali_{(n)}}(\mathrm{DIM}_j; i_1,...,i_k). \tag{3.17}$$

Step 3: The approximation error of the quasi-Monte Carlo method is bounded by a term proportional to the discrepancy of the set H. Therefore, according to the Koksma-Hlawka inequality [Caflisch, 1998], the error of $\widehat{\mathrm{RDIM}}_j$ is bounded as follows:

$$\epsilon = \left| \frac{1}{N} \sum_{i=1}^{N} \mathrm{DIM}_j(\boldsymbol{X}^i) - \int_{[0,1]^n} \mathrm{DIM}_j(\mathbf{u})\mathrm{d}\mathbf{u} \right| \leq V(\mathrm{DIM}_j)\mathrm{D}_N^*(H) \tag{3.18}$$

Step 4: The error bound in step 3 leads to the conclusion that the point sets with small star discrepancy guarantee small errors in quasi-Monte Carlo estimation over $[0,1]^n$. This is true not only when the integration domain is normalized to $[0,1]^n$, but also for the integration domains contained in $[0,1]^n$. One can expect a low discrepancy if the proportion of points falls in to the arbitrary set Q is close to its measure [Caflisch, 1998]. Some examples of low-discrepancy sequences include van der Corput sequence, Halton sequence and Sobol sequence.

For an integer $d \ \geq 2$, let $Z_d = \{0,1,...,d-1\}$. Every integer $m \geq 0$ has a unique digit expansion [Niederreiter [1992]]

$$m = \sum_{j=0}^{\infty} b_j(m)d^j \tag{3.19}$$

in base d, where $b_j(m) \in Z_d$ for all $j \geq 0$ and $b_j(m) = 0$ for all sufficiently large j. i.e., the sum in equation (3.19) is finite.
For an integer $d \ \geq 2$, the radical-inverse function ϕ_d in base d is

$$\phi_d(m) = \sum_{j=0}^{\infty} b_j(m)d^{-j-1} \text{ for all integers } \ m \geq 0 \tag{3.20}$$

where m is given by its digit expansion (3.19) in base d.

Let us consider the discrepancy of a Halton sequence. For an integer $d \ \geq 2$, the van der Corput sequence in base d is the sequence $x_0, x_1, \cdots$ with $x_m = \phi_d(m)$ for all

$m \geq 0$. However, this sequence can be extended as follows to produce a low-discrepancy multi-dimensional sequence which leads to a Halton sequence.

Definition 3. For a given dimension $n \geq 1$, let $h_1, ..., h_n$ be integers greater than two. Then, using the radical inversion function ϕ_d in equation (3.20), the Halton sequence in the bases $h_1, ..., h_n$ as the sequence $x_0, x_1, \cdots$ which is defined as

$$\mathbf{x}_m = (\phi_{h_1}(m), ..., \phi_{h_n}(m)) \in [0,1)^n \text{ for all } m \geq 0. \tag{3.21}$$

For $n = 1$, this definition reduces to van der Corput sequence. By following the above definitions and the theorem given in Niederreiter [1992] we provide an upper bound of the start discrepancy as follows:

Theorem 3.2.2. *[Niederreiter, 1992] If H is the Halton sequence in the pairwise relatively prime bases $h_1, ..., h_n$ (If every pair of the bases is coprime, then the set of the bases is said to be pairwise relatively prime) then*

$$D_N^*(H) < \frac{n}{N} + \frac{1}{N} \prod_{i=1}^{n} \left(\frac{h_i - 1}{2 \log h_i} \log N + \frac{h_i + 1}{2} \right) \text{ for all } N \geq 1. \tag{3.22}$$

Further it is simplified as

$$D_N^*(H) \leq \left(\prod_{i=1}^{n} \frac{h_i - 1}{2 \log h_i} \right) N^{-1} (\log N)^n + O(N^{-1} (\log N)^{n-1}) \quad for \ \ N \geq 2. \tag{3.23}$$

We have mentioned all necessary partial results to prove theorem (3.2.1).

Proof. (**Theorem 3.2.1**)
By equation (3.18), it is clear that ϵ is bounded by

$$\epsilon \leq V(\mathrm{DIM}_j) \mathrm{D}_N^*(H)$$

and from equation (3.23) we have

$$D_N^*(H) \leq N^{-1} (\log N)^n$$

It is clear that the star discrepancy of a Halton sequence is dominated by the term $N^{-1} (\log N)^n$. Therefore, by equation (3.18), we have an error bound of $\mathrm{O}(N^{-1}(\log N)^n)$ for RDIM. □

3.3 RDIM as a screening method

Screening methods foresee the evaluation of the model at the limited number of locations in $\mathcal{X}$. The primary goal of screening design is to identify the least important model inputs, while maintaining a reasonable number of model evaluations. Screening methods are used within the *factor fixing* setting. In a *factor fixing* setting, analysts are interested in identifying the least important model inputs with a reduced number of model evaluations hence the least important variables are fixed to their base values. Most of the screening methods are based on the so-called "One At a Time"(OAT) design, where each input is varied by itself while fixing others. Several reviews on screening methods are available in the literature (Sanchez et al. [2005];Kleijnen [2009]). Among such methods, Morris method [Morris, 1991] is the most commonly used. The method allows to analyse the model inputs into three groups: inputs having negligible effects, inputs having large linear effects without interactions and inputs having large non-linear and/or interaction effects. This method considers segmenting the model input ranges in finite number of levels in a deterministic framework.

Since with the newly introduced sensitivity measure RDIM, one can identify non-influential variables (or influential variables, i.e., duality of detection), we claim that RDIM can be seen as a screening method in a probabilistic frame work. We discuss here two such similar methods associated with the randomized evaluation of partial derivatives; DGSM [Sobol' and Kucherenko, 2009] and DELSA [Rakovec et al., 2014]. Later, we will compare numerically RDIM with these methods.

3.3.1 Derivative based global sensitivity measures

DGSM are considered within the family of screening methods. Sobol' and Kucherenko [2009] define DGSM of X_i as:

$$\nu_i = \mathbb{E}_{\boldsymbol{X}}\Big[\Big(\frac{\partial g(\boldsymbol{X})}{\partial x_i}\Big)^2\Big] = \int \Big(\frac{\partial g(\boldsymbol{x})}{\partial x_i}\Big)^2 \mathrm{d}\mu_{\boldsymbol{X}}(\boldsymbol{x}) \tag{3.24}$$

provided that $\dfrac{\partial g}{\partial x_i}$ is square integrable and $c \leq \left|\dfrac{\partial g}{\partial x_i}\right| \leq C$. Further, in the same work the authors have established a link between ν_i and S_i^T (total sensitivity index defined in equation (2.15)):

$$S_i^T \leq \nu_i/\pi^2\, \mathbb{V}(Y) \tag{3.25}$$

where $\mathbb{V}(Y)$ is the total variance defined in the equation (2.11). The link in equation (3.25) is defined when the given the model inputs lie in the unit hypercube $[0,1]^n$ with Lebesgue measure $\mathrm{d}\boldsymbol{x} = \mathrm{d}x_1\mathrm{d}x_2...\mathrm{d}x_n$. Moreover, if the corresponding probability density function of $\mu_{\boldsymbol{X}}$ is normal with model input variances σ_i^2, Sobol' and Kucherenko [2009]

obtain the link between S_i^T and ν_i as:

$$S_i^T \leq \nu_i \sigma_i^2 / \mathbb{V}(Y). \tag{3.26}$$

However, ν_i has been motivated by the Morris importance measure $\mu_i = \int_{H^n} |\partial y / \partial x_i| \, \mathrm{d}x$. It is reported in Sobol' and Kucherenko [2009] that μ_i and ν_i are equivalent from practical point of view and linked as $\nu_i \leq C\mu_i$ and $\mu_i \leq \sqrt{\nu_i}$, where C is the upper bound of the partial derivative. Hence, The upper bound in equation (3.25) can be useful for both ν_i and μ_i. On the other hand, Campolongo et al. [2007] suggested a modified version of the Morris importance measure which was also based on absolute values of partial derivatives and was named as μ^*. Further, it was reported that in some practical problems this measure had good agreements with the rankings of Sobol total indices (S_i^T), but no formal proof of the relationship between μ_i^* and S_i^T was provided.

Additionally, DGSM have been largely studied in Lamboni et al. [2013a] and Kucherenko et al. [2009]. These authors claim that DGSM can be efficiently estimated in most of the cases using quasi-Monte Carlo samples of size 100 to 1000 and thus they are computationally more efficient than variance based methods, especially for high dimensional cases. We noticed that DGSM are not necessarily denominated in the same units (since DGSM are not normalized measures), hence can not directly be used in a *factor prioritization* setting. To over come this situation, the formal links in equation (3.25) and equation (3.26) can be used to rank the inputs according to their importance. Lamboni et al. [2013b] recently extended this link for any complex model and for any input variable X_i, that has a Boltzmann probability measure $\mu_i(x)$ on $\mathbb{R}$. A measure is said to be a Boltzmann measure if it is absolutely continuous with respect to the Lebesgue measure and its density is of the form $k \exp[-\beta(x)]$, with $\beta(\cdot)$ a continuous function and k a normalizing constant. The well known class of log-concave probability measures belong to the class of Boltzmann probability measures. In this case, $\beta(\cdot)$ is a convex function. The following theorem gives the generalized formal link between Sobol' indices and DGSM.

Theorem 3.3.1. *[Lamboni et al., 2013b] If* $g \in L^2(\mathbb{R})$, $\dfrac{\partial g}{\partial x_i} \in L^2(\mathbb{R})$, X_i *are independent and the law of* X_i *is a Boltzmann probability measure, we have*

$$V_i^T \leq \Upsilon_i \tag{3.27}$$

with

$$\Upsilon_i = D[\mu_i(x)]\nu_i$$

and

$$D[\mu_i(x)] = 4\left[\sup_{x \in \mathbb{R}} \frac{min(F_i(x), 1 - F_i(x))}{f_i(x)}\right]^2$$

where $F_i(\cdot)$ is the cumulative probability function of X_i and $f_i(\cdot)$ is the probability density function of X_i. The upper bounds Υ_i provide accurate judgements on input sensitivities when total Sobol' indices cannot be estimated efficiently for expensive models with considerable less amount of cpu time. However, it is not always guaranteed that Υ_i provides accurate rankings on the model inputs. To support this fact, we can refer to a counterexample discussed in section (7) of Sobol' and Kucherenko [2009] where the rankings of upper bounds do not coincide with the rankings of S_i^T, i.e.,$\Upsilon_i > \Upsilon_j \nRightarrow S_{T_i} > S_{T_j}$. In addition, despite the upper bounds can be computed numerically, if the analyst impose a mixture of distribution for $\boldsymbol{X}$, the upper bounds can not be compared with the total Sobol' indices (ANOVA expansion is not defined, see page 14).

3.3.2 DELSA

We now present the DELSA method by Rakovec et al. [2014] . This method shares the same intuition of evaluating a local sensitivity measure at a number of randomized sample points in the model input space as RDIM and DGSM. However, DELSA uses a different local statistic. It is constructed in a way that allows direct comparison to the Sobol' sensitivity indices and thus it can be considered as an alternative to global sensitivity indices that is obtained at a lower computational cost.

The randomized local measure in DELSA is based on multiple factors, i.e., partial derivative $\left(\partial g/\partial x_j\right)$, predicted variance ($\mathbb{V}_L(Y)$ of the model output) and prior input variances (s_i^2). The predicted variance $\mathbb{V}_L(Y)$ [Hill and Tiedeman, 2007] is defined as

$$\mathbb{V}_L(Y) = \left(\left.\frac{\partial g}{\partial \boldsymbol{X}}\right|_k\right)^T (\mathbf{Q}^T \boldsymbol{W} \mathbf{Q})^{-1} \left(\left.\frac{\partial g}{\partial \boldsymbol{X}}\right|_k\right) \tag{3.28}$$

where $\boldsymbol{Q}$ is a matrix of both $\partial y_i/\partial x_j$ (y_i being the i^{th} observation) and prior information with M rows and n columns based on either classical or Bayesian statistical arguments. Classical statistical arguments are based on sampling methods; Bayesian statistical arguments are, at least in part, based on belief [Bolstad, 2007]. $\boldsymbol{W}$ is a matrix of weights of the observations with M rows and M columns. The weighting used approximates the reliability of the prior information. The value of M depends on the problem considered. For model calibration problems with no prior information, M would be the number of observations. If prior information are available, $M = N + M_p$, where N is the number of observations and M_p is the number of prior information equations (for prior information equations refer page 32 of Hill and Tiedeman [2007]). The additional rows of $\boldsymbol{Q}$ often have zero entries for the parameters (in this context model inputs) where no prior information is available. Equation (3.28) produces values identical to the total variance in equation (2.11) under some conditions including the linearity of Y with respect to the model inputs.

For comparison with Sobol indices, Rakovec et al. [2014] do some arrangements to $\mathbb{V}_L(Y)$ in such a way that it produces comparable results with Sobol' sensitivity indices. First, they do not include observations in $\boldsymbol{Q}$, but only prior information on parameters since they are primary concern is into parameters. In that way $\boldsymbol{Q}$ becomes an identity matrix with n dimension. Secondly, $\boldsymbol{W}$ is considered as a diagonal matrix with $\big[\frac{1}{12}(x_{i,max} - x_{i,min})^2)\big]^{-1}$ being the diagonal elements for $i = 1, 2, ..., n$. The motivation of the choice of $\boldsymbol{W}$ lies on the Sobol sampling method. In this sampling, the probability that an input can take a value within its range ($[x_{i,min}, x_{i,max}]$) is constant, which is consistent with a uniform probability distribution. Therefore, to produce equivalent results as Sobol, the prior variance in DELSA needs to be defined as a variance for uniform distribution with parameters $x_{i,min}$ and $x_{i,max}$. After defining the predicted variance, the authors define the first order sensitivity measure of DELSA for the i^{th} input at a given sample point k as:

$$S^i_{L1} = \frac{\left|\frac{\partial g}{\partial x_i}\right|^2_k s_i^2}{\mathbb{V}_L(Y)} \tag{3.29}$$

For an example, consider a case with three model inputs and we are interested to see the predicted variance associated with Sobol' indices. i.e.,

$$\mathbb{V}_L(Y) = \left|\frac{\partial g}{\partial x_1}\right|_k s_1^2 + \left|\frac{\partial g}{\partial x_2}\right|_k s_2^2 + \left|\frac{\partial g}{\partial x_3}\right|_k s_3^2 \tag{3.30}$$

with s_1^2,s_2^2 and s_3^2 are input prior variances (s_i^2 being the variance of a uniform distribution with parameters $x_{i,min}$ and $x_{i,max}$). Simulation studies in Rakovec et al. [2014] show that for a given sample of points in the model input space, $\mathbb{V}_L(Y)$ (in equation (3.30), variance of DELSA method) and $\mathbb{V}(Y)$ (in equation (2.11), variance of Sobol method) produce quit similar results. However, Sobol values are slightly larger, as expected given that the local methods used in this context do not account for model input interactions.

The cost of calculating S^i_{L1} at N sample points using a quasi random sequence is $N(n+1)$ where as the first order sensitivity indices of Sobol' need $N_s(n+1) * N$, where N_s is the Sobol' sample size. Hence, $N = 1$ provides the sensitivity measure calculated at one location and evidently it is a local statistic. In summary, calculation of the Sobol sensitivity measure distributed in model input space is computationally expensive [Rakovec et al., 2014].

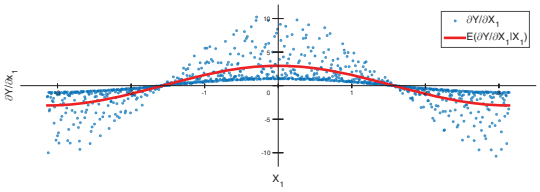
The study of DELSA mainly includes the comparison with variance based /Sobol' sensitivity indices. The comparison is made through empirical cumulative distribution (full frequency distribution), surface plots and box plots of S_i and S^i_{L1}. Two hydrologic models with 2 and 14 model inputs are investigated and for each sample size (100,1000 and 10 000 etc), the variation of Sobol index was higher than its variation of the S^i_{L1}.

The results of the study showed that in both cases, Sobol' and DELSA identified similar important and unimportant variables.

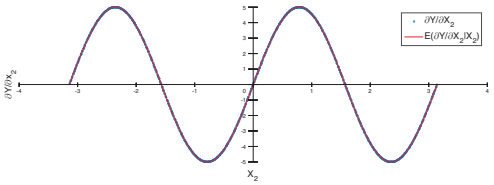
3.4 Managerial insight of RDIM

In this section, we are interested in the insights that an analyst/decision maker can obtain by the estimation of RDIM. Some of those questions includes *What is the direction of change implied by a model input change?, What are the least important model inputs (so they can be fixed at their base value)? and what is the change in model output implied by a change of a group of model inputs?*. Hence, one can certainly chose an appropriate sensitivity analysis method to answer these stated questions. If the question is answered with uncertainty of model inputs, global sensitivity analysis is recommended whereas if the question is related to a given point in the model input space, local sensitivity is advisable. Therefore, before conducting the sensitivity analysis, a precise formulation of the questions is necessary for the selection of an appropriate sensitivity method. This process goes under the name of formulating the sensitivity *settings* (introduced in the first chapter) for the investigation at hand. In fact, having available both the realizations of the model and of its derivatives, the analyst can answer not only a *factor prioritization* and *factor fixing* setting in an informed way, but also the *direction of change* and *joint sensitivity* settings. In the reminder, we explore how the estimation of RDIM allows us to provide answer within the four above mentioned settings.

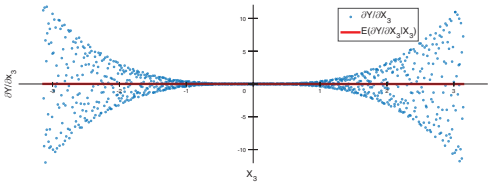
Direction of Change: To answer the question of the decision maker *do model input changes cause the model output to increase or decrease*, the *direction of change* setting is used. As Samuelson (1941) states: *Will an increase in demand raise or lower price*?. This is a typical problem in economics as well as in many applications where the analysts are interested to know whether an increase (decrease) in a model input results an increase (decrease) in model output. In this case, the model output can be a risk metric or an expected utility or a net present value, etc. Then, it is natural to ask the "what if "question of whether, when inputs are changed, risk or expected utility or net present value increase or decrease, respectively. With our proposed sensitivity index, one can easily answer this question by observing the sign of partial derivatives that summarizes the overall consequence of a change in an input variable with respect to model output. A straightforward method to visualize the sign of change of the model with respect to a single input is to use a derivative scatterplot, *D-scatterplot*. If the realizations of partial derivatives are all in the first two upper/lower quadrants, then the model is non-decreasing/decreasing whereas if the partial derivatives have both positive and negative signs, it confirms that the model is non-monotonic.



(a) Partial derivatives with respect to x_1.



(b) Partial derivatives with respect to x_2.



(c) Partial derivatives with respect to x_3.

Figure 3.1: D-plots of Ishigami function.

To illustrate consider the Ishigami test function written in the form

$$y = \sin x_1 + 5 \sin^2 x_2 + 0.1 x_3^4 \sin x_1 \tag{3.31}$$

where $x_i \overset{iid}{\sim} U[-\pi, \pi]$. We generate a sample of $\boldsymbol{X}$ and evaluate the partial derivatives of the Ishigami model. The scatterplots of the partial derivatives are reported in figure (3.1). As figure (3.1) illustrates, signs of partial derivatives have a mix behaviour with positive and negative signs for all three model inputs. This means that the model is non-monotonic with respect to each model input. Like wise, the decision maker can check the monotonicity property of a given model by plotting the partial derivatives with respect to each model input.

These results, however, can be used to obtain additional information. We can, in fact, treat the scatterplots of the derivatives as "regular scatterplots" and plot the expectation of the partial derivatives. That is, we can compute

$$\mathbb{E}\left(\frac{\partial y}{\partial x_1}\middle| x_1\right) = \mathbb{E}\left(\cos x_1 + 0.1\, x_3^4 \cos x_1 \middle| x_1\right) = \cos x_1 + 0.1 \cos x_1\, \mathbb{E}(x_3^4)$$

$$\mathbb{E}\left(\frac{\partial y}{\partial x_2}\middle| x_2\right) = \mathbb{E}\left(10 \cos x_2\, \sin x_2 \middle| x_2\right) = 10\, \cos\, x_2\, \sin\, x_2$$

$$\mathbb{E}\left(\frac{\partial y}{\partial x_3}\middle| x_3\right) = \mathbb{E}(0.4\, x_3^3\, \sin\, x_1 | x_3) = 0.4\, x_3^3\, \mathbb{E}(\sin\, x_1).$$

Factor Fixing: Here, we wish to establish *which model inputs* can be fixed at their base case value (such as mean) and hence the relative importance setting is used. By utilizing $|\text{RDIM}_i|$, the decision maker can rank the model inputs based on their individual impact on the output.

Joint Sensitivity: To answer the question of the decision maker *what is the joint effect of a subset of model inputs on the mode output*, the *joint sensitivity* setting is used. The answer is straightforward thanks to the additivity property of RDIM (see proposition 1). In this way, it is very feasible to evaluate the joint effect of any subset of input variables from a single simulation run.

3.5 Numerical Studies

The first part of this section includes several toy examples that have been used as test cases to check the consistency of the estimation procedure of RDIM. Primarily, we observed the convergence plots of RDIM to its theoretical value. By using a given data estimation approach, one can also estimate from the dataset the variance-based and moment-independent global sensitivity measures of the model inputs. In the second part of this section we discuss this intuition with direct application to a well known case study in the sensitivity analysis literature, namely, the probabilistic risk assessment model of the advanced test reactor (ATR) sequence. We have available both the datasets of derivatives and of realizations of the model output for this computer code. We then run a comparison between randomized local sensitivity measures (RDIM, DELSA and DGSM), variance-based and moment independent sensitivity measures, discussing the ranking agreement as well as the alternative insights obtained by their simultaneous utilization.

3.5.1 Analytical Test Cases of RDIM

We start with multilinear models. Let

$$y = g(\boldsymbol{x}) = \sum_{u=1}^{n} \prod_{k=1}^{u} (1 + x_k) = a_i(x_{\sim i})x_i + b_i(x_{\sim i})$$

be a multilinear model with $\boldsymbol{X} \sim f_{\boldsymbol{X}}$ and $a_i(x_{\sim i})$ and $b_i(x_{\sim i})$ be functions of all x_j's except x_i. Then $\dfrac{\partial Y}{\partial x_j} = a_j(x_{\sim j})$. We obtain the analytical expressions of DIM for the two hypotheses explained in section (3.2.1) for a model input x_j:

$$\text{H}_1 : \text{DIM}_j(\boldsymbol{x}) = \frac{a_j(x_{\sim j})}{\sum_{i=1}^{n} a_i(x_{\sim i})}$$
$$\text{H}_2 : \text{DIM}_j(\boldsymbol{x}) = \frac{a_j(x_{\sim j})x_j}{\sum_{i=1}^{n} a_i(x_{\sim i})x_i}$$

Thus, RDIM_j is

$$\begin{aligned} \text{H}_1 :&\text{RDIM}_j = \mathbb{E}_{\boldsymbol{X}}[\text{DIM}_j(\boldsymbol{X})] = \mathbb{E}_{\boldsymbol{X}}\Big[\frac{a_j(X_{\sim j})}{\sum_{i=1}^{n} a_i(X_{\sim i})}\Big] \\ \text{H}_2 :&\text{RDIM}_j = \mathbb{E}_{\boldsymbol{X}}[\text{DIM}_j(\boldsymbol{X})] = \mathbb{E}_{\boldsymbol{X}}\Big[\frac{a_j(X_{\sim j})X_j}{\sum_{i=1}^{n} a_i(X_{\sim i})X_i}\Big]. \end{aligned} \tag{3.32}$$

Now, we consider two particular cases of the multilinear models namely additive and multiplicative models.

Additive models

Let

$$y = \sum_{i=1}^{n} a_i x_i \tag{3.33}$$

with $\boldsymbol{X} \sim f_{\boldsymbol{X}}$. Then $\frac{\partial Y}{\partial x_j} = a_j$. We obtain the analytical expressions of DIM for the two hypotheses for a model input x_j:

$$\begin{aligned} \text{H}_1 :&\text{DIM}_j(\boldsymbol{x}) = \frac{a_j}{\sum_{i=1}^{n} a_i} \\ \text{H}_2 :&\text{DIM}_j(\boldsymbol{x}) = \frac{a_j x_j}{\sum_{i=1}^{n} a_i x_i} \end{aligned}$$

Thus, RDIM_j is

$$\begin{aligned} \text{H}_1 :&\text{RDIM}_j = \mathbb{E}_{\boldsymbol{X}}[\text{DIM}_j(\boldsymbol{X})] = \frac{a_j}{\sum_{i=1}^{n} a_i} \\ \text{H}_2 :&\text{RDIM}_j = \mathbb{E}_{\boldsymbol{X}}[\text{DIM}_j(\boldsymbol{X})] = \mathbb{E}_{\boldsymbol{X}}\Big[\frac{a_j X_j}{\sum_{i=1}^{n} a_i X_i}\Big] \end{aligned} \tag{3.34}$$

Remark 1. RDIM in an additive model under uniform perturbations is the same under any model input distribution. (see equation (3.34)).

Multiplicative models

Let

$$y = \prod_{i=1}^{n} x_i^{a_i} \tag{3.35}$$

with $\boldsymbol{X} \sim f_{\boldsymbol{X}}$. Then $\frac{\partial Y}{\partial x_j} = \left(\prod_{s=1,s\neq j}^{n} x_s^{a_s}\right)\ a_j x_j^{a_j-1}$. We obtain the analytical expressions of DIM for the two hypotheses for a model input x_j:

$$\begin{aligned}
\mathrm{H}_1 :\mathrm{DIM}_j(\boldsymbol{x}) &= \frac{\left(\prod_{s=1,s\neq j}^{n} x_s^{a_s}\right)\ a_j x_j^{a_j-1}}{\sum_{i=1}^{n}\left(\prod_{s=1,s\neq i}^{n} x_s^{a_s}\right)\ a_i x_i^{a_i-1}} = \frac{\left(\frac{a_j}{x_j}\right)}{\sum_{i=1}^{n}\left(\frac{a_i}{x_i}\right)} \\
\mathrm{H}_2 :\mathrm{DIM}_j(\boldsymbol{x}) &= \frac{\left(\prod_{s=1,s\neq j}^{n} x_s^{a_s}\right)\ a_j x_j^{a_j}}{\sum_{i=1}^{n}\left(\prod_{s=1,s\neq i}^{n} x_s^{a_s}\right)\ a_i x_i^{a_i}} = \frac{a_j}{\sum_{i=1}^{n} a_i}
\end{aligned}$$

Thus, RDIM_j is

$$\begin{aligned}
\mathrm{H}_1 :\mathrm{RDIM}_j &= \mathbb{E}_{\boldsymbol{X}}[\mathrm{DIM}_j(\boldsymbol{X})] = \mathbb{E}_{\boldsymbol{X}}\Big[\frac{\left(\frac{a_j}{X_j}\right)}{\sum_{i=1}^{n}\left(\frac{a_i}{X_i}\right)}\Big] \\
\mathrm{H}_2 :\mathrm{RDIM}_j &= \mathbb{E}_{\boldsymbol{X}}[\mathrm{DIM}_j(\boldsymbol{X})] = \frac{a_j}{\sum_{i=1}^{n} a_i}
\end{aligned} \tag{3.36}$$

Remark 2. RDIM in a multiplicative model under proportional perturbations is the same under any model input distribution (see equation (3.36)). Moreover, it is interesting to see the duality of RDIM under H_1 of a linear additive model and under H_2 of a multiplicative model where they have a similar structure associated with the coefficients.

3.5.2 Test Cases

In this section we provide several test cases. The aim of these experiments is to explore the convergence of the estimation procedure of RDIM across various sample sizes. We provide the additive and multiplicative cases with three model inputs by imposing different distributions for the model inputs and then we provide the well known test case in SA literature, the Ishigami function along with a comparison with alternative SA indices ; δ_i, S_i and S_i^T.

Test case 1

Let $Y = 4X_1 + 7X_2 + 9X_3$, where $X_i \overset{i.i.d}{\sim} U[0,1]$ generated from a Halton sequence. Then, the partial derivatives are $\dfrac{\partial y}{\partial x_1} = 4$, $\dfrac{\partial y}{\partial x_2} = 7$ and $\dfrac{\partial y}{\partial x_3} = 9$. The theoretical values of

RDIM_j for $j = 1, 2, 3$ for proportional perturbations are reported below.

$$\text{RDIM}_1 = \int_0^1 \int_0^1 \int_0^1 \frac{4x_1}{4x_1 + 7x_2 + 9x_3} \mathrm{d}x_1 \mathrm{d}x_2 \mathrm{d}x_3 = 0.21543$$
$$\text{RDIM}_2 = \int_0^1 \int_0^1 \int_0^1 \frac{7x_2}{4x_1 + 7x_2 + 9x_3} \mathrm{d}x_1 \mathrm{d}x_2 \mathrm{d}x_3 = 0.35153$$
$$\text{RDIM}_3 = \int_0^1 \int_0^1 \int_0^1 \frac{9x_3}{4x_1 + 7x_2 + 9x_3} \mathrm{d}x_1 \mathrm{d}x_2 \mathrm{d}x_3 = 0.43304.$$

Table (3.1) illustrates the numerical values of RDIM across different sample sizes.

Table 3.1: Simulation results of test case 1

	Sample Size $(N)(\times 10^2)$									
	10	20	30	40	50	60	70	80	90	100
RDIM_1	0.21547	0.21553	0.21542	0.21537	0.21553	0.21546	0.21548	0.21543	0.21547	0.21544
RDIM_2	0.35128	0.35148	0.35153	0.35156	0.35145	0.35152	0.35149	0.35151	0.35150	0.351527
RDIM_3	0.43326	0.43299	0.43305	0.43307	0.43302	0.43302	0.43303	0.43306	0.43302	0.43304

Figure (3.2) shows the convergence plots of RDIM_1, RDIM_2 and RDIM_3 across sample sizes for test case 1. The numerical values have good agreements on their corresponding theoretical values. The convergence is obtained at $N = 2000$.

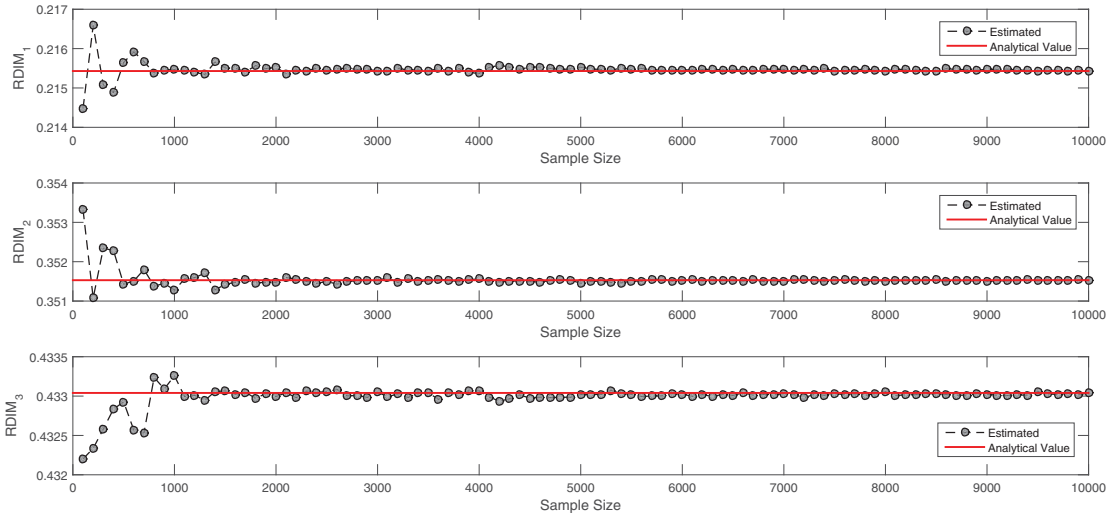


Figure 3.2: Convergence plot of test case 1 under proportional perturbations

Test Case 2

Let us consider the same linear model in test case 1 by assuming X_i (independent) comes from a two component Gaussian mixture distribution such that

$X_1 \sim 0.2N(3,1) + 0.8N(2,0.5)$
$X_2 \sim 0.6N(2.5,0.8) + 0.4N(1.2,0.4)$
$X_3 \sim 0.5N(1,0.2) + 0.5N(6,0.7)$.

Moreover, let the corresponding marginal densities be $f_{X_1}(x_1)$, $f_{X_2}(x_2)$ and $f_{X_3}(x_3)$, respectively. Under H_2, the theoretical values of RDIM index are reported below.

$$\text{RDIM}_1 = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\left(\frac{4x_1}{4x_1+7x_2+9x_3}\right)f_{X_1}(x_1)f_{X_2}(x_2)f_{X_3}(x_3)\mathrm{d}x_1\mathrm{d}x_2\mathrm{d}x_3 = 0.203$$
$$\text{RDIM}_2 = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\left(\frac{7x_2}{4x_1+7x_2+9x_3}\right)f_{X_1}(x_1)f_{X_2}(x_2)f_{X_3}(x_3)\mathrm{d}x_1\mathrm{d}x_2\mathrm{d}x_3 = 0.298$$
$$\text{RDIM}_3 = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\left(\frac{9x_3}{4x_1+7x_2+9x_3}\right)f_{X_1}(x_1)f_{X_2}(x_2)f_{X_3}(x_3)\mathrm{d}x_1\mathrm{d}x_2\mathrm{d}x_3 = 0.50.$$

The corresponding numerical values of RDIM across various sample sizes for the test case 2 are given in table (3.2). Figure (3.3) shows the convergence plots of RDIM_1, RDIM_2 and

Table 3.2: Simulation results of test case 2

	Sample Size $(N)(\times 10^2)$									
	10	20	30	40	50	60	70	80	90	100
RDIM_1	0.2082	0.2034	0.2022	0.2066	0.1973	0.2057	0.2041	0.2037	0.2010	0.2029
RDIM_2	0.2993	0.3024	0.2973	0.2936	0.2977	0.2974	0.2947	0.2999	0.2931	0.2983
RDIM_3	0.4925	0.4942	0.5004	0.4998	0.5049	0.4969	0.5013	0.4964	0.5059	0.4989

RDIM_3 across sample sizes for test case 2. The numerical values have good agreements on their corresponding theoretical values. The convergence is obtained at $N = 5000$.

Test Case 3

Consider the function $Y = {X_1}^6{X_2}^9{X_3}^8$ where $X_i \overset{iid}{\sim} U[0,1]$. The partial derivatives are

$\frac{\partial y}{\partial x_1} = 6{x_1}^5{x_2}^9{x_3}^8$, $\frac{\partial y}{\partial x_2} = 9{x_1}^6{x_2}^8{x_3}^8$ and $\frac{\partial y}{\partial x_3} = 8{x_1}^6{x_2}^9{x_3}^7$.

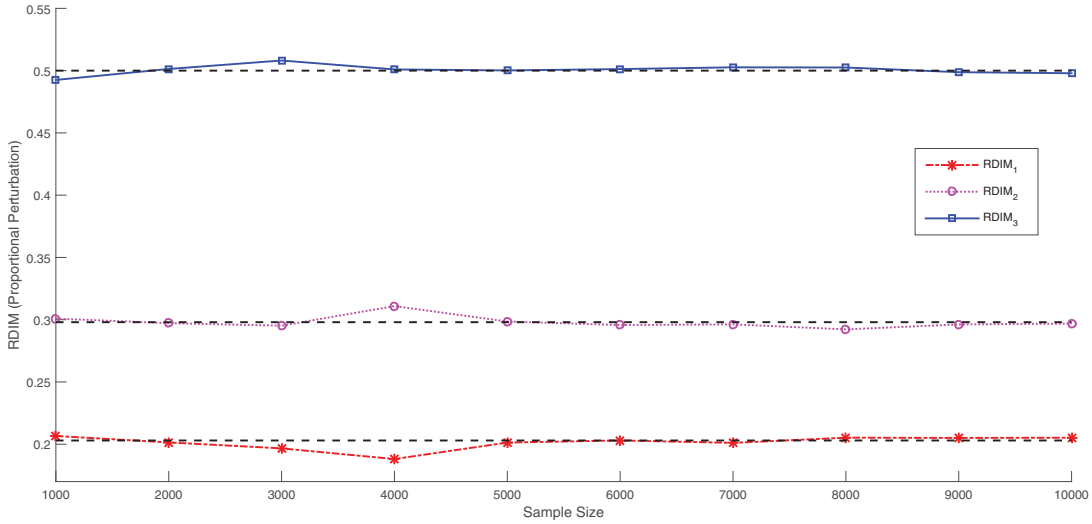


Figure 3.3: Convergence plot of test case 2

Under H_1,

$$\text{RDIM}_1 = \int_0^1 \int_0^1 \int_0^1 \left(\frac{6x_2x_3}{6x_2x_3 + 9x_1x_3 + 8x_1x_2} \right) \mathrm{d}x_1 \mathrm{d}x_2 \mathrm{d}x_3 = 0.2763$$
$$\text{RDIM}_2 = \int_0^1 \int_0^1 \int_0^1 \left(\frac{9x_1x_3}{6x_2x_3 + 9x_1x_3 + 8x_1x_2} \right) \mathrm{d}x_1 \mathrm{d}x_2 \mathrm{d}x_3 = 0.3783$$
$$\text{RDIM}_3 = \int_0^1 \int_0^1 \int_0^1 \left(\frac{8x_1x_2}{6x_2x_3 + 9x_1x_3 + 8x_1x_2} \right) \mathrm{d}x_1 \mathrm{d}x_2 \mathrm{d}x_3 = 0.3454.$$

The corresponding numerical values of RDIM for the test case 3 are reported in table (3.3).

Table 3.3: Simulation results of test case 3

	Sample Size $(N)(\times 10^2)$									
	10	20	30	40	50	60	70	80	90	100
RDIM_1	0.2759	0.2763	0.2762	0.2763	0.2763	0.2763	0.2763	0.2763	0.2763	0.2763
RDIM_2	0.3783	0.3784	0.3783	0.3783	0.3783	0.3783	0.3783	0.3783	0.3783	0.3783
RDIM_3	0.3458	0.3453	0.3455	0.3455	0.3454	0.3454	0.3454	0.3454	0.3454	0.3454

Figure (3.4) shows the convergence plots of RDIM_1, RDIM_2 and RDIM_3 across sample sizes for test case 3. The numerical values have good agreements on their corresponding theoretical values. The convergence is obtained at $N = 2000$.

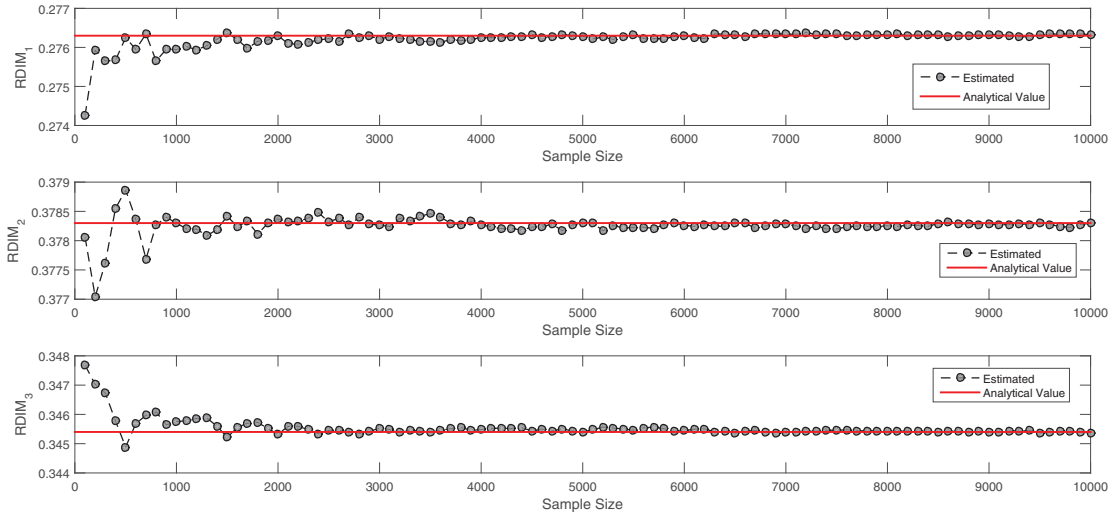


Figure 3.4: Convergence plot of test case 3

Test Case 4

Let us consider the same model in test case 3 but with $X_i \overset{iid}{\sim} exponential(0.8)$.
Under H_1,

$$\text{RDIM}_1 = \int_0^\infty \int_0^\infty \int_0^\infty \left(\frac{6x_2x_3}{6x_2x_3 + 9x_1x_3 + 8x_1x_2}\right)\left(0.8^3 e^{-0.8(x_1+x_2+x_3)}\right) \mathrm{d}x_1\mathrm{d}x_2\mathrm{d}x_3 = 0.282$$

$$\text{RDIM}_2 = \int_0^\infty \int_0^\infty \int_0^\infty \left(\frac{9x_1x_3}{6x_2x_3 + 9x_1x_3 + 8x_1x_2}\right)\left(0.8^3 e^{-0.8(x_1+x_2+x_3)}\right) \mathrm{d}x_1\mathrm{d}x_2\mathrm{d}x_3 = 0.373$$

$$\text{RDIM}_3 = \int_0^\infty \int_0^\infty \int_0^\infty \left(\frac{8x_1x_2}{6x_2x_3 + 9x_1x_3 + 8x_1x_2}\right)\left(0.8^3 e^{-0.8(x_1+x_2+x_3)}\right) \mathrm{d}x_1\mathrm{d}x_2\mathrm{d}x_3 = 0.344.$$

The corresponding numerical values of RDIM for the test case 4 are reported in table (3.4).

Table 3.4: Simulation results of test case 4

	Sample Size $(N)(\times 10^2)$									
	10	20	30	40	50	60	70	80	90	100
RDIM_1	0.2818	0.2823	0.2821	0.2822	0.2823	0.2822	0.2823	0.2823	0.2823	0.28233
RDIM_2	0.3734	0.3733	0.3733	0.3733	0.3733	0.3733	0.3733	0.3733	0.3733	0.3733
RDIM_3	0.3448	0.3444	0.3446	0.3445	0.3444	0.3445	0.3444	0.3445	0.3444	0.3444

The plots in figure (3.5) show that the estimates tend to the corresponding analytical values as the sample size increases.

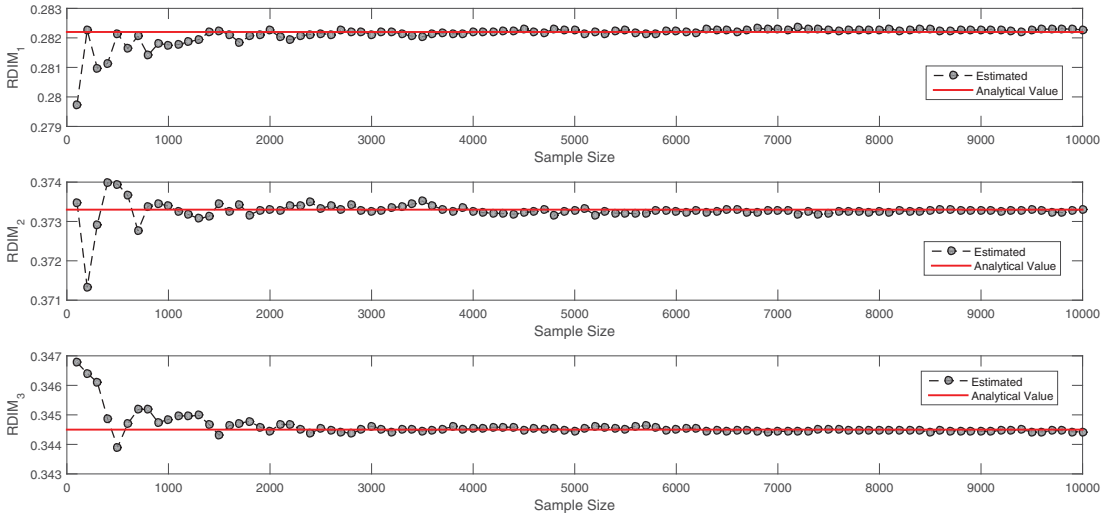


Figure 3.5: Convergence plot of test case 4

Test case 5

Let us consider the same model in test case 3 but with $X_i \overset{iid}{\sim} Beta(2,1)$.
Under H_1,

$$\text{RDIM}_1 = \int_0^1 \int_0^1 \int_0^1 \left(\frac{6x_2x_3}{6x_2x_3 + 9x_1x_3 + 8x_1x_2} \right) 8x_1x_2x_3 \ \mathrm{d}x_1\mathrm{d}x_2\mathrm{d}x_3 = 0.266$$
$$\text{RDIM}_2 = \int_0^1 \int_0^1 \int_0^1 \left(\frac{9x_1x_3}{6x_2x_3 + 9x_1x_3 + 8x_1x_2} \right) 8x_1x_2x_3 \ \mathrm{d}x_1\mathrm{d}x_2\mathrm{d}x_3 = 0.387$$
$$\text{RDIM}_3 = \int_0^1 \int_0^1 \int_0^1 \left(\frac{8x_1x_2}{6x_2x_3 + 9x_1x_3 + 8x_1x_2} \right) 8x_1x_2x_3 \ \mathrm{d}x_1\mathrm{d}x_2\mathrm{d}x_3 = 0.347.$$

The numerical values of RDIM for test case 5 are given in table (3.5). Its corresponding convergence plot is shown in figure (3.6). The numerical values have good agreements on their corresponding theoretical values and also the plots given in figure (3.6) show that the estimates tend to the corresponding analytical values as the sample size increases.

Table 3.5: Simulation results of test case 5

	Sample Size $(N)(\times 10^2)$									
	10	20	30	40	50	60	70	80	90	100
RDIM_1	0.2662	0.2663	0.2662	0.2663	0.2663	0.2663	0.2663	0.2663	0.2663	0.2663
RDIM_2	0.3866	0.3868	0.3866	0.3866	0.3867	0.3867	0.3867	0.3867	0.3867	0.3867
RDIM_3	0.3472	0.3469	0.3471	0.3471	0.3471	0.3471	0.3471	0.3471	0.3471	0.3471

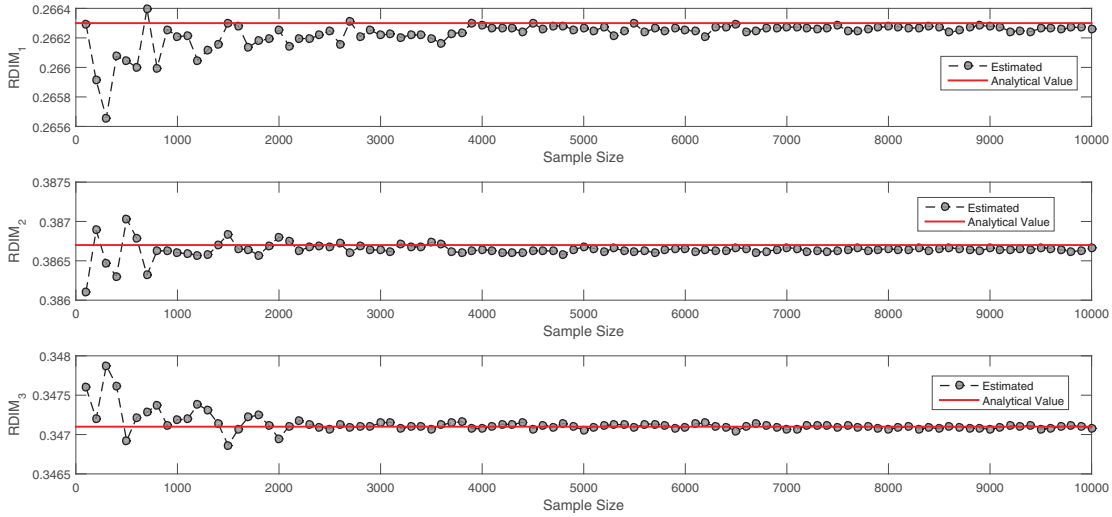


Figure 3.6: Convergence plot of test case 5

Table 3.6: Simulation results of test case 6

	Sample Size $(N)(\times 10^2)$									
	10	20	30	40	50	60	70	80	90	100
RDIM_1	0.2690	0.2740	0.2763	0.2825	0.2778	0.2737	0.2719	0.2737	0.2758	0.2749
RDIM_2	0.3635	0.3785	0.3823	0.3793	0.3790	0.3778	0.3803	0.3794	0.3789	0.3786
RDIM_3	0.3674	0.3476	0.3414	0.3382	0.3432	0.3486	0.3479	0.3470	0.3453	0.3466

So far the model inputs of the test cases we considered were independent. However, the convergence plots had good agreements on their corresponding theoretical values. Next, we consider a test case with correlated model inputs to see the performance of the estimator across sample sizes.

Test case 6

Consider a multiplicative model $Y = X_1^6 X_2^9 X_3^8$, where X_i's are multivariate normal random variables with $\mu = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$ and $\text{Cov}(\boldsymbol{X}) = \begin{bmatrix} 1 & 0.01 & 0.01 \\ 0.01 & 1 & 0.01 \\ 0.01 & 0.01 & 1 \end{bmatrix}$.

The numerical values of RDIM for different sample sizes are reported in table (3.6) and their corresponding plots are given in figure (3.7). The plots show that the estimates tend to the corresponding analytical values as the sample size increases.

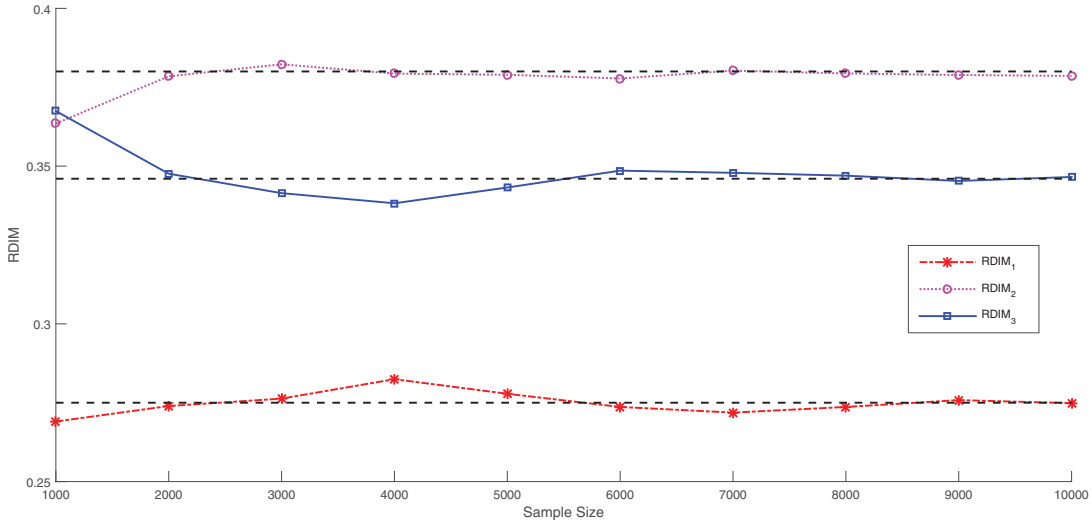


Figure 3.7: Convergence plot of test case 6

Test case 7 - Ishigami function

Let $Y = g(X_1, X_2, X_3) = \sin X_1 + a \sin^2 X_2 + b\, X_3^4 \sin X_1$ with $X_i \overset{iid}{\sim} U(-\pi, \pi)$ generated using Halton sequence.

We compare the performance of RDIM with variance based and Borogonovo's δ method. The results are tabulated in table (3.7). RDIM and δ rank X_2 as the most important model input. On the other hand Sobol' indices rank X_1 as the most important model input.

The convergence plot of RDIM of the Ishigami function is given in figure (3.8). The

Table 3.7: A comparison of global importance measures with RDIM_i for test case 7

Parameter	RDIM_i	δ_i	S_i	$\text{ST}i$
X_1	0.11	0.33	0.39	0.62
X_2	0.73	0.39	0.29	0.34
X_3	0.16	0.28	0.02	0.28

convergence to the theoretical values is obtained at $N = 6000$.

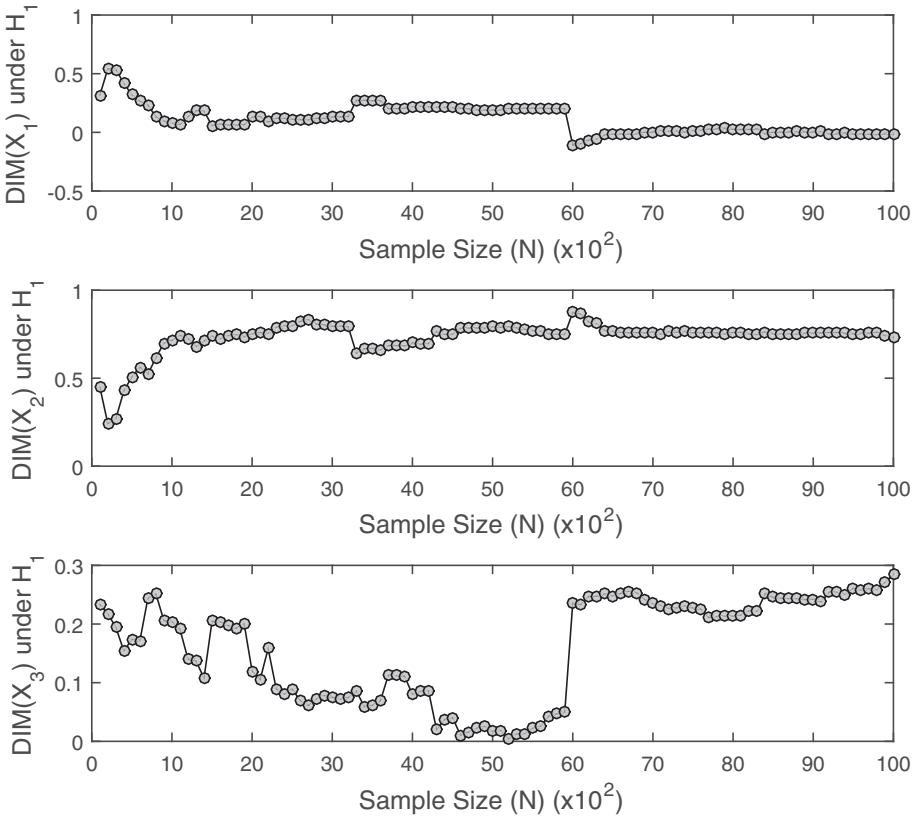


Figure 3.8: Convergence plot of RDIM of test case 7

Test case 8 - A toy model with interactions

Let

$$\begin{aligned} y = {} & 10 + 3 * X_1 + 3 * X_2 + 3 * X_3 + 12 * X_4 + 1.5 * X_1 * X_2 \\ & + 1.5 * X_1 * X_3 + 20 * X_1 * X_4 + 2 * X_2 * X_3 + 10 * X_2 * X_4 \\ & + 10 * X_3 * X_4 + 1.5 * X_1 * X_2 * X_3 + 10 * X_2 * X_3 * X_4 \\ & + 10 * X_1 * X_3 * X_4 + 10 * X_1 * X_2 * X_4 + 5 * X_1 * X_2 * X_3 * X_4 \end{aligned}$$

Table 3.8: Simulation Results of test case 8

	Sample Size $(N)(\times 10^2)$									
	10	20	30	40	50	60	70	80	90	100
RDIM_1	0.2201	0.2202	0.2201	0.2202	0.2202	0.2201	0.2202	0.2202	0.2202	0.2202
RDIM_2	0.1797	0.1795	0.1796	0.1796	0.1796	0.1796	0.1796	0.1796	0.1796	0.1796
RDIM_3	0.1795	0.1795	0.1795	0.1796	0.1796	0.1796	0.1796	0.1796	0.1796	0.1796
RDIM_4	0.4207	0.4208	0.4207	0.4206	0.4207	0.4207	0.4207	0.4206	0.4206	0.4207

with $X_i \overset{iid}{\sim} U(0,1),\ i = 1,2,3,4$ generated using Halton sequence. Then, the partial derivatives are

$$\frac{\partial y}{\partial x_1} = 3 + 1.5x_2 + 1.5x_3 + 20x_4 + 1.5x_2x_3 + 10x_3x_4 + 10x_2x_4 + 5x_2x_3x_4$$
$$\frac{\partial y}{\partial x_2} = 3 + 1.5x_1 + 2x_3 + 10x_4 + 1.5x_1x_3 + 10x_3x_4 + 10x_1x_4 + 5x_1x_3x_4$$
$$\frac{\partial y}{\partial x_3} = 3 + 1.5x_1 + 2x_2 + 10x_4 + 1.5x_1x_2 + 10x_2x_4 + 10x_1x_4 + 5x_1x_2x_4$$
$$\frac{\partial y}{\partial x_4} = 12 + 20x_1 + 10x_2 + 10x_3 + 10x_2x_3 + 10x_1x_3 + 10x_1x_2 + 5x_1x_2x_3$$

The theoretical values of RDIM_j for $j = 1,2,3,4$ for proportional perturbations are reported below. The plots given in figure (3.9) show that the estimates tend to the corresponding analytical values as the sample size increases.

$$\text{RDIM}_1 = \int_0^1 \cdots \int_0^1 \frac{\frac{\partial y}{\partial x_1}x_1}{\sum_{i=1}^4 \frac{\partial y}{\partial x_i}x_i}\ \mathrm{d}x_1 \cdots \mathrm{d}x_4 = 0.22014$$
$$\text{RDIM}_2 = \int_0^1 \cdots \int_0^1 \frac{\frac{\partial y}{\partial x_2}x_2}{\sum_{i=1}^4 \frac{\partial y}{\partial x_i}x_i}\ \mathrm{d}x_1 \cdots \mathrm{d}x_4 = 0.1796$$
$$\text{RDIM}_3 = \int_0^1 \cdots \int_0^1 \frac{\frac{\partial y}{\partial x_3}x_3}{\sum_{i=1}^4 \frac{\partial y}{\partial x_i}x_i}\ \mathrm{d}x_1 \cdots \mathrm{d}x_4 = 0.1796$$
$$\text{RDIM}_4 = \int_0^1 \cdots \int_0^1 \frac{\frac{\partial y}{\partial x_4}x_4}{\sum_{i=1}^4 \frac{\partial y}{\partial x_i}x_i}\ \mathrm{d}x_1 \cdots \mathrm{d}x_4 = 0.42067.$$

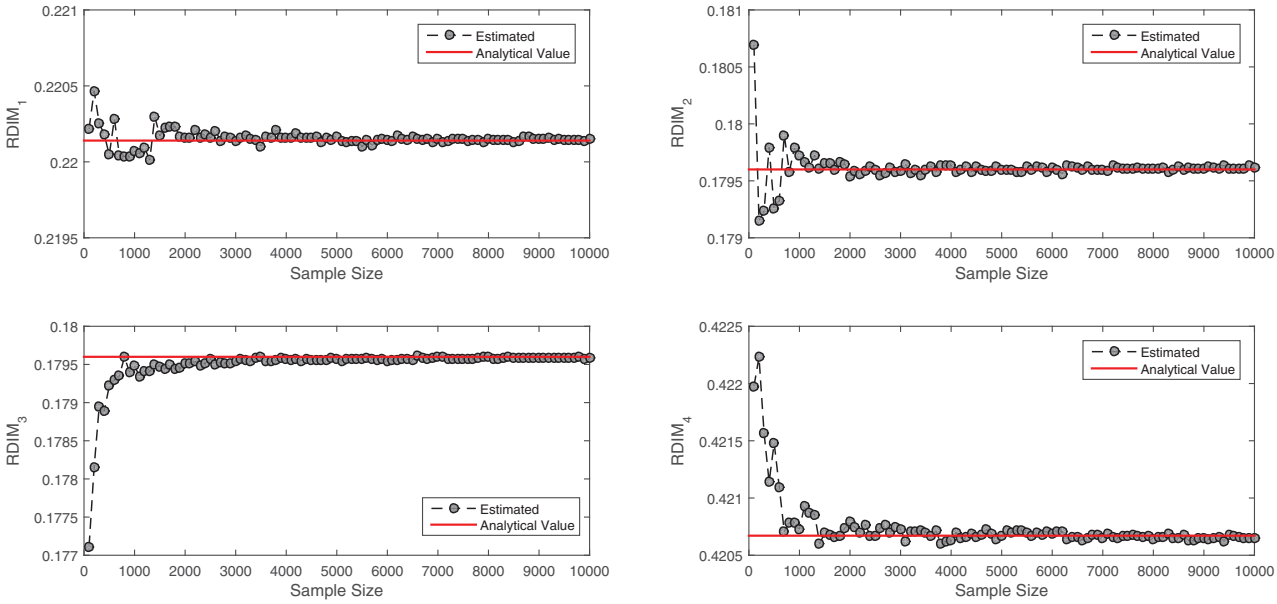


Figure 3.9: Convergence plot of test case 8

3.5.3 Application

The Advanced Test Reactor Large Loss of Coolant Accident Sequence

We apply RDIM to a Probability Safety Assessment (PSA) Model: the large loss of coolant accident (LLOCA) PSA model of the advanced test reactor (ATR) which determines the core damage frequency of a nuclear test reactor located at the Idaho National Laboratories in the USA. The reason for using the model is its previous utilization in global sensitivity studies [Borgonovo et al., 2003].

PSA is an established technique to numerically quantify risk measures in nuclear power plants. It sets out to determine what undesired scenarios can occur, with which likelihood, and what the consequences could be. In addition, it can produce indirect information such as the importance of individual risk contributors. The risk metric of interest in this context is the core damage frequency (CDF).

The first step in a PSA is to identify a top event and trace out the different hazards that could lead to this event. System failures are identified and quantified by system models like Fault Trees (FT) which deduce logical combinations of simpler events. At the lowest level, the Basic Events (BE)(e.g.,cooling pump fails to run, emergency pump fails to start, operator fails to actuate valve) of the fault trees are assigned probability distributions. These probability distributions are propagated up through the tree logic to reach a probability distribution of the top event. Hence, each basic event probability is associated with a parameter [Borgonovo and Apostolakis, 2001]. Note that due to epistemic uncertainty, same parameter can characterize several basic event probabilities and

therefore, the number of parameters are less than the number of basic events. The response of the plant itself to each group of Initiating Events (IE) is usually modelled by the use of Event Trees (ET). They provide sequences that, depending on successes or failures of relevant systems, lead either to a safe or to a core damage state. This methodology is known as the linked fault tree methodology. To summarize, the PSA methodology is a logical, deductive technique which specifies an undesired top event and uses fault trees and event trees to model the various parallel and sequential combinations of failures that might lead to an undesired event (e.g. core damage). The number of failure combinations that might lead to core damage increases exponentially with the number of modelled components. Consequently, effective computer codes and quantification techniques are necessary to solve any large scale problem.

At the parameter level, the risk metric, CDF, becomes a function of 31 distinct parameters [1], the 31^{st} being the initiating event frequency (see also Borgonovo et al. [2003] for details about the ATR model).

$$\text{CDF} = g(x_1, x_2, ..., x_{31}) \tag{3.37}$$

The model in equation (3.37) is non-additive and non-linear. We now perform global sensitivity analysis to this model as the model inputs being the 31 distinct parameters $(x_1, x_2, ..., x_{31})$ and the model output being the CDF. We generated a sample of size $N = 32000$ from a log-normal distribution with mean values being the corresponding point estimate failure probabilities (see Table 1 in page 108 of Borgonovo et al. [2003]) and error factor being 10 according to Borgonovo et al. [2003]. Further, no correlation on the model inputs have been assumed.

The results of the sensitivity analysis at the parameter level are reported in table (3.9). We name the RDIM evaluated under uniform and proportional perturbations as RDIM1_j and RDIM2_j, respectively. In order to rank the parameters according to their importance, we use RDIM2_j since the parameters have different units. The rankings of DIM of Borgonovo and Apostolakis [2001] is also reported in table (3.9). We note that there is a discrepancy between the rankings of the local (DIM)(see Borgonovo et al. [2003] for the points DIM are evaluated for each parameter) and global (RDIM) importance measures as expected. In particular, 12 parameters (marked with "$*$"in table (3.9)) are ranked in the same position by both DIM and RDIM.

Now, let us interpret the results of table (3.9) with the help of the settings discussed in section 4.

Direction of Change. All first-order partial derivatives are positive as shown in the *D*-scatterplots in figures (3.10), (3.11), (3.12) and (3.13) which implies that the model is monotonic increasing. Note that also the signs of RDIM of all parameters are positive

[1] In this application the 31 parameters associated with BE probabilities are the model inputs.

which implies that all parameters have positive impacts on the CDF. That is each positive shift in basic event probability increases the CDF. This result follows from the coherent structure of the system (Borgonovo et al. [2003]).

Factor Prioritization. From table (3.9) and figure (3.14), we note that the most important parameter is the 31^{st} parameter which is the initiating event frequency f_{LLOCA} that is associated with the initiating event: LLOCA. The second most important parameter is x_{19} which is associated with the basic event "level control faults".

Joint Sensitivity. The joint sensitivity is straightforward thanks to the additivity property of RDIM. We note that the relative cumulative sensitivity exceeds 50% for parameters x_{31} and x_{19}. Around 23% of the importance on the parameters is associated with x_{12}, x_{10}, x_{11} and x_5 (see figure (3.14) for the relative cumulative sensitivity).

3.5.4 Comparisons among different sensitivity measures for the ATR model

In this section we are interested to compare the rankings obtained from RDIM of our benchmark model with the rankings obtained from other global sensitivity measures. In this respect, we see that averaging a local measure over the model input space can be considered as a global sensitivity measure.

We first take in to account the comparison of RDIM and DELSA. These methods share the same intuition of randomizing normalized derivative based local sensitivity measures across the model input space. Figure (3.15)(a) shows the box plots of S_{L1} (the local measure used in DELSA) across thousand quasi random sample points of the thirty one parameters on a common scale. The higher the variation of a box plot the higher the significance of the corresponding parameter. For instance, x_{31} is the most important parameter followed by x_{12}, x_{21} and x_{13}. These rankings also agree with the mean values of S_{L1} ; 0.43801 , 0.3539, 0.0937, 0.065 and 0.017 of x_{31}, x_{12}, x_{21} and x_{13}, respectively. The empirical cumulative frequency distribution of S_{L1} of the variability across the model input space shown in figure (3.15) (b) also agrees with the parameter (or model input) rankings. Figure (3.16) shows the scatterplots of DELSA statistic of each parameter plotted against the CDF, the risk metric. Here we make an observation. Apart of unimportant parameters, the plots of most important parameters are scattered more which are in this case x_{31}, x_{12}, x_{21} and x_{13}.

Table 3.9: RDIM and its ranking of ATR model at the parameter level

Parameter (x_i)	RDIM1$_i$	RDIM2$_i$	RDIM1 rankings	RDIM2 rankings	DIM rankings Borgonovo et al. [2003]
x_1	1×10^{-6}	0.009835	29	16*	16*
x_2	0.00065	0.009835	16	16*	16*
x_3	0.00924	0.002191	2	24*	24*
x_4	0.00924	0.03194	2	8	10
x_5	0.00924	0.04108	2	6	7
x_6	4.13×10^{-5}	0.00494	18	21	22
x_7	0.00413	0.00268	13	23	25
x_8	4.13×10^{-5}	0.01155	18	15	20
x_9	4.13×10^{-5}	0.00741	18	20	21
x_{10}	0.00924	0.06964	2	4*	4*
x_{11}	0.00924	0.04705	2	5	6
x_{12}	3.27×10^{-5}	0.07399	21	3*	3*
x_{13}	8.64×10^{-6}	0.01604	27	12	11
x_{14}	3.27×10^{-5}	0.01527	22	13	12
x_{15}	0.00326	0.01519	14	14	13
x_{16}	3.27×10^{-5}	0.00468	23	22	19
x_{17}	0.00296	0.00012	15	28*	28*
x_{18}	1.21×10^{-5}	0.00896	24	19	15
x_{19}	0.00924	0.07973	2	2*	2*
x_{20}	0.00034	0.02119	17	10	9
x_{21}	1.20×10^{-5}	0.02938	25	9	5
x_{22}	1.20×10^{-5}	0.00168	26	25	23
x_{23}	0.00924	0.01918	2	11	14
x_{24}	0.00924	0.00978	2	18*	18*
x_{25}	0.00924	0.03514	2	7	8
x_{26}	8.45×10^{-6}	3.5932×10^{-6}	28	29*	29*
x_{27}	0.00924	0.00072	2	27*	27*
x_{28}	0.00924	0.00097	2	26	26
x_{29}	2.29×10^{-8}	1.7882×10^{-6}	30	31	30
x_{30}	2.29×10^{-8}	1.8050×10^{-6}	30	30*	30*
x_{31}	0.88	0.42982	1	1*	1*

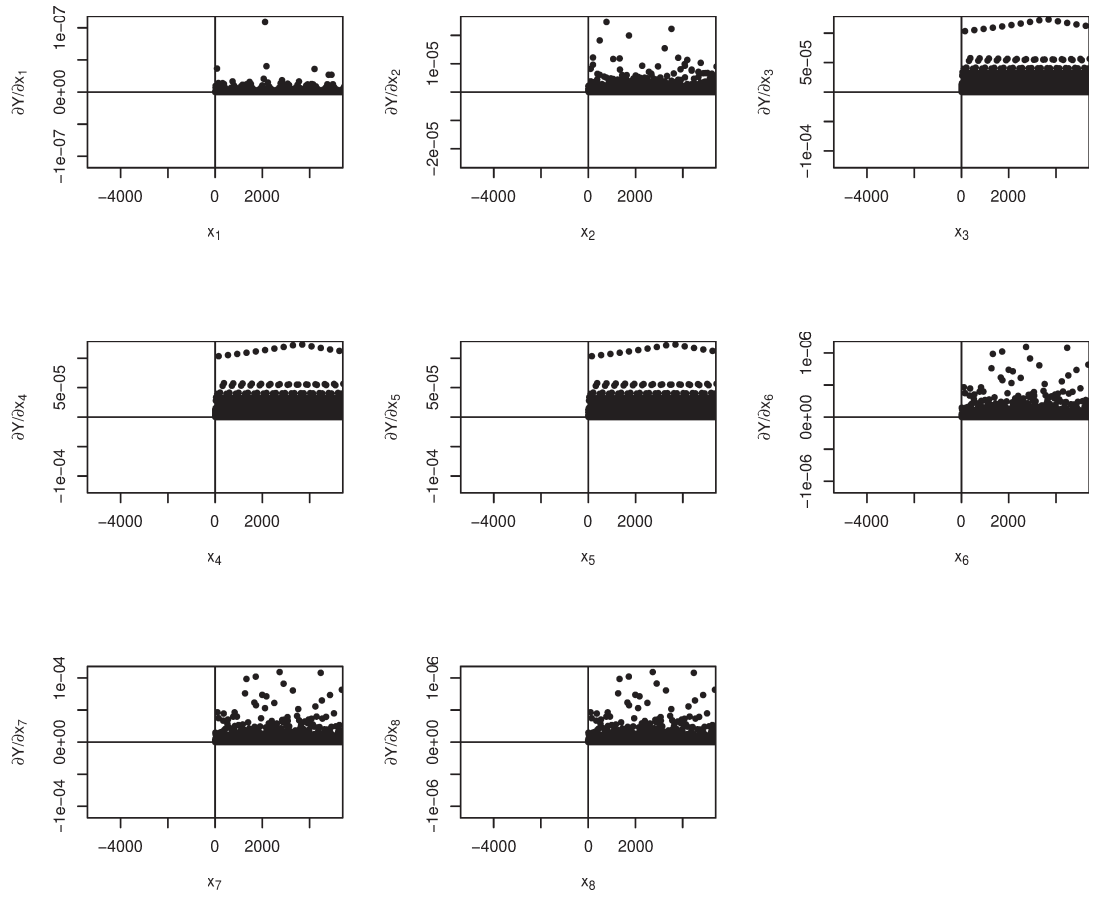


Figure 3.10: D-plots of parameters $x_1 - x_8$

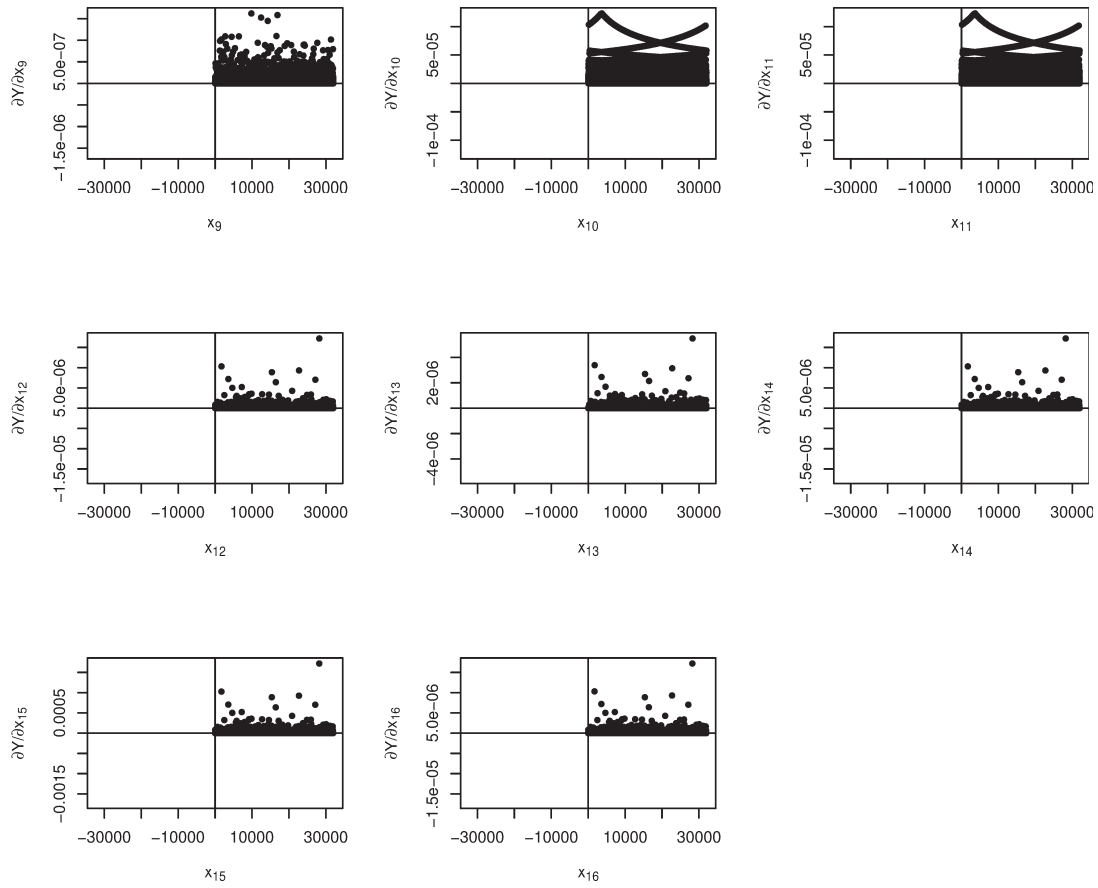


Figure 3.11: D-plots of parameters $x_9 - x_{16}$

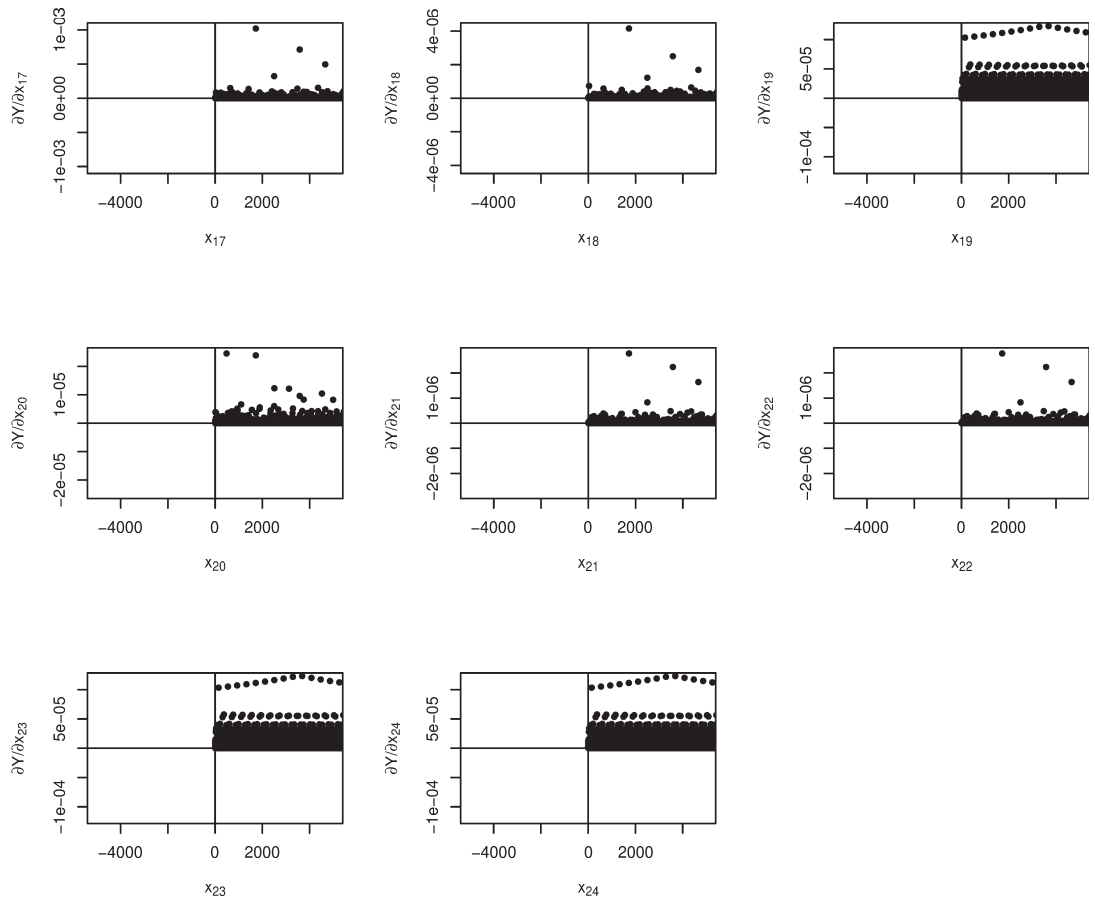


Figure 3.12: D-plots of parameters $x_{17} - x_{24}$

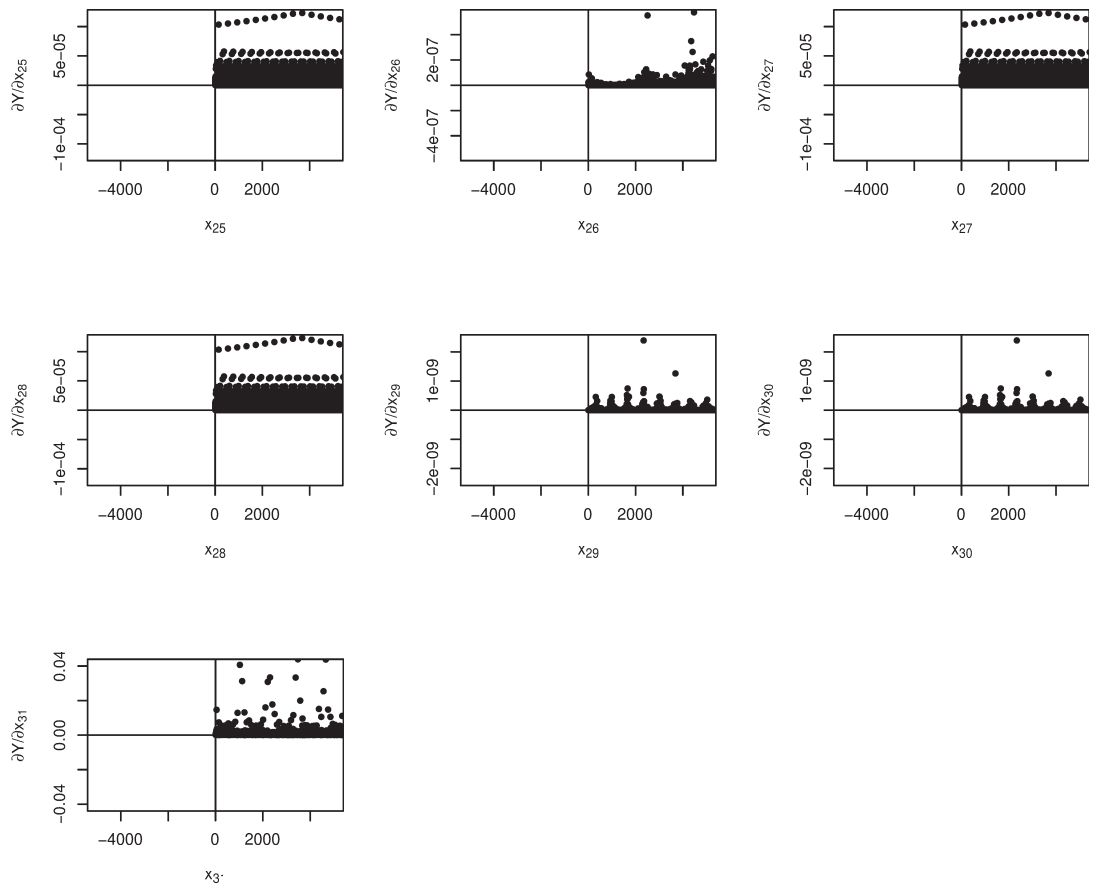


Figure 3.13: D-plots of parameters $x_{25} - x_{31}$

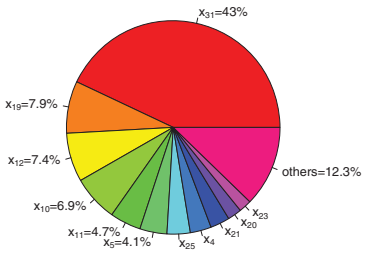
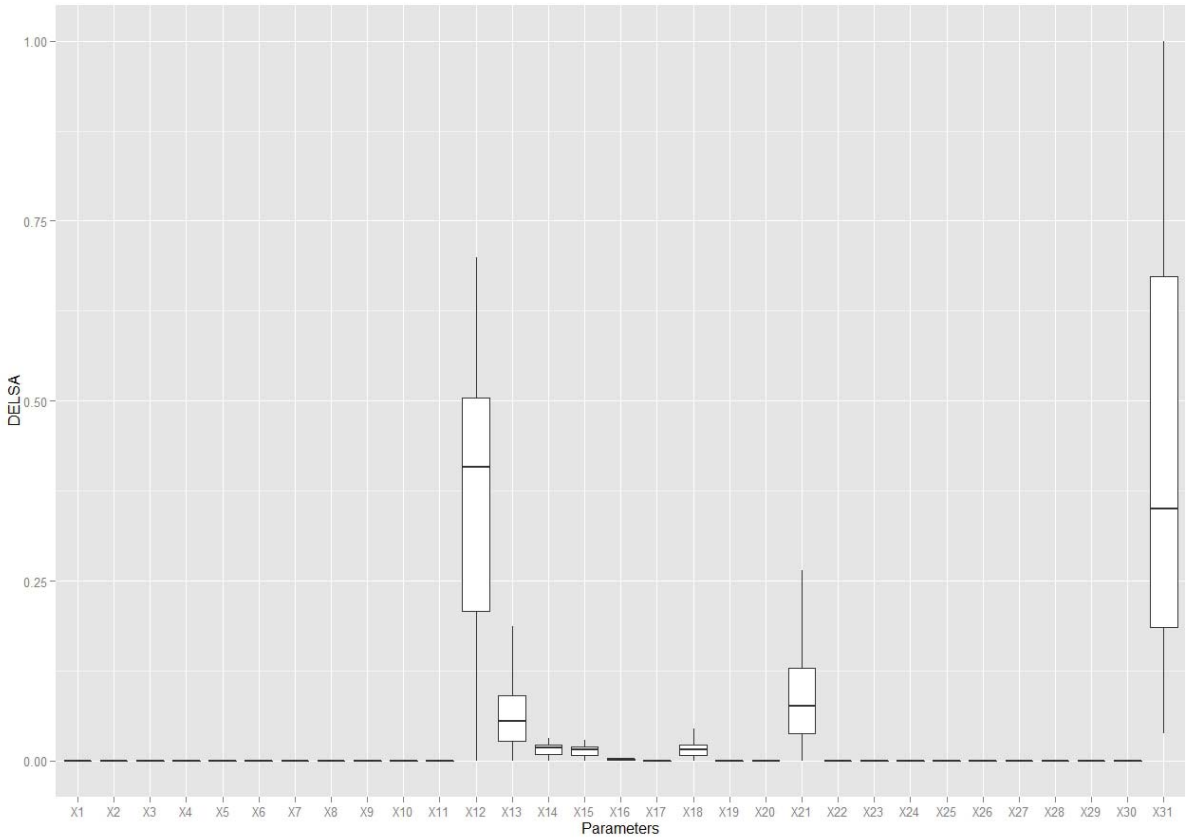
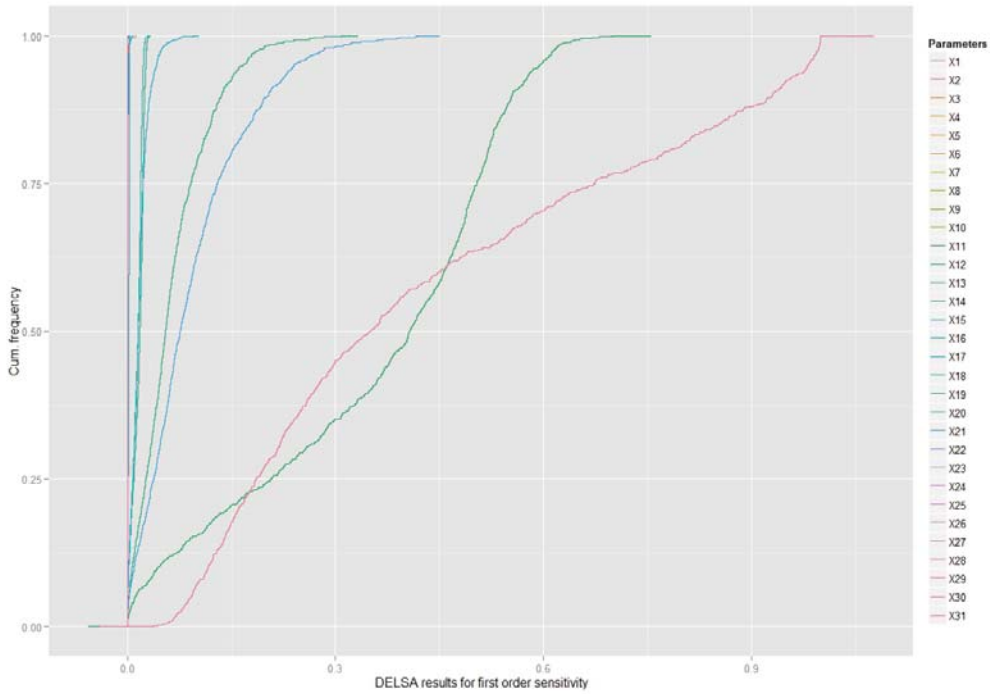


Figure 3.14: Relative importance with respect to RDIM2 of ATR model at parameter level



(a) DELSA for parameters of ATR Model



(b) Cumulative frequency distribution of S_{L1} of the variability across the parameter space using DELSA method

Figure 3.15: Distribution of S_{L1} of DELSA

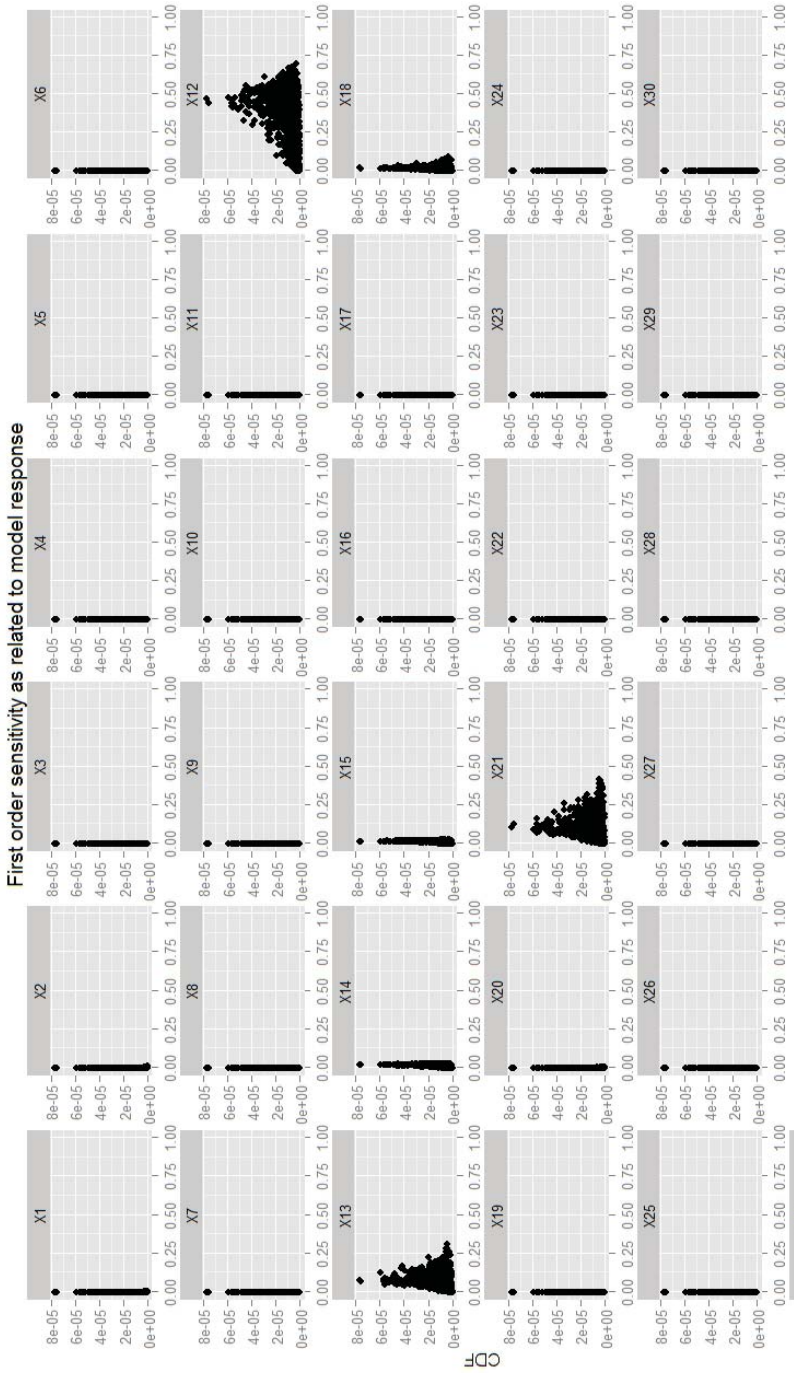


Figure 3.16: Scatter plots of S^j_{L1} of DELSA, related to CDF of ATR model for $N = 1000$.

Figures (3.17), (3.18) and (3.19) show the box plots of the distribution of the local measures (DIM and S_{L1}) used in the both methods, RDIM and DELSA of parameters of the ATR model. The parameter, f_{LLOCA} being the 31^{st} has been detected as the most influential parameter by both methods. The results show an overall agreement with DELSA and RDIM in identification in most important model inputs. For these model inputs we note a lower variability in the estimates of RDIM method with respect to estimates of DELSA method. However, if we consider model inputs with intermediate importance we note that some model inputs that are identified as having an impact by RDIM are not identified by DELSA. We believe that this is due to the fact that DELSA assumes a linearisation of the input-output mapping which is not implied by RDIM. Moreover, we compare other global sensitivity indices discussed in chapter 2, namely DGSM (Υ_i), β_i^{KS}, δ_i, β_i^{Ku} and S_i. The results are given in table (3.10). The f_{LLOCA} is ranked in the first position by all methods. We notice that DELSA and Sobol first index do not detect x_{19} as important while other methods detect x_{19} as important. However, overall the rankings of all methods have good agreements.

3.6 Summary

In summary, we have proposed a new bridge between local and global sensitivity analyses in this chapter. We showed that this new bridge, RDIM, helps the decision maker to identify importance of different input variables without imposing many assumptions, for example, the independence assumption among model inputs. Moreover, the proposed method can also be used with mixture probability density function for the model input vector $\boldsymbol{X}$, given the model is differentiable. With the proposed measure, we showed that one can evaluate the joint sensitivity of any subsets of the model inputs in a single simulation run which computationally efficient.

For the accuracy of RDIM, we have also proved the convergence rate to see how RDIM works for different sample sizes in terms of its estimation. Beside this, to show the effectiveness of RDIM, we compared with some global sensitivity indices already introduced in the literature such as transformation invariant global sensitivity statistics, DGSM and DELSA. DELSA has particularly been compared because both methods follow the same intuition of distributing a local sensitivity measure across the model input space. It is important to mention that our proposed method can only be implemented given the model is differentiable or if the derivatives exist. Therefore, future work is needed to develop a bridge that can apply when the model is not differentiable.

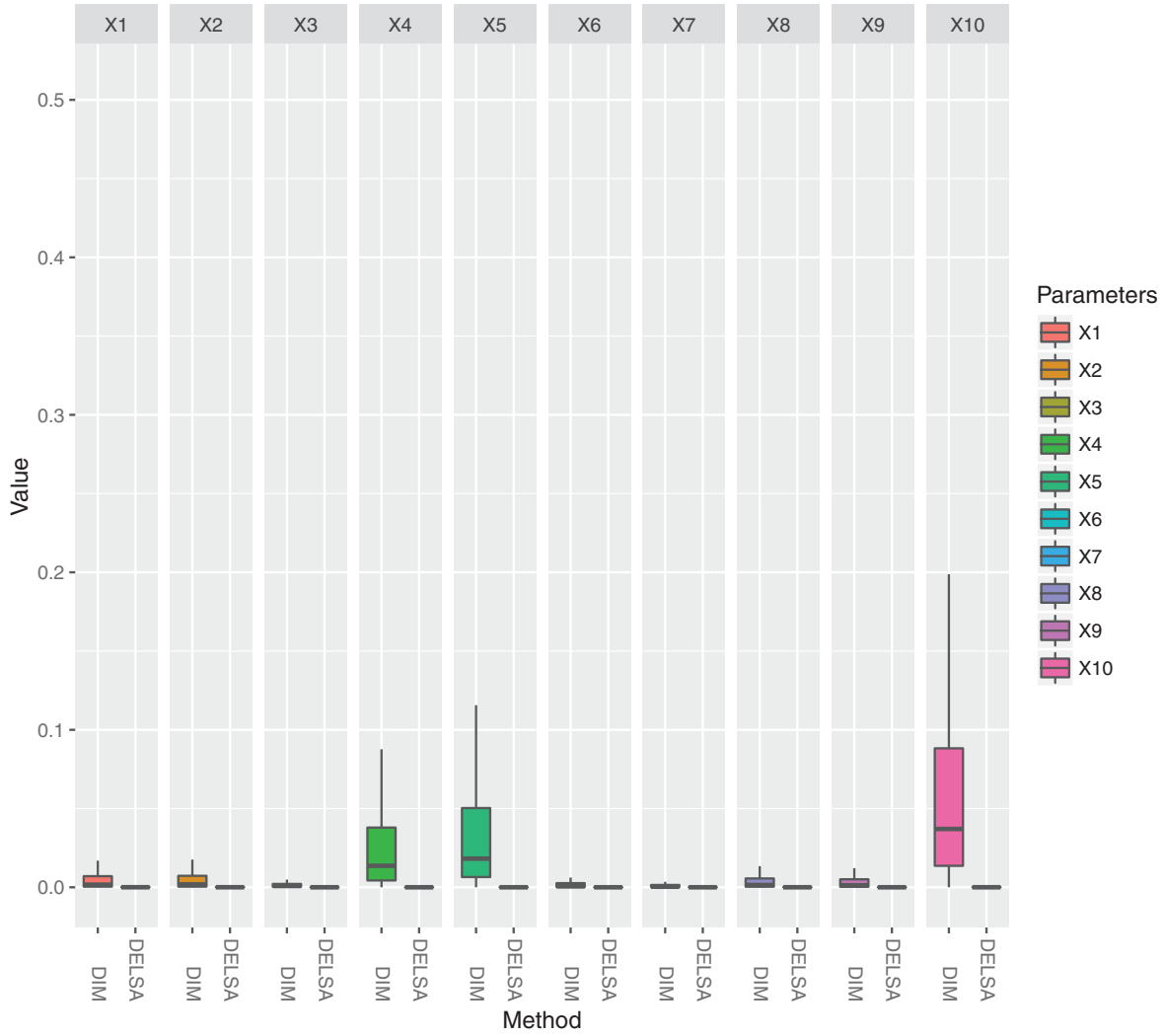


Figure 3.17: Comparison of the distribution of DIM and S_{L1} for ATR model

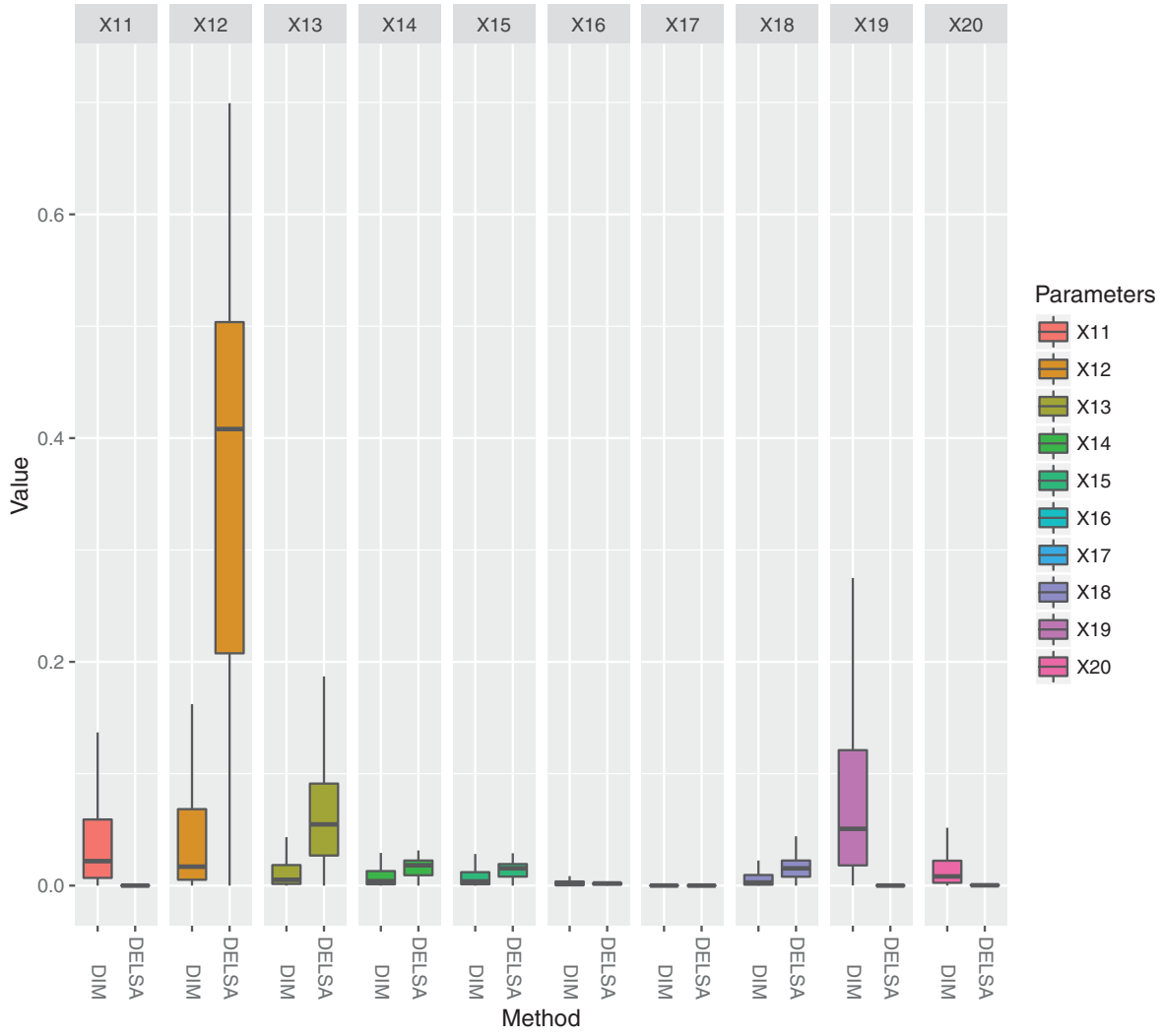


Figure 3.18: Comparison of the distribution of DIM and S_{L1} for ATR model

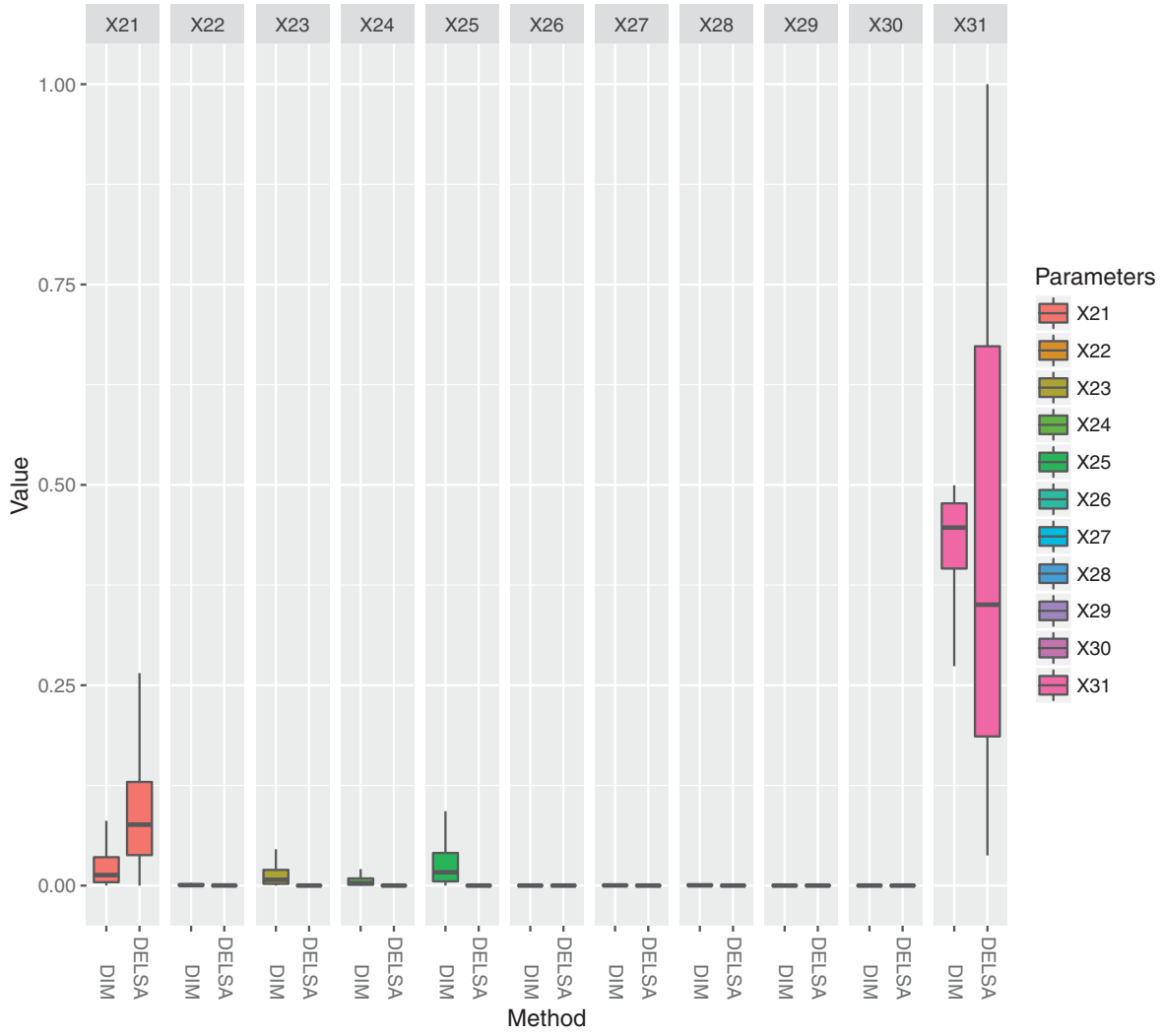


Figure 3.19: Comparison of the distribution of DIM and S_{L1} for ATR model

Table 3.10: Comparisons among different sensitivity measures for ATR model parameters

Parameter	RDIM	DELSA	Υ_i	β_i^{KS}	δ_i	β_i^{Ku}	S_i
x_1	0.00983(16)	0.00019 (11)	15	0.0206(24)	0.01692(29)	0.03024(25)	0.00104(13)
x_2	0.00984(16)	0.0002(10)	17	0.0237(18)	0.03091(15)	0.03237(18)	0.00112(11)
x_3	0.00219(24)	1.9×10^{-8}(26)	25	0.02479(14)	0.02696(17)	0.03175(19)	**0.00368(3)**
x_4	0.03194(8)	6.182×10^{-6}(21)	14	0.03315(9)	0.03535(12)	0.03912(10)	0.00058(25)
x_5	0.04108(6)	0.00001(18)	12	0.03716(6)	0.04119(7)	0.04159(9)	0.0013(9)
x_6	0.00494(21)	0.00001(19)	23	0.02159(22)	0.02628(19)	0.03343(17)	0.00059(24)
x_7	0.00268(23)	3.828×10^{-6}(22)	24	0.01554(31)	0.00912(31)	0.02642(31)	0.00057(26)
x_8	0.01155(15)	0.00004(14)	21	0.02109(23)	0.02058(24)	0.03102(21)	0.00052(30)
x_9	0.00741(20)	0.00002(16)	22	0.01940(26)	0.02004(25)	0.0309(23)	0.00157(7)
x_{10}	0.06964(4)	0.00004(15)	6	0.05628(4)	0.05780(4)	0.05914(4)	0.00231(4)
x_{11}	0.04705(5)	0.00002(17)	10	0.04041(5)	0.04173(6)	0.04352(8)	0.00072(17)
x_{12}	**0.07399(3)**	**0.3539(2)**	**2**	**0.06812(2)**	**0.07224(2)**	**0.07211(2)**	**0.06044(2)**
x_{13}	0.01604(12)	0.06510(4)	4	0.02267(19)	0.02553(21)	0.02885(28)	0.00121(10)
x_{14}	0.01527(13)	0.01578(6)	7	0.025 (13)	0.03341(13)	0.035263(14)	0.002(5)
x_{15}	0.01519(14)	0.01358(7)	8	0.02435 (16)	0.02979(16)	0.03427(15)	0.00105(12)
x_{16}	0.00468(22)	0.00167(8)	16	0.0201(25)	0.02106(23)	0.02959(26)	0.00069(19)
x_{17}	0.00012(28)	1.352×10^{-6}(24)	27	0.01733(29)	0.01399(30)	0.02955(27)	0.00062(22)
x_{18}	0.00896(19)	0.01697(5)	9	0.02218 (20)	0.02474(22)	0.03411(16)	0.00060(23)
x_{19}	**0.07973(2)**	0.00006(13)	5	**0.06440(3)**	**0.06665(3)**	**0.06733(3)**	0.0018(6)
x_{20}	0.02119(10)	0.00051(9)	11	0.02640(12)	0.02587(20)	0.03158(20)	0.00054(29)
x_{21}	0.02938(9)	**0.0937(3)**	**3**	0.03383(7)	0.0389(10)	0.03731(12)	0.000961(15)
x_{22}	0.00168(25)	0.00016(12)	19	0.01668(7)	0.01745(28)	0.02847(29)	0.00154(8)
x_{23}	0.01918(11)	1.76×10^{-6}(23)	18	0.02382(17)	0.02689(18)	0.03098(22)	0.00068(20)
x_{24}	0.00978(18)	4.285×10^{-7}(25)	20	0.01893(27)	0.01869(27)	0.02808(30)	0.00099(14)
x_{25}	0.03514(7)	7.514×10^{-6}(20)	13	0.03371 (8)	0.03717(11)	0.03806(11)	0.00056(28)
x_{26}	3.59×10^{-6}(29)	1.33×10^{-6}(29)	29	0.03242(10)	0.05024(5)	0.04968(5)	0.00057(27)
x_{27}	0.00072(27)	1.924×10^{-9}(28)	28	0.01869(28)	0.01881(26)	0.03089(24)	0.00042(31)
x_{28}	0.00097(26)	3.582×10^{-9}(27)	26	0.02781 (11)	0.04040(9)	0.04361(7)	0.00069(18)
x_{29}	1.7882×10^{-6}(31)	3.66×10^{-12}(31)	31	0.02159(21)	0.03234(14)	0.03622(13)	0.00081(16)
x_{30}	1.8050×10^{-6}(30)	3.790×10^{-12}(30)	30	0.02436(15)	0.0408(8)	0.04383(6)	0.00067(21)
x_{31}	**0.42982(1)**	**0.4380(1)**	**1**	**0.45534(1)**	**0.51862(1)**	**0.51677(1)**	**0.06720(1)**

Chapter 4

Stochastic Differential Importance Measure

This chapter proposes a differential sensitivity measure in the case the quantity of interest is the expected value of the model output. After the formal definition of the sensitivity measure, an extension of the score function method is proposed for the estimation of the newly defined sensitivity measure.

4.1 Motivation

In the previous chapter we dealt with deterministic models in which, once observed $\boldsymbol{X}$, the value of the model output is unique. In this chapter we deal with the case in which $\boldsymbol{X}$ is not observable, but instead its distributional parameters are available. This is due to the assumption that a probability distribution, $f(\boldsymbol{x};\boldsymbol{\theta})$ of $\boldsymbol{X}$ is known. We refer to Saltelli and Tarantola [2002c] for further details about having these distributions available. Given the probability distribution of $\boldsymbol{X}$, we formally write $\boldsymbol{X}|\boldsymbol{\theta} \sim f(\boldsymbol{x};\boldsymbol{\theta})$. So given $\boldsymbol{X} = \boldsymbol{x}$, $y = g(\boldsymbol{x})$ is known, but since $\boldsymbol{X}$ is not observable, Y is random with a distribution induced by $f(\cdot;\boldsymbol{\theta})$. Thus, the model response is stochastic when considered as a function of θ [Chick, 2001].

That is, given a fixed $\boldsymbol{\theta}$, we do not obtain a deterministic value of Y, but obtain a distribution. As Chick [2001] points out, in these situations the decision maker is often interested in the expected value of the model output, $\mathbb{E}_{\boldsymbol{\theta}}[g(\boldsymbol{X})]$, which becomes the quantity of interest and we are interested in evaluating the sensitivity of the expectation of $Y = g(\boldsymbol{X})$ with respect to model input distributional parameters. Usually, $\mathbb{E}_{\boldsymbol{\theta}}[g(\boldsymbol{X})]$ is called the performance measure of a stochastic system and it is always a function of $\boldsymbol{\theta}$, $l(\boldsymbol{\theta})$ (denoting the function as l).

Formally, $\mathbb{E}_{\boldsymbol{\theta}}[g(\boldsymbol{X})]$ is the expected output of the stochastic model whose value is

dependent on a simulation parameter vector $\boldsymbol{\theta}$ such that

$$l(\boldsymbol{\theta}) = \mathbb{E}_{\boldsymbol{\theta}}[g(\boldsymbol{X})] \tag{4.1}$$
$$l(\boldsymbol{\theta}) = \int \cdots \int g(\boldsymbol{x}) f(\boldsymbol{x}; \boldsymbol{\theta}) \, \mathrm{d}\boldsymbol{x}$$

where $g(\cdot)$ is a deterministic model for which the analytical expression is either unknown or very complicated, so one has to resort to Monte Carlo simulation. For example consider discrete event simulation systems such as a queuing system with service rate (μ) and arrival rate (λ). Then, μ and λ are the distributional parameters ($\boldsymbol{\theta} = (\mu, \lambda)$) of the mean waiting time, which is defined by the expected value of $Y = g(\boldsymbol{X})$. In such situations, our goal is to find the sensitivity of the mean waiting time to the arrival and service rates.

To assess the sensitivity, we propose the *stochastic differential importance measure (SDIM)*. SDIM indicates how sensitive $\mathbb{E}_{\boldsymbol{\theta}}[g(\boldsymbol{X})]$ is to small changes in the distributional parameters $\boldsymbol{\theta}$, and can thus be used to identify the most significant components of $\boldsymbol{\theta}$. We believe that SDIM provides guidance for design and operational decisions and plays an important role in selecting system parameters that optimize certain performance measures. Moreover, it allows the quantification of the relative contribution of a component or a group of components on the mean of the output when changes occur simultaneously in several parameters' values in the system.

To estimate SDIM we propose an estimator based on the likelihood ratio method (LRM) also known as the score function method. LRM has been widely used to estimate derivatives of the expectation of a random variable through simulations (Glasserman and Liu [2007]; Rubinstein and Shapiro [1993]). It provides an alternative approach to derivative estimation and does not require the differentiability of $g(\boldsymbol{X})$. The LRM estimator of SDIM is easy to use when the density $f(\boldsymbol{x}; \boldsymbol{\theta})$ and its derivatives are readily available especially in global sensitivity analysis where the model input distribution is known in advance most of the time. The LRM does not require any smoothness in the performance measure since it is based on the differentiation of probability densities. In the next subsection we formalize the definition of SDIM.

4.1.1 Definition of SDIM

We start with a particular point, say $\boldsymbol{\theta}^0 = (\theta_1^0, \cdots, \theta_j^0, \cdots, \theta_m^0)$ in the model input distributional parameter space, $\Theta \subseteq \mathbb{R}^m$ and consider the value assumed by the performance measure $\mathbb{E}_{\boldsymbol{\theta}}[g(\boldsymbol{X})]$ (which is a function of $\boldsymbol{\theta}$ and $Y = g(\boldsymbol{X})$) when the parameters are fixed at this point. Assuming the availability of partial derivatives of $\mathbb{E}_{\boldsymbol{\theta}}[g(\boldsymbol{X})]$ with respect to $\boldsymbol{\theta} = (\theta_1, ..., \theta_m)$, one can compute any derivative based sensitivity measure of the model output mean. For example, when DIM is of interest, we define DIM of the θ_j^{th}

distributional parameter at $\boldsymbol{\theta}^0$ as SDIM_{θ_j}

$$\text{SDIM}_{\theta_j}(\boldsymbol{\theta}^0) = \frac{\left.\frac{\partial \mathbb{E}_{\boldsymbol{\theta}}[g(\boldsymbol{X})]}{\partial \theta_j}\right|_{\boldsymbol{\theta}^0} \mathrm{d}\theta_j}{\sum_{i=1}^{m} \left.\frac{\partial \mathbb{E}_{\boldsymbol{\theta}}[g(\boldsymbol{X})]}{\partial \theta_i}\right|_{\boldsymbol{\theta}^0} \mathrm{d}\theta_i}. \tag{4.2}$$

The change in $\mathbb{E}_{\boldsymbol{\theta}}[g(\boldsymbol{X})]$ depends on how input distributional parameters are varied and this is reflected by the value of SDIM. As we explained in Chapter 3, SDIM can also be defined in the following two particular cases:

H_1 : Uniform perturbations: $\mathrm{d}\theta_i = \mathrm{d}\theta_j \ \forall \ i, j$

$$\text{SDIM}_{\theta_j}(\boldsymbol{\theta}^0) = \frac{\left.\frac{\partial \mathbb{E}_{\boldsymbol{\theta}}[g(\boldsymbol{X})]}{\partial \theta_j}\right|_{\boldsymbol{\theta}^0}}{\sum_{i=1}^{m} \left.\frac{\partial \mathbb{E}_{\boldsymbol{\theta}}[g(\boldsymbol{X})]}{\partial \theta_i}\right|_{\boldsymbol{\theta}^0}}. \tag{4.3}$$

H_2 : Proportional perturbations: $\dfrac{\mathrm{d}\theta_i}{\theta_i^0} = \dfrac{\mathrm{d}\theta_j}{\theta_j^0} \ \forall \ i, j$

$$\text{SDIM}_{\theta_j}(\boldsymbol{\theta}^0) = \frac{\left.\frac{\partial \mathbb{E}_{\boldsymbol{\theta}}[g(\boldsymbol{X})]}{\partial \theta_j}\right|_{\boldsymbol{\theta}^0} \theta_j^0}{\sum_{i=1}^{m} \left.\frac{\partial \mathbb{E}_{\boldsymbol{\theta}}[g(\boldsymbol{X})]}{\partial \theta_i}\right|_{\boldsymbol{\theta}^0} \theta_i^0}. \tag{4.4}$$

The condition under which one should apply H_1 or H_2 depends on the model and the problem at hand. For instance, SDIM_{θ_j}s are not comparable under H_1 when the input distributional parameters have different units, instead H_2 is recommended. Moreover, SDIM posses the additivity property. We present the following example to give a clear idea to the readers about the definition of SDIM.

Example: Suppose the model of interest is given by $Y = X_1^2 + X_2^2 + X_3^2$, where $X_i \sim exp(\theta_i)$, that is, $\boldsymbol{\theta} = (\theta_1, \theta_2, \theta_3)$. Then the expectation of Y is

$$l(\boldsymbol{\theta}) = \mathbb{E}_{\boldsymbol{\theta}}[g(\boldsymbol{X})] = \frac{2}{\theta_1^2} + \frac{2}{\theta_2^2} + \frac{2}{\theta_3^2}$$

which is a function of $\boldsymbol{\theta}$. The corresponding partial derivatives are $\dfrac{\partial \mathbb{E}_{\boldsymbol{\theta}}[g(\boldsymbol{X})]}{\partial \theta_j} = \dfrac{-4}{\theta_j^3}$ for $j = 1, 2, 3$. Let us write the explicit expressions of SDIM at $\boldsymbol{\theta}^0 = (\theta_1^0, \theta_2^0, \theta_3^0)$ for both H_1

and H_2 as

$$\text{SDIM}_{\theta_j}(\boldsymbol{\theta}^0) = \frac{\frac{1}{(\theta_j^0)^3}}{\sum_{i=1}^{3}\frac{1}{(\theta_i{}^0)^3}} \qquad \text{(Uniform perturbations)}$$

$$\text{SDIM}_{\theta_j}(\boldsymbol{\theta}^0) = \frac{\frac{1}{(\theta_j^0)^2}}{\sum_{i=1}^{3}\frac{1}{(\theta_i^0)^2}} \qquad \text{(Proportional perturbations)}$$

In the above example, we have considered a very simple model where the partial derivatives were available in explicit form. However in a practical situation the model is usually either very complex or intractable and we have a simulation code instead of a tractable expression., e.g., queuing and reliability models. In such situations, the partial derivatives are obtained numerically and therefore, we propose estimating SDIM by exploiting the partial derivatives obtained via LRM.

The following subsection introduces some preliminaries along with the method of likelihood ratio to estimate the gradients and SDIM of the performance measure with respect to the distributional parameter vector, $\boldsymbol{\theta}$.

4.1.2 Estimation of SDIM

An important requirement for gradient estimation using LRM is the interchange between differentiation and integration. The following theorem provides sufficient conditions for such interchange.

Theorem 4.1.1. *(Interchanging Differentiation and Integration see e.g. Rubinstein and Shapiro [1993]) Let the function $h(\boldsymbol{x};\boldsymbol{\theta})$ be differentiable at $\boldsymbol{\theta}^0 \in \mathbb{R}^m$. Denote the corresponding gradient by $\nabla_{\boldsymbol{\theta}} h(\boldsymbol{x};\boldsymbol{\theta}^0)$. We assume that as a function of $\boldsymbol{x}$ this gradient is integrable. If there exists a neighbourhood Θ of $\boldsymbol{\theta}^0$ and an integral function $M(\boldsymbol{x};\boldsymbol{\theta}^0)$ such that for all $\boldsymbol{\theta} \in \Theta$*

$$\frac{\left|h(\boldsymbol{x};\boldsymbol{\theta}) - h(\boldsymbol{x};\boldsymbol{\theta}^0)\right|}{\|\boldsymbol{\theta} - \boldsymbol{\theta}^0\|} \leq M(\boldsymbol{x};\boldsymbol{\theta}^0) \tag{4.5}$$

then

$$\nabla_{\boldsymbol{\theta}} \int h(\boldsymbol{x};\boldsymbol{\theta})\mathrm{d}\boldsymbol{x}\Big|_{\boldsymbol{\theta}=\boldsymbol{\theta}^0} = \int \nabla_{\boldsymbol{\theta}} h(\boldsymbol{x};\boldsymbol{\theta}^0)\mathrm{d}\boldsymbol{x} \tag{4.6}$$

A special case where differentiation and integration can be interchanged arises in the theory of exponential families that can be summarized by the following theorem.

Theorem 4.1.2. *(Interchange in Exponential Families, see e.g. Rubinstein and Shapiro*

[1993]) For any function ϕ for which

$$\int \phi(\boldsymbol{x}) e^{\boldsymbol{\eta}^T \boldsymbol{t}(\boldsymbol{x})} \mathrm{d}\boldsymbol{x} < \infty,$$

the integral as a function of $\boldsymbol{\eta}$ has partial derivatives of all orders, for all $\boldsymbol{\eta}$ in the interior of the natural parameter space. Moreover, these derivatives can be obtained by differentiating under the integral sign. That is,

$$\nabla_{\boldsymbol{\eta}} \int \phi(\boldsymbol{x}) e^{\boldsymbol{\eta}^T \boldsymbol{t}(\boldsymbol{x})} \mathrm{d}\boldsymbol{x} = \int \phi(\boldsymbol{x}) t(\boldsymbol{x}) e^{\boldsymbol{\eta}^T \boldsymbol{t}(\boldsymbol{x})} \mathrm{d}\boldsymbol{x}$$

Now, we explain the main idea of the LRM for gradient estimation [Rubinstein, 1989]. The goal of the LRM is to estimate the gradients of $l(\boldsymbol{\theta})$ with respect to the distributional parameter vector $\boldsymbol{\theta}$ of the performance measure $l(\boldsymbol{\theta})$.

Consider the case where $\boldsymbol{\theta}$ is a scalar (denoted by θ instead of $\boldsymbol{\theta}$) and assume that the parameter set Θ is an open interval on the real line. Furthermore, suppose that for all $\boldsymbol{x}$ the probability density function $f(\boldsymbol{x}; \theta)$ is continuously differentiable in θ and that there exists an integrable function $k(\boldsymbol{x})$ such that

$$\left| g(\boldsymbol{x}) \frac{\mathrm{d}\, f(\boldsymbol{x}; \theta)}{\mathrm{d}\theta} \right| \leq k(\boldsymbol{x}) \tag{4.7}$$

for all $\theta \in \Theta$.

Following theorem (4.1.1), the differentiation and integration are interchangeable, so that differentiation of $\mathbb{E}_{\boldsymbol{\theta}}[g(\boldsymbol{X})]$ yields

$$\begin{aligned} \frac{\mathrm{d}\mathbb{E}_{\boldsymbol{\theta}}[g(\boldsymbol{X})]}{\mathrm{d}\theta} =& \frac{\mathrm{d}}{\mathrm{d}\theta} \int g(\boldsymbol{x}) f(\boldsymbol{x}; \theta) \mathrm{d}\boldsymbol{x} = \int g(\boldsymbol{x}) \frac{\mathrm{d} f(\boldsymbol{x}; \theta)}{\mathrm{d}\theta} \mathrm{d}\boldsymbol{x} \\ =& \int g(\boldsymbol{x}) \frac{\mathrm{d} f(\boldsymbol{x}; \theta)}{\mathrm{d}\theta} \frac{f(\boldsymbol{x}; \theta)}{f(\boldsymbol{x}; \theta)} \mathrm{d}\boldsymbol{x} \\ =& \int g(\boldsymbol{x}) \frac{\mathrm{d}\ \ln f(\boldsymbol{x}; \theta)}{\mathrm{d}\theta} f(\boldsymbol{x}; \theta) \mathrm{d}\boldsymbol{x} = \mathbb{E}\left[g(\boldsymbol{X}) \frac{\mathrm{d}\ln f(\boldsymbol{X}; \theta)}{\mathrm{d}\theta} \right] \\ =& \mathbb{E}\left[g(\boldsymbol{X}) \mathcal{S}(\theta; \boldsymbol{X}) \right] \end{aligned} \tag{4.8}$$

where

$$\mathcal{S}(\theta; \boldsymbol{x}) = \frac{\mathrm{d} \ln f(\boldsymbol{x}; \theta)}{\mathrm{d}\theta} \tag{4.9}$$

is the score function (SF) that is viewed as a function of θ for a given $\boldsymbol{x}$. Similar arguments

Table 4.1: Score functions for commmonly used distributions

Distribution	$f(x;\boldsymbol{\theta})$	$\mathcal{S}(\boldsymbol{\theta};x)$
Bin(n,p)	$\binom{n}{x}p^x(1-p)^{n-x}$	$\frac{x-np}{p(1-p)}$
Poi(λ)	$\frac{\lambda^x e^{-\lambda}}{x!}$	$\frac{x}{\lambda}-1$
Exp(λ)	$\lambda e^{-\lambda x}$	$\lambda^{-1}-x$
Gamma(α,λ)	$\frac{\lambda^\alpha x^{\alpha-1}e^{-\lambda x}}{\Gamma(\alpha)}$	$\Big(\ln(\lambda x)-\frac{\Gamma'(\alpha)}{\Gamma(\alpha)},\, \alpha\lambda^{-1}-x\Big)^T$
Weib(α,λ)	$\alpha\lambda(\lambda x)^{\alpha-1}e^{-(\lambda x)^\alpha}$	$(\alpha^{-1}+\ln(\lambda x)[1-(\lambda x)^\alpha],\, \frac{\alpha}{\lambda}[1-(\lambda x)^\alpha])^T$
$N(\mu,\sigma^2)$	$\frac{1}{\sigma\sqrt{2\pi}}e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2}$	$(\sigma^{-2}(x-\mu),-\sigma^{-1}+\sigma^{-3}(x-\mu)^2)^T$

allow us to represent the gradient of $\mathbb{E}_{\boldsymbol{\theta}}[g(\boldsymbol{X})]$ for the case in which θ is a vector.

$$\begin{aligned}\nabla_{\boldsymbol{\theta}}\mathbb{E}_{\boldsymbol{\theta}}[g(\boldsymbol{X})] =& \nabla_{\boldsymbol{\theta}}\int g(\boldsymbol{x})f(\boldsymbol{x};\boldsymbol{\theta})\mathrm{d}\boldsymbol{x}\\ =& \int g(\boldsymbol{x})\nabla_{\boldsymbol{\theta}}f(\boldsymbol{x};\boldsymbol{\theta})\mathrm{d}\boldsymbol{x}\\ =& \int g(\boldsymbol{x})\frac{\nabla_{\boldsymbol{\theta}}f(\boldsymbol{x};\boldsymbol{\theta})}{f(\boldsymbol{x};\boldsymbol{\theta})}f(\boldsymbol{x};\boldsymbol{\theta})\mathrm{d}\boldsymbol{x}\\ =& \int g(\boldsymbol{x})[\nabla_{\boldsymbol{\theta}}\, lnf(\boldsymbol{x};\boldsymbol{\theta})]f(\boldsymbol{x};\boldsymbol{\theta})\mathrm{d}\boldsymbol{x}\\ =& \mathbb{E}_{\boldsymbol{\theta}}\big[g(\boldsymbol{X})\mathcal{S}(\boldsymbol{\theta};\boldsymbol{X})\big]\end{aligned} \tag{4.10}$$

where

$$\mathcal{S}(\boldsymbol{\theta};\boldsymbol{x}) = \nabla_{\boldsymbol{\theta}}\ln f(\boldsymbol{x};\boldsymbol{\theta}) \tag{4.11}$$

is the score function of $f(\boldsymbol{x};\boldsymbol{\theta})$ and $\nabla \ln f(\boldsymbol{x};\boldsymbol{\theta})^T$ presents the transpose of the column vector $\nabla \ln f(\boldsymbol{x};\boldsymbol{\theta})$ of the partial derivatives of $\ln f(\boldsymbol{x};\boldsymbol{\theta})$. Table (4.1) represents the score functions calculated from equation (4.11) for some commonly used input distributions. As an example, for a Gamma(α,β) distribution, we let $\boldsymbol{\theta}=(\alpha,\beta)$.

In general the quantities $\nabla_{\boldsymbol{\theta}}\mathbb{E}_{\boldsymbol{\theta}}[g(\boldsymbol{X})]$ are not available analytically, since the response $\mathbb{E}_{\boldsymbol{\theta}}[g(\boldsymbol{X})]$ is not available. They can be estimated, however, via a single simulation as

$$\widehat{\nabla_{\boldsymbol{\theta}}\mathbb{E}_{\boldsymbol{\theta}}[g(\boldsymbol{X})]} = \frac{1}{N}\sum_{i=1}^{N} g(\boldsymbol{X_i})\mathcal{S}(\boldsymbol{\theta};\boldsymbol{X_i}). \tag{4.12}$$

It is clear from equations (4.8) and (4.10) that $\frac{1}{N}\sum_{i=1}^{N} g(\boldsymbol{X_i})\mathcal{S}(\boldsymbol{\theta};\boldsymbol{X_i})$ is an unbiased esti-

mator of $\nabla_{\boldsymbol{\theta}}\mathbb{E}_{\boldsymbol{\theta}}[g(\boldsymbol{X})]$). Having estimated the partial derivatives, we propose a simulation based estimator for SDIM_{θ_j} which can be computed from the same simulation used to estimate the derivatives:

$$\widehat{\text{SDIM}}_{\theta_j} = \frac{\widehat{\frac{\partial \mathbb{E}_{\boldsymbol{\theta}}[g(\boldsymbol{X})]}{\partial \theta_j}} \mathrm{d}\theta_j}{\sum_{i=1}^{m} \widehat{\frac{\partial \mathbb{E}_{\boldsymbol{\theta}}[g(\boldsymbol{X})]}{\partial \theta_i}} \mathrm{d}\theta_i}. \tag{4.13}$$

To explain better, we provide the following example about the estimation of SDIM_{θ_j}.

Example: Let $Y = g(\boldsymbol{X}) = \max\{X_1^2 + 3, X_2^2 + 2\}$, where $\boldsymbol{X} = (X_1, X_2)$ is a two dimensional vector with independent components, $X_1 \sim exp(\theta_1)$ and $X_2 \sim exp(\theta_2)$. We are interested in estimating SDIM_{θ_j} with respect to the distributional parameter vector $\boldsymbol{\theta} = (\theta_1, \theta_2)$. For this, we have

$$\widehat{\nabla_{\boldsymbol{\theta}}\mathbb{E}_{\boldsymbol{\theta}}[g(\boldsymbol{X})]} = \frac{1}{N}\sum_{i=1}^{N} g(\boldsymbol{X_i})\mathcal{S}(\boldsymbol{\theta}; \boldsymbol{X_i})$$

where

$$\mathcal{S}(\boldsymbol{\theta}; \boldsymbol{X}_i) = \begin{bmatrix} \theta_1^{-1} - X_{1i} \\ \theta_2^{-1} - X_{2i} \end{bmatrix}$$

More explicitly,

$$\widehat{\frac{\partial \mathbb{E}_{\boldsymbol{\theta}}[g(\boldsymbol{X})]}{\partial \theta_1}} = \frac{1}{N}\sum_{i=1}^{N} g(\boldsymbol{X}_i)(\theta_1^{-1} - X_{1i})$$

$$\widehat{\frac{\partial \mathbb{E}_{\boldsymbol{\theta}}[g(\boldsymbol{X})]}{\partial \theta_2}} = \frac{1}{N}\sum_{i=1}^{N} g(\boldsymbol{X}_i)(\theta_2^{-1} - X_{2i})$$

By using equation (4.13), SDIM_{θ_j} under uniform perturbations can be estimated by

$$\widehat{\text{SDIM}}_{\theta_j} = \frac{\widehat{\frac{\partial \mathbb{E}_{\boldsymbol{\theta}}[g(\boldsymbol{X})]}{\partial \theta_j}}}{\sum_{i=1}^{m} \widehat{\frac{\partial \mathbb{E}_{\boldsymbol{\theta}}[g(\boldsymbol{X})]}{\partial \theta_i}}}.$$

Note that SDIM is a local measure of $\boldsymbol{\theta}$. To estimate SDIM simultaneously at several random points in the parameter space (Θ), we shall apply the importance sampling technique. For this, let $z(\boldsymbol{x})$ be the importance sampling density, assuming, that the support of $z(\boldsymbol{x})$ contains the support of $g(\boldsymbol{x})f(\boldsymbol{x}; \boldsymbol{\theta})$ for all $\boldsymbol{\theta} \in \Theta$. If not stated otherwise, we assume that the importance sampling probability density function lies in the same para-

metric family as the original probability density function $f(\boldsymbol{x};\boldsymbol{\theta})$. That is, $z(\boldsymbol{x}) = f(\boldsymbol{x};\boldsymbol{\theta}')$ for some $\boldsymbol{\theta}' \in \Theta$. Then, $\nabla_{\boldsymbol{\theta}}\mathbb{E}_{\boldsymbol{\theta}}[g(\boldsymbol{X})]$ can be written as [Rubinstein, 1989]

$$\nabla_{\boldsymbol{\theta}}\mathbb{E}_{\boldsymbol{\theta}}[g(\boldsymbol{X})] = \mathbb{E}_{\boldsymbol{\theta}}[g(\boldsymbol{X})\mathcal{S}(\boldsymbol{\theta};\boldsymbol{X})\Lambda(\boldsymbol{X};\boldsymbol{\theta})], \tag{4.14}$$

where

$$\Lambda(\boldsymbol{x};\boldsymbol{\theta}) = \frac{f(\boldsymbol{x};\theta)}{z(\boldsymbol{x})} \tag{4.15}$$

is the likelihood ratio of $f(\boldsymbol{x};\boldsymbol{\theta})$ and $z(\boldsymbol{x})$. Therefore, the likelihood ratio estimator of $\nabla_{\boldsymbol{\theta}}\mathbb{E}_{\boldsymbol{\theta}}[g(\boldsymbol{X})]$ can be then written as

$$\widehat{\nabla_{\boldsymbol{\theta}}\mathbb{E}_{\boldsymbol{\theta}}[g(\boldsymbol{X})]} = \frac{1}{N}\sum_{i=1}^{N} g(\boldsymbol{X_i})\mathcal{S}(\boldsymbol{\theta};\boldsymbol{X_i})\Lambda(\boldsymbol{X_i};\boldsymbol{\theta}) \tag{4.16}$$

where $\boldsymbol{X_1}$,...,$\boldsymbol{X}_N$ is a random sample from $z(\boldsymbol{x})$, and $\widehat{\nabla_{\boldsymbol{\theta}}\mathbb{E}_{\boldsymbol{\theta}}[g(\boldsymbol{X})]}$ is an unbiased estimator of $\nabla_{\boldsymbol{\theta}}\mathbb{E}_{\boldsymbol{\theta}}[g(\boldsymbol{X})]$ for all $\boldsymbol{\theta}$. This means that by varying $\boldsymbol{\theta}$ and keeping z fixed we can, in principle, estimate unbiasedly the whole response surface $\{\nabla_{\boldsymbol{\theta}}\mathbb{E}_{\boldsymbol{\theta}}[g(\boldsymbol{X})], \boldsymbol{\theta} \in \Theta\}$ from the same simulation. Then, equation (4.16) can be re-written as

$$\widehat{\nabla_{\boldsymbol{\theta},\boldsymbol{\theta}'}\mathbb{E}_{\boldsymbol{\theta}}[g(\boldsymbol{X})]} = \frac{1}{N}\sum_{i=1}^{N} g(\boldsymbol{X_i})\mathcal{S}(\boldsymbol{\theta};\boldsymbol{X_i})\Lambda(\boldsymbol{X_i};\boldsymbol{\theta},\boldsymbol{\theta}') \tag{4.17}$$

with $\Lambda(\boldsymbol{x};\boldsymbol{\theta},\boldsymbol{\theta}') = f(\boldsymbol{x};\boldsymbol{\theta})/f(\boldsymbol{x};\boldsymbol{\theta}')$. Thus, it allows the estimation of $\nabla_{\boldsymbol{\theta}}\mathbb{E}_{\boldsymbol{\theta}}[g(\boldsymbol{X})]$ and SDIM simultaneously for different values of $\boldsymbol{\theta}$ using a single sample of size N from the importance sampling probability density function $f(\boldsymbol{x};\boldsymbol{\theta}')$.

Algorithm 1 Estimation of SDIM for multiple values of $\boldsymbol{\theta}$

1. Generate a sample $\boldsymbol{X}_1, \cdots, \boldsymbol{X}_N$ from the importance sampling probability density function $f(\boldsymbol{x};\boldsymbol{\theta}')$ which must be chosen in advance.
2. Calculate the model output $g(\boldsymbol{X}_i)$ and the scores $\mathcal{S}(\boldsymbol{\theta};\boldsymbol{X}_i)$, $i = 1, \cdots, N$ for the desired parameter value $\boldsymbol{\theta}$.
3. Calculate $\widehat{\text{SDIM}_{\theta_j}}$ using equations (4.17) and (4.13).

From Algorithm 1 it follows that to estimate SDIM_{θ_j} for all $j = 1, \cdots, m$, it is sufficient to have at our disposal a realization of the output process $g(\boldsymbol{X})$ and a realization of the score function based on a sample $\boldsymbol{X}_1, \cdots, \boldsymbol{X}_N$, i.e., N realizations for each X_i, obtained from the importance sampling probability density function $f(\boldsymbol{x};\boldsymbol{\theta}')$. Thus, the complexity of the model can be overcome. The next section is devoted to the application of SDIM in discrete event systems to evaluate the sensitivity of the performance measure with respect to the distributional parameters.

4.2 Application: Discrete Event Systems (DES)

Discrete-event systems are often used to model many real world complex systems in science and engineering. The behaviour of such systems is identified via a sequence of discrete events, which causes the system to change from one state to another. Examples include traffic systems, flexible manufacturing systems, computer communications systems, inventory systems, production lines and flow networks. A discrete event system can be classified as either static or dynamic. The former is called a discrete-event static system (DESS), while the latter is called a discrete-event dynamic system (DEDS). The major difference is that DESS do not evolve over time, while DEDS do. A coherent reliability system is a classical example of a DESS, with a sample performance given by, for instance, the failure time of a component. A queueing system, is an example of a DEDS, with a sample performance given by, for instance, the waiting time of a customer in the queue. In this chapter, we deal with sensitivity analysis for both DESS and DEDS.

Let $l(\boldsymbol{\theta}) = \mathbb{E}_{\boldsymbol{\theta}}[g(\boldsymbol{X})]$ be the performance measure of one system, where $g(\boldsymbol{X})$ is the sample performance driven by an input vector $\boldsymbol{X}$ having a cumulative distribution (cdf) $F(\boldsymbol{x}, \boldsymbol{\theta})$. Here $\boldsymbol{\theta}$ is a vector of parameters lying in a parameter set $\Theta \subset \mathbb{R}^m$. For example the performance measure in a traffic light system can be a vehicle's average delay as it proceeds from a given point of origin to a given destination and in a coherent lifetime systems it can be the mean time to failure of the system.

Most of the real-world DES must be studied numerically. Thus, initially, sensitivity analysis of DES was performed using crude Monte Carlo methods which was based on finite-difference estimation of the gradients. But it has been proved in literature that his might be a time consuming and often inaccurate procedure. For example, it requires at least $(n + 1)$ simulation runs to estimate the gradient, where n is the number of design variables. Later on, two new methods were introduced for sensitivity analysis called perturbation analysis (Suri and Zazanis [1988];Xi-ren [1985]) and LRM (Rubinstein [1989]). As we have mentioned in the previous section LRM entails only perturbation and differentiation of the underlying probability density function $f(\boldsymbol{x}, \boldsymbol{\theta}) = \mathrm{d}F(\boldsymbol{x}, \boldsymbol{\theta})/\mathrm{d}\boldsymbol{x}$. Note that there is no need for an analytical expression of $g(\boldsymbol{X})$ which in fact is not available in most practical applications.

4.2.1 SDIM for Discrete Event Static Systems

In this subsection we study two cases regarding a notable example in reliablity: the bridge system where it is a DESS. First, we evaluate the sensitivity of the mean shortest path and secondly, we evaluate the sensitivity of the mean time to failure of the system, with respect to a distributional parameter vector. Reliability systems play a major role in the design of all kinds of computing systems. Due to environmental effects like manufactur-

ing tolerance, cosmic rays and also ageing effects such as electro-migration, the system components are susceptible to failure. Given these conditions, reliability importance measures have traditionally helped designers in redundancy allocation and consequently to access the importance of the components. A variety of reliability importance measures have been introduced in the literature to answer different sensitivity questions in many applications. We refer to Kuo and Zhu [2012b], Aven and Nokland [2010] and Kuo and Zhu [2012a] for reviews of the existing reliability importance measures. In this study we consider SDIM as a novel differential based importance measure in reliability applications. It is an extension of partial derivatives for models with stochastic output (with respect to distributional parameters). The advantages are that it allows one to consider simultaneous changes in the parameters thanks to the additivity property. Also, in the case where the parameters have alternative units (e.g., consider two random variables length with uniform distribution (θ) and time with exponential distribution (λ). Then, λ and θ have different units), it allows to consider a proportional change perturbation and, therefore, to rank the corresponding inputs. Then, using SDIM one can answer sensitivity questions both in a *factor prioritization*, *factor fixing* and *direction of change* settings.

Case Study 1: Consider the undirected graph shown in figure (4.1), illustrating a bridge network. A bridge network can be specified by a collection of vertices (or nodes) and a set of edges joining selected pairs of vertices. Suppose we wish to estimate SDIM_{θ_j} for $j = 1, \cdots, 5$ of the mean shortest path between vertices A and B, with respect to the distributional parameters of the random lengths $X_1, \cdots, X_5$ of the links. This becomes an important question such as in world wide web where the mean shortest path facilitates the quick transfer of information and reduces costs. The efficiency of mass transfer in a metabolic network can be judged by studying the shortest path between two vertices. In this respect, SDIM provides information about the most sensitive paths for the corresponding shortest paths between the given vertices. The mean shortest path can be expressed as $l(\boldsymbol{\theta}) = \mathbb{E}_{\boldsymbol{\theta}}[g(\boldsymbol{X})]$, where

$$Y = g(\boldsymbol{X}) = \min\{X_1 + X_4, X_1 + X_3 + X_5, X_2 + X_3 + X_4, X_2 + X_5\}.$$

and let us assume that $X_i \sim U[0, \theta_i]$, $i = 1, \cdots, 5$. Then

$$f(\boldsymbol{x}, \boldsymbol{\theta}) = \prod_{i=1}^{5} \frac{\boldsymbol{I}_{\{0<x_i<\theta_i\}}}{\theta_i}.$$

This is a typical example where the interchange of gradients and integral is not appropriate, because of the discontinuities at $\theta_1, \cdots, \theta_5$. However, the situation can easily be fixed by including a continuity correction, a method when a discrete distribution is

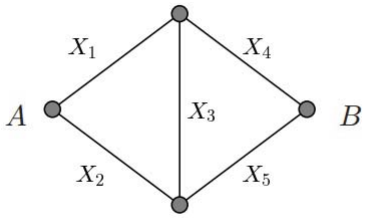


Figure 4.1: The bridge network with corresponding lengths.

approximated by a continuous distribution. Then, the derivative with respect to θ_1 is

$$\begin{aligned}\frac{\partial}{\partial\theta_1}\mathbb{E}_{\boldsymbol{\theta}}[g(\boldsymbol{X})] &= \frac{\partial}{\partial\theta_1}\int_0^{\theta_1}\Big(\int_0^{\theta_2}\cdots\int_0^{\theta_5} g(\boldsymbol{x})\frac{1}{\theta_1\cdots\theta_5}\mathrm{d}x_2\cdots\mathrm{d}x_5\Big)\mathrm{d}x_1 \\ &= \int_0^{\theta_2}\cdots\int_0^{\theta_5} g(\theta_1,x_2,\cdots,x_5)\frac{1}{\theta_1\cdots\theta_5}\mathrm{d}x_2\cdots\mathrm{d}x_5 - \frac{1}{\theta_1}\int g(\boldsymbol{x})f(\boldsymbol{x};\boldsymbol{\theta})\mathrm{d}\boldsymbol{x} \\ &= \frac{1}{\theta_1}\big(\mathbb{E}_{\boldsymbol{\theta}}[g(\boldsymbol{X}^*)] - \mathbb{E}_{\boldsymbol{\theta}}[g(\boldsymbol{X})]\big)\end{aligned}$$

where $\boldsymbol{X}\sim f(\boldsymbol{x};\boldsymbol{\theta})$ and $\boldsymbol{X}^*\sim f(\boldsymbol{x};\boldsymbol{\theta}|x_1=\theta_1)$. Both $\mathbb{E}_{\boldsymbol{\theta}}[g(\boldsymbol{X}^*)]$ and $\mathbb{E}_{\boldsymbol{\theta}}[g(\boldsymbol{X})]$ can easily be estimated via Monte Carlo. The other partial derivatives follow by symmetry. Now we are interested to estimate SDIM for five parameter combinations across sample sizes $N=10^5,10^6,10^7$. Tables (4.2) and (4.3) show results of $\widehat{\text{SDIM}}$ under uniform and proportional perturbations for different parameter settings of $(\theta_1,\theta_2,\theta_3,\theta_4,\theta_5)$. We observed that $\widehat{\text{SDIM}}$ was stable across sample sizes. It is clear that when the parameter values change the importance of the lengths consequently changes.

Case Study 2: In this study we consider the bridge network shown in figure (4.2) consisting of five components. Consider the following corresponding structure function (ψ) of this system. The structure function is a model that determines the status of the system given the status of its components. We use the structure function to compute the system mean time to failure (MTTF).

$$\psi = (\varphi_1\wedge\varphi_2)\vee(\varphi_3\wedge\varphi_4)\vee(\varphi_1\wedge\varphi_4\wedge\varphi_5)\vee(\varphi_2\wedge\varphi_3\wedge\varphi_5)$$

where

$$\varphi_i = \begin{cases}1 \text{ component } i \text{ has failed}\\ 0 \text{ component } i \text{ is working correctly.}\end{cases}$$

To apply SDIM we consider the system MTTF as the performance measure of the bridge network. In particular, we are interested in the effect of the failure of component i on the

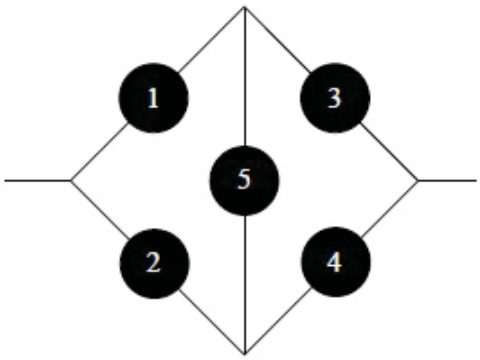


Figure 4.2: Bridge Network with five components

system MTTF:

$$\text{MTTF} = \mathbb{E}(T) = \int_0^\infty t\, f(t)\, \mathrm{d}t$$

where, $f(t)$ is the probability density of system failure time (t). An alternative way of expressing MTTF is

$$\text{MTTF} = \mathbb{E}\Big[\max\Big\{\min(T_1, T_2), \min(T_3, T_4), \min(T_1, T_4, T_5), \min(T_2, T_3, T_5)\Big\}\Big] \qquad (4.18)$$

where T_i is the failure time of the i^{th} component. In practise the Weibull distribution is commonly used to model the ageing effect of the components and thus we assume that T_i has a Weibull distribution with corresponding parameters α_i and λ_i.

Table 4.2: SDIM under uniform perturbations of different parameter combinations across different sample sizes for case study 1

Parameters ($\boldsymbol{\theta}_0$)	$N = 10^5$					$N = 10^6$					$N = 10^7$				
	$SDIM_1$	$SDIM_2$	$SDIM_3$	$SDIM_4$	$SDIM_5$	$SDIM_1$	$SDIM_2$	$SDIM_3$	$SDIM_4$	$SDIM_5$	$SDIM_1$	$SDIM_2$	$SDIM_3$	$SDIM_4$	$SDIM_5$
(1,0.5,1.5,2,1)	0.0551	0.4630	0.0057	0.0347	0.4416	0.0541	0.4636	0.0056	0.0340	0.4428	0.0542	0.4636	0.0056	0.0340	0.4426
(5,6,8.5,3,2)	0.2423	0.2071	0.0045	0.2478	0.2984	0.2422	0.2066	0.0044	0.2479	0.2988	0.2425	0.2065	0.0044	0.2484	0.2982
(1,2,3,1,2)	0.4632	0.0364	0.0030	0.4610	0.0364	0.4618	0.0368	0.0030	0.4615	0.0369	0.4620	0.0366	0.0030	0.4618	0.0366
(1,1,1,1,1)	0.2446	0.2445	0.0221	0.2450	0.2437	0.2445	0.2446	0.0223	0.2442	0.2444	0.2443	0.2446	0.0222	0.2443	0.2446
(0.3,0.2,0.5,0.6,1)	0.3084	0.2259	0.0171	0.3514	0.0972	0.3064	0.2280	0.0174	0.3510	0.0972	0.3065	0.2280	0.0174	0.3508	0.0973

Table 4.3: SDIM under proportional perturbations of different parameter combinations across different sample sizes for case study 1

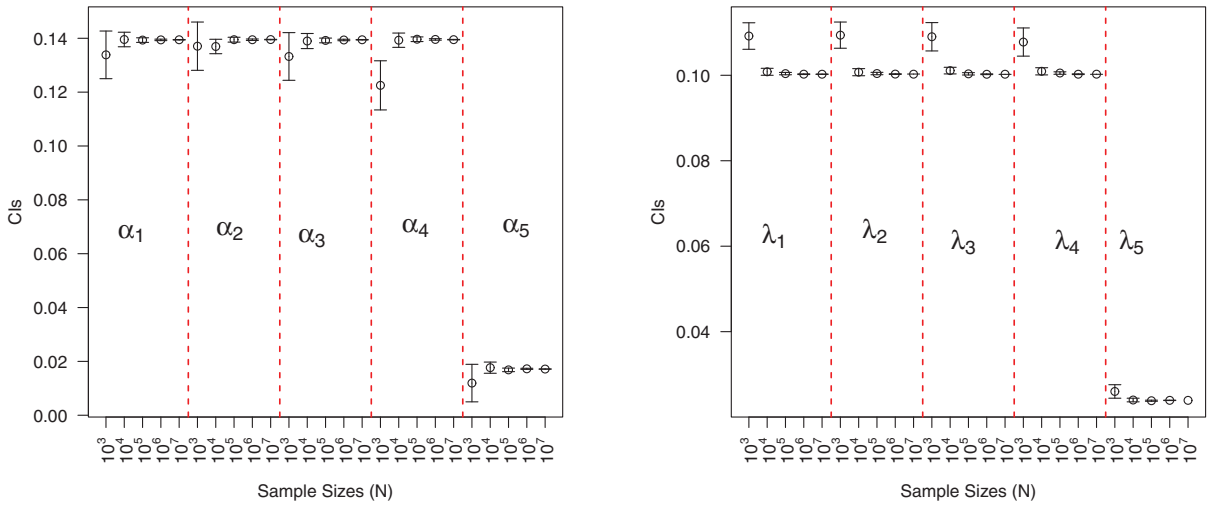
Parameters ($\boldsymbol{\theta}_0$)	$N = 10^5$					$N = 10^6$					$N = 10^7$				
	$SDIM_1$	$SDIM_2$	$SDIM_3$	$SDIM_4$	$SDIM_5$	$SDIM_1$	$SDIM_2$	$SDIM_3$	$SDIM_4$	$SDIM_5$	$SDIM_1$	$SDIM_2$	$SDIM_3$	$SDIM_4$	$SDIM_5$
(1,0.5,1.5,2,1)	0.0673	0.2880	0.0106	0.0842	0.5499	0.0678	0.2875	0.0106	0.0849	0.5492	0.0674	0.2878	0.0105	0.0845	0.5499
(5,6,8.5,3,2)	0.3159	0.3247	0.0098	0.1947	0.1548	0.3172	0.3229	0.0099	0.1950	0.1550	0.3164	0.3235	0.0099	0.1946	0.1557
(1,2,3,1,2)	0.4286	0.0683	0.0078	0.4268	0.0686	0.4273	0.0684	0.0082	0.4277	0.0684	0.4281	0.0679	0.0082	0.4280	0.0678
(1,1,1,1,1)	0.2452	0.2440	0.0221	0.2441	0.2446	0.2441	0.2447	0.0223	0.2445	0.2444	0.2443	0.2446	0.0222	0.2443	0.2446
(0.3,0.2,0.5,0.6,1)	0.2013	0.1009	0.0192	0.4641	0.2145	0.2022	0.1003	0.0192	0.4638	0.2144	0.2025	0.1004	0.0192	0.4637	0.2141

To study the bridge system, we consider four different cases where we assign fixed parameter values.

Case 1: Decreasing hazard rate : the system fails less

$$\alpha = (0.5, 0.5, 0.5, 0.5, 0.5)$$
$$\lambda = (1, 1, 1, 1, 1)$$

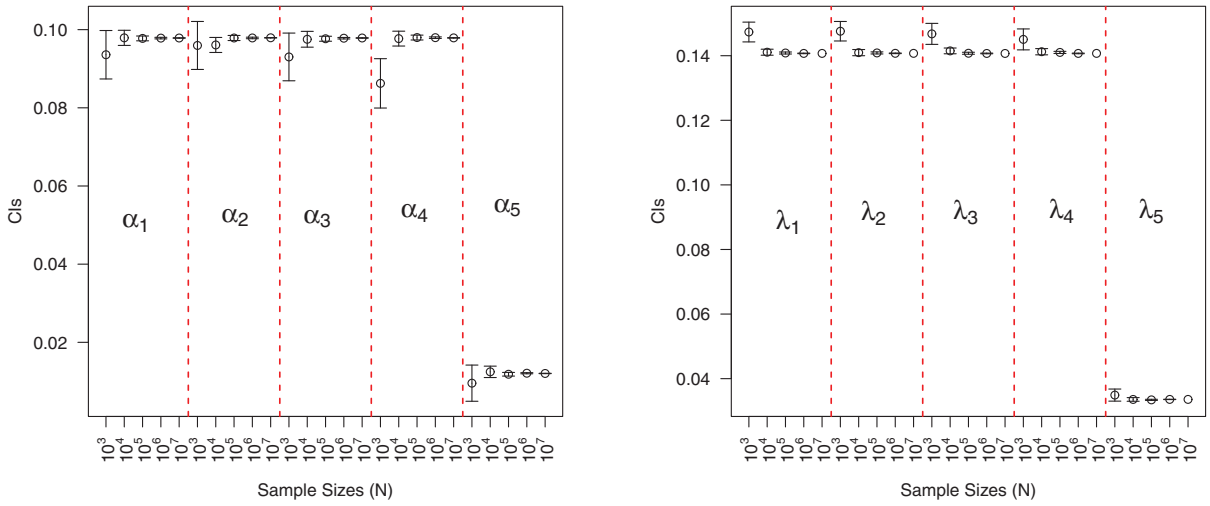
Figures (4.3) and (4.4) show the confidence intervals of SDIM of the parameter values specified for α_i and λ_i, $i = 1, \cdots, 5$ with bootstrap sample size with $n = 500$ Monte Carlo repetitions. It is clear that as the sample size N increases the confidence intervals become narrow. Thus, the performance of $\widehat{\text{SDIM}}$ is good across sample sizes. Moreover, one can



(a) (b)

Figure 4.3: Confidence intervals of SDIM of α (a) and λ (b) under uniform perturbations (Case 1).

compute the joint sensitivity of the model output with respect to the parameters of the model input distribution of a component by using the additivity property of SDIM. For instance, the joint sensitivity of the parameters of the fifth component (under uniform perturbation) is $\widehat{\text{SDIM}}_{(\alpha_5,\lambda_5)} = \widehat{\text{SDIM}}_{\alpha_5} + \widehat{\text{SDIM}}_{\lambda_5} = 0.017150 + 0.023923 = 0.041073$, where $\widehat{\text{SDIM}}_{\alpha_5}$ and $\widehat{\text{SDIM}}_{\lambda_5}$ are the mean values for $n = 500$. In this case, under both uniform and proportional perturbations, we observe that the fifth component has less importance while other components have similar importance but with different values of SDIM of α_1 to α_4 and λ_1 to λ_4.



(a) (b)

Figure 4.4: Confidence intervals of SDIM of α (a) and λ (b) under proportional perturbations (Case 1).

Case 2: Increasing hazard rate : the system fails more often

$$\alpha = (1.5, 1.5, 1.5, 1.5, 1.5)$$
$$\lambda = (1, 1, 1, 1, 1)$$

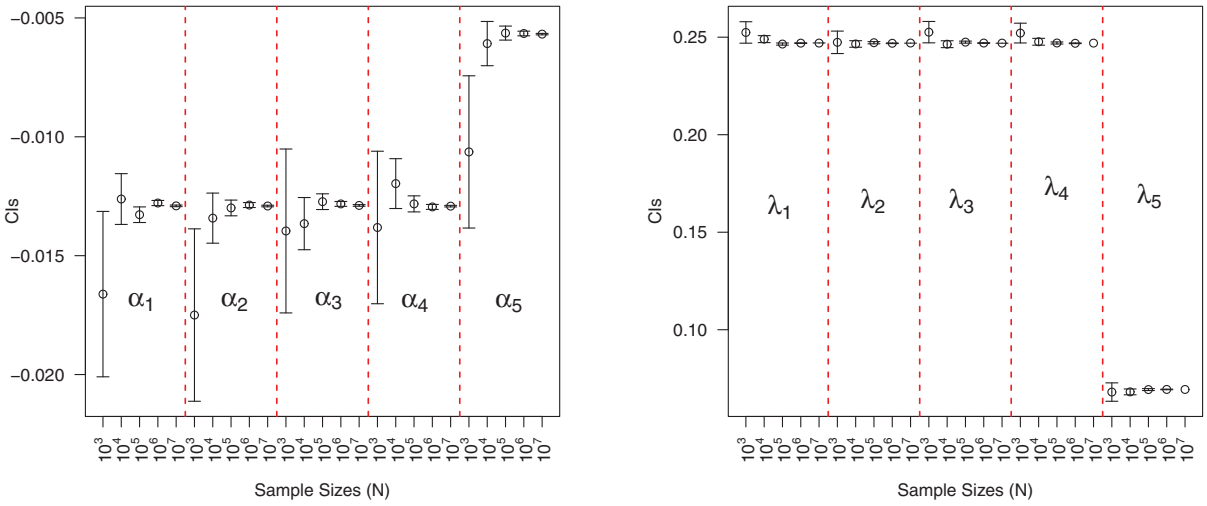
The corresponding graphs for this case are shown in figures (4.5) and (4.6). The parameter values are chosen as specified for α_i and λ_i, $i = 1, \cdots, 5$ with $n = 500$ Monte Carlo repetitions. It is clear that also in this case as the sample size increases, the confidence intervals become narrow. Thus, the estimator of SDIM performs well across different sample sizes. Moreover, for increasing hazard rate, in both uniform and proportional perturbations, λ_1 to λ_4 and α_1 to α_4 have equal importance while λ_5 has the least importance in MTTF.

Case 3: In this case we consider constant failure rates.

$$\alpha = (1, 1, 1, 1, 1)$$
$$\lambda = (1, 1, 1, 1, 1)$$

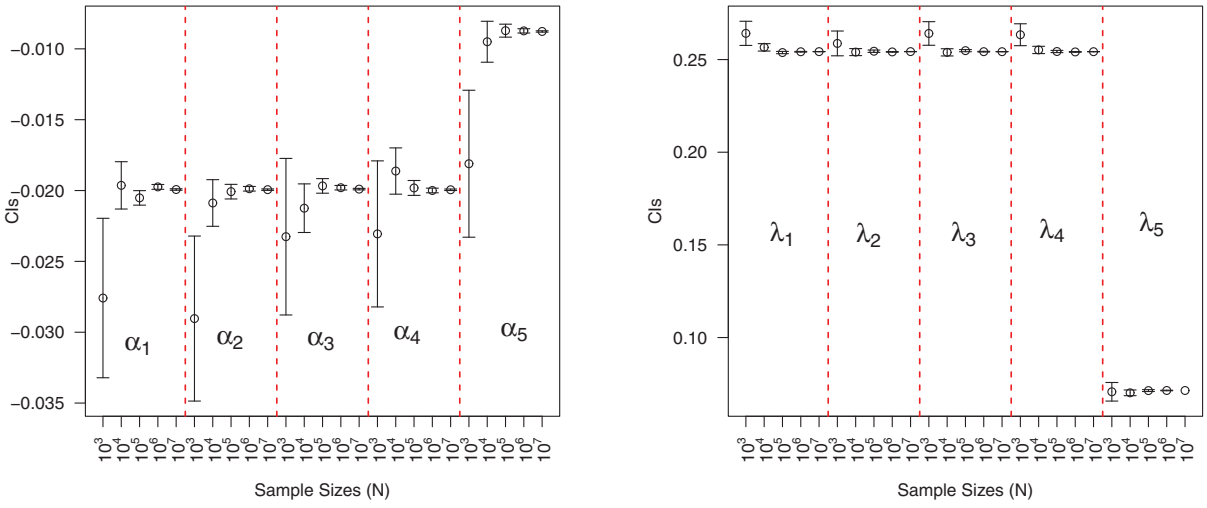
Given the system components have constant failure rates, figures (4.7) and (4.8) show the performance of the SDIM estimator across sample sizes. We observe that the mean values of SDIM are the same for both uniform and proportional perturbations.

Case 4: In this case we consider the following parameter setting.



(a) (b)

Figure 4.5: Confidence intervals of SDIM of α (a) and λ (b) under uniform perturbations (Case 2).

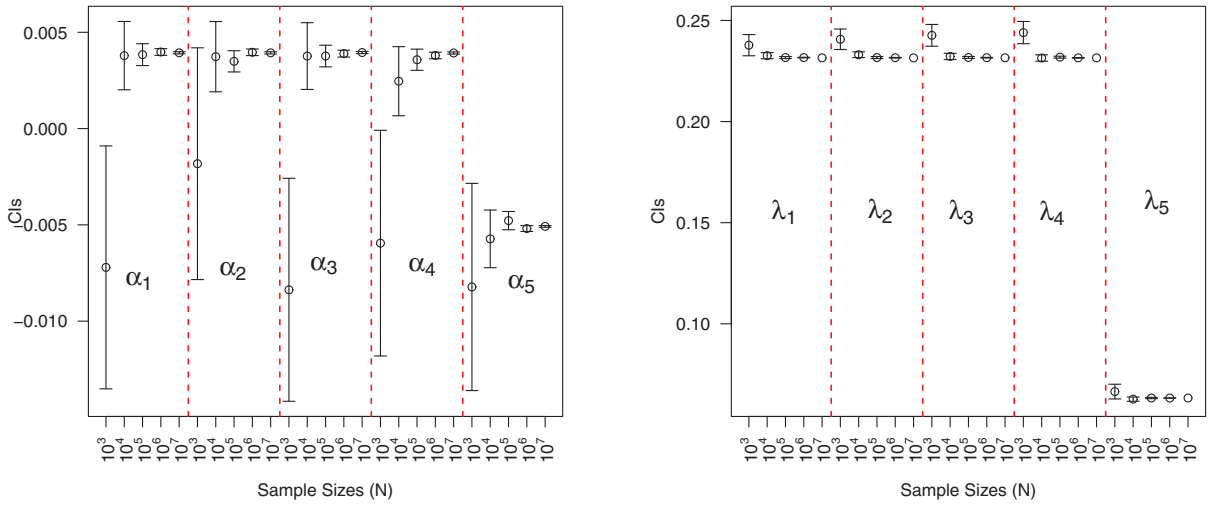


(a) (b)

Figure 4.6: Confidence intervals of SDIM of α (a) and λ (b) under proportional perturbations (Case 2).

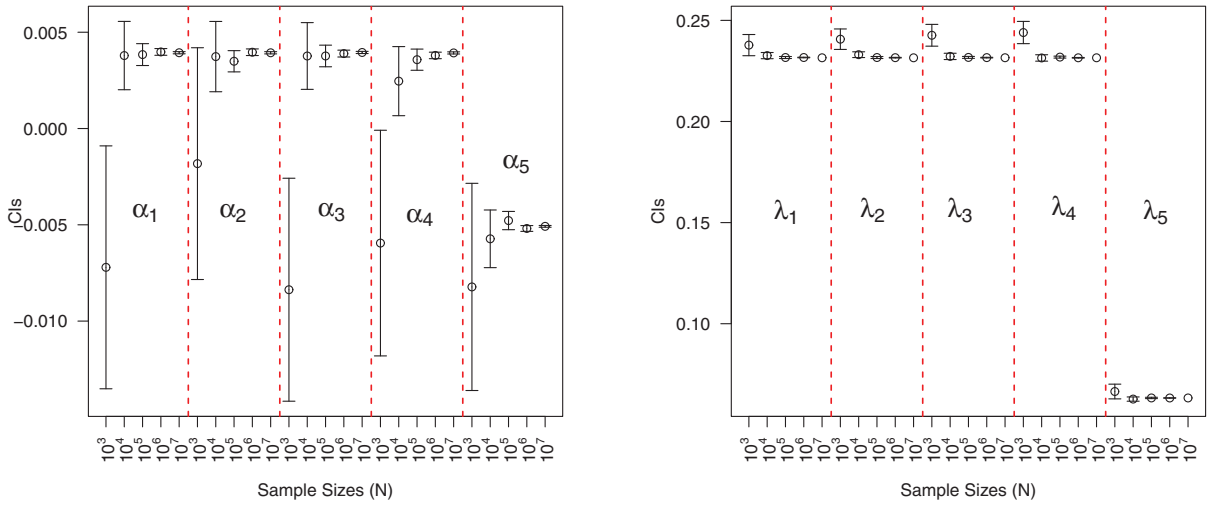
$$\alpha = (6, 8, 6, 5, 8)$$

$$\lambda = (10, 20, 30, 40, 50)$$



(a) (b)

Figure 4.7: Confidence intervals of SDIM of α (a) and λ (b) under uniform perturbations (Case 3).



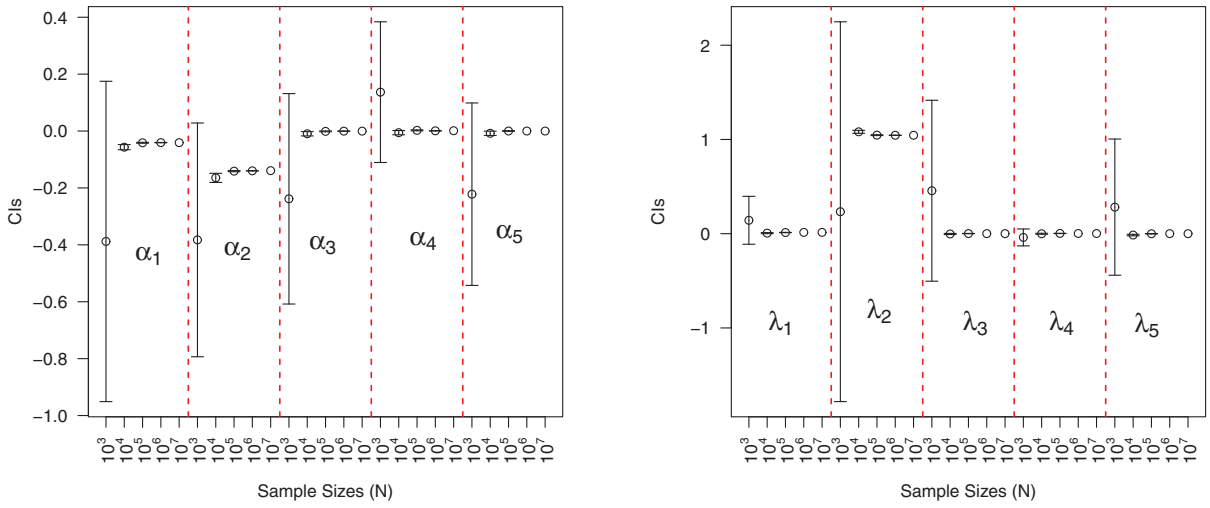
(a) (b)

Figure 4.8: Confidence intervals of SDIM of α (a) and λ (b) under proportional perturbations (Case 3).

The corresponding confidence intervals of SDIM are shown in figures (4.9) and (4.10) and we observed that the performance of $\widehat{\text{SDIM}}$ is good across sample sizes in the sense that the confidence intervals become smaller as the sample size (N) increases.

In this subsection we studied two cases of discrete event static systems and evaluated

parameter sensitivities of the sample performance. From the numerical study, we observed that the performance of the proposed estimator was good across sample sizes since the confidence intervals of SDIM shrank as the sample size increased. In the next sub-section we compute parameter sensitivities in a $GI/G/1$ queueing system.

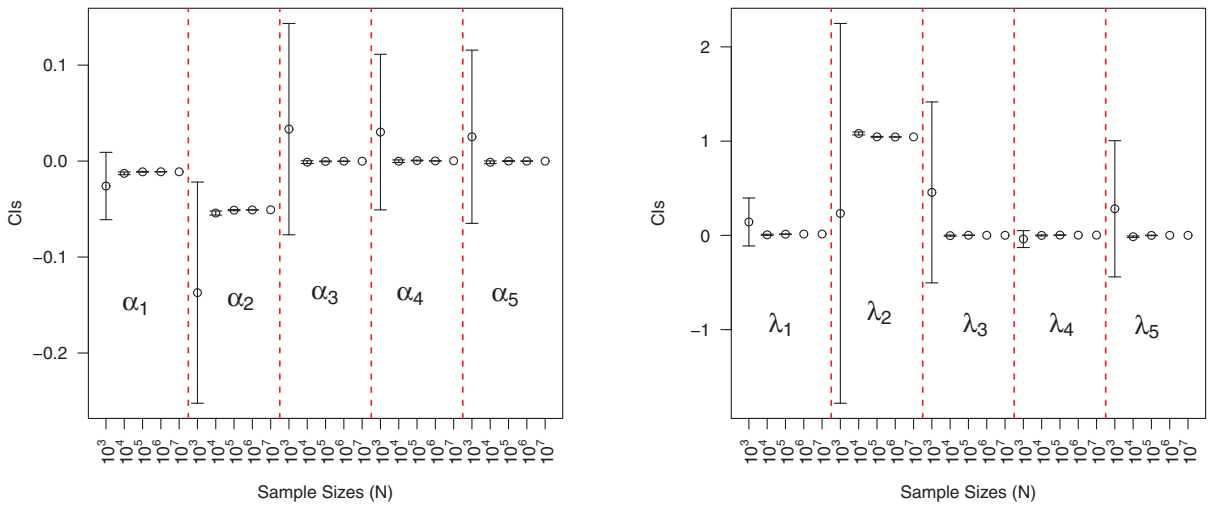


(a) (b)

Figure 4.9: Confidence intervals of SDIM of α (a) and λ (b) under uniform perturbations (Case 4).

4.2.2 SDIM for Discrete Event Dynamic Systems

Let $\boldsymbol{X}_1, \boldsymbol{X}_2, ...$ be an input sequence of n-dimensional random vectors driving an output process $Y = \{Y_t, t = 0, 1, 2, \cdots\}$. That is, $Y_t = Y_t(\mathbf{X_t})$ for some function Y_t, where the vector $\mathbf{X}_t = (\boldsymbol{X}_1, \boldsymbol{X}_2, ..., \boldsymbol{X}_t)$ represents the history of the input process up to time t. Let $f_t(\mathbf{x_t}; \boldsymbol{\theta})$ be the probability density function of $\mathbf{X_t}$ which depends on some parameter $\boldsymbol{\theta}$. Suppose that $\{Y_t\}$ is a regenerative process with a regenerative cycle of length T. Given a stochastic process $Y = \{Y_t, t = 0, 1, 2, \cdots\}$, suppose there exists a random time T such that $\{Y_{t+T}, t = 0, 1, 2, \cdots\}$ has the same distribution as Y and is independent of the past, $\{Y_t, 0 \leq t \leq T\}$, then we say that Y regenerated at time T, meaning that it has stochastically "started over again ", as if it was time $t = 0$ again, and its future is independent of its past. A typical example is the waiting time process in a $GI/G/1$ system.



(a) (b)

Figure 4.10: Confidence intervals of SDIM of α (a) and λ (b) under proportional perturbations (Case 4).

The expected steady performance, $l(\boldsymbol{\theta})$ for such systems can be written as

$$l(\boldsymbol{\theta}) = \frac{\mathbb{E}_{\boldsymbol{\theta}}[R]}{\mathbb{E}_{\boldsymbol{\theta}}[T]} = \frac{\mathbb{E}_{\boldsymbol{\theta}}\left[\sum_{t=1}^{T} Y_t(\mathbf{X}_t)\right]}{\mathbb{E}_{\boldsymbol{\theta}}[T]} \tag{4.19}$$

where R is the reward during a cycle. Our goal is to estimate SDIM of $l(\boldsymbol{\theta}) = \mathbb{E}_{\boldsymbol{\theta}}[R]/\mathbb{E}_{\boldsymbol{\theta}}[T]$ with respect to $\boldsymbol{\theta}$. For that, first we start by defining an estimator for $\nabla l(\boldsymbol{\theta})$ [Rubinstein and Shapiro, 1993]. Then, we plug it in equation (4.13) to obtain an estimator of SDIM.

We consider the estimation of $\nabla l_R(\boldsymbol{\theta})$ where $l_R(\boldsymbol{\theta}) = \mathbb{E}_{\boldsymbol{\theta}}[R]$ when the $\{\boldsymbol{X}_i\}$ are iid with probability density function $f(\boldsymbol{x};\boldsymbol{\theta})$, thus $f_t(\mathbf{x}_t) = \prod_{i=1}^{t} f(\boldsymbol{x}_i)$. Let $z(\boldsymbol{x})$ be any importance sampling probability density function, and let $z_t(\mathbf{x}_t) = \prod_{i=1}^{t} z(\boldsymbol{x}_i)$. From Rubinstein and Shapiro [1993], it can be shown that $l_R(\boldsymbol{\theta})$ can be represented as

$$l_R(\boldsymbol{\theta}) = \mathbb{E}_z\left[\sum_{t=1}^{T} Y_t(\mathbf{X}_t)\Lambda_t(\mathbf{X}_t;\boldsymbol{\theta})\right] \tag{4.20}$$

where $\mathbf{X}_t \sim z_t(\mathbf{x})$ and $\Lambda_t(\mathbf{X}_t;\boldsymbol{\theta}) = f_t(\mathbf{x}_t;\boldsymbol{\theta})/z_t(\mathbf{x}_t) = \prod_{j=1}^{t} f(\boldsymbol{X}_j;\boldsymbol{\theta})/z(\boldsymbol{X}_j)$. Further, in order to proceed, we write

$$\sum_{t=1}^{T} Y_t = \sum_{t=1}^{\infty} Y_t I_{\{T\geq t\}}. \tag{4.21}$$

Note that $T = T(\mathbf{X}_t)$ is completely determined by $\mathbf{X}_t$, therefore the indicator $I_{\{T\geq t\}}$ can

be viewed as a function of $\mathbf{x}_t$; we write $I_{\{T\geq t\}}(\mathbf{x}_t)$. Hence the expectation of $Y_t I_{\{T\geq t\}}$ is

$$\begin{aligned}\mathbb{E}_{\boldsymbol{\theta}}[Y_t I_{\{T\geq t\}}] &= \int Y_t(\mathbf{x}_t) I_{\{T\geq t\}}(\mathbf{x}_t) f_t(\mathbf{x}_t;\boldsymbol{\theta})\, \mathrm{d}\mathbf{x}_t \\ &= \int Y_t(\mathbf{x}_t) I_{\{t\geq t\}}(\mathbf{x}_t) \Lambda_t(\mathbf{x}_t;\boldsymbol{\theta}) z_t(\mathbf{x}_t)\, \mathrm{d}\mathbf{x}_t \\ &= \mathbb{E}_z[Y_t(\mathbf{X}_t) I_{\{T\geq t\}}(\mathbf{X}_t) \Lambda_t(\mathbf{X}_t;\boldsymbol{\theta})].\end{aligned} \tag{4.22}$$

The result in equation (4.20) follows by combining equations (4.21) and (4.22). For the case where $Y_t \equiv 1$, equation (4.20) reduces to

$$\mathbb{E}_{\boldsymbol{\theta}}[T] = \mathbb{E}_z\left[\sum_{t=1}^{T} \Lambda_t\right] \tag{4.23}$$

abbreviating $\Lambda_t(\mathbf{X}_t;\boldsymbol{\theta})$ to Λ_t. In a similar manner under interchangeability of the differentiation and expectation operators, one can write [Rubinstein and Shapiro, 1993]

$$\nabla l_R(\boldsymbol{\theta}) = \mathbb{E}_z\left[\sum_{t=1}^{T} Y_t \mathcal{S}_t \Lambda_t\right] \tag{4.24}$$

where $\mathcal{S}_t$ is the score function corresponding to $f_t(\mathbf{x}_t;\boldsymbol{\theta})$. Given a sample $\{\boldsymbol{X}_{11}, ..., \boldsymbol{X}_{T_1 1}, \boldsymbol{X}_{12}, \cdots, \boldsymbol{X}_{T_2 2}, \cdots, \boldsymbol{X}_{1N}, \cdots, \boldsymbol{X}_{T_N N}\}$ of N regenerative cycles from the probability density function $z(\boldsymbol{x})$, using equation (4.24), we can estimate $\nabla l_R(\boldsymbol{\theta})$ by simulation as

$$\widehat{\nabla l_R}(\boldsymbol{\theta}) = \frac{1}{N}\sum_{i=1}^{N}\sum_{t=1}^{T_i} Y_{ti}\mathcal{S}_{ti}\Lambda_{ti} \tag{4.25}$$

with

$$\Lambda_{ti} = \prod_{j=1}^{t} \frac{f(\boldsymbol{X}_{ji};\boldsymbol{\theta})}{z(\boldsymbol{X}_{ji})} \tag{4.26}$$

with $\boldsymbol{X}_{ji} \sim z(\boldsymbol{x})$. Moreover, the score function process $\{\mathcal{S}_t\}$ is given by

$$\mathcal{S}_t = \sum_{j=1}^{t} \nabla f(\boldsymbol{X}_j;\boldsymbol{\theta}). \tag{4.27}$$

Let us return to $l(\boldsymbol{\theta}) = \mathbb{E}_{\boldsymbol{\theta}}[R]/\mathbb{E}_{\boldsymbol{\theta}}[T]$ and its partial derivatives. In view of equation (4.24) and the fact that $T = \sum_{t=1}^{T} 1$ can be viewed as a special case of equation (4.20), with $Y_t \equiv 1$, then one can write $l(\boldsymbol{\theta})$ as

$$l(\boldsymbol{\theta}) = \frac{\mathbb{E}_z[\sum_{t=1}^{T} Y_t \Lambda_t]}{\mathbb{E}_z[\sum_{t=1}^{T} \Lambda_t]} \tag{4.28}$$

and by direct differentiation of equation (4.28) the partial derivatives of $l(\boldsymbol{\theta})$ with respect to $\boldsymbol{\theta}$ are obtained as [Rubinstein and Shapiro, 1993]

$$\nabla l(\boldsymbol{\theta}) = \frac{\mathbb{E}_z[\sum_{t=1}^{T} Y_t \Lambda_t \mathcal{S}_t]}{\mathbb{E}_z[\sum_{t=1}^{T} \Lambda_t]} - \frac{\mathbb{E}_z[\sum_{t=1}^{T} Y_t \Lambda_t]}{\mathbb{E}_z[\sum_{t=1}^{T} \Lambda_t]} . \frac{\mathbb{E}_z[\sum_{t=1}^{T} \Lambda_t \mathcal{S}_t]}{\mathbb{E}_z[\sum_{t=1}^{T} \Lambda_t]}. \tag{4.29}$$

Note that $\Lambda_t = \Lambda_t(\mathbf{X}_t; \boldsymbol{\theta})$ is a function of $\boldsymbol{\theta}$ but $Y_t = Y_t(\mathbf{X}_t)$ is not. Then the estimator of $\nabla l(\boldsymbol{\theta})$ is

$$\widehat{\nabla l}(\boldsymbol{\theta}) = \frac{\sum_{i=1}^{N} \sum_{t=1}^{T_i} Y_{ti} \Lambda_{ti} \mathcal{S}_{ti}}{\sum_{i=1}^{N} \sum_{t=1}^{T_i} \Lambda_{ti}} - \frac{\sum_{i=1}^{N} \sum_{t=1}^{T_i} Y_{ti} \Lambda_{ti}}{\sum_{i=1}^{N} \sum_{t=1}^{T_i} \Lambda_{ti}} . \frac{\sum_{i=1}^{N} \sum_{t=1}^{T_i} \Lambda_{ti} \mathcal{S}_{ti}}{\sum_{i=1}^{N} \sum_{t=1}^{T_i} \Lambda_{ti}}. \tag{4.30}$$

The following table illustrates the steps of the algorithm to estimate SDIM for multiple values of $\boldsymbol{\theta}$.

Algorithm 2 Estimation of SDIM for multiple values of $\boldsymbol{\theta}$

1. Generate a random sample $\{\boldsymbol{X}_{11}, ..., \boldsymbol{X}_{T_1 1}, \boldsymbol{X}_{12}, \cdots, \boldsymbol{X}_{T_2 2}, \cdots, \boldsymbol{X}_{1N}, \cdots, \boldsymbol{X}_{T_N N}\}$ where $\tau = \sum_{i=1}^{N} T_i$, from $z(\boldsymbol{x})$.
2. Generate the output process $\{Y_t\}$ and $\{\Lambda_t \mathcal{S}_t\}$.
3. Calculate $\widehat{\nabla l}(\boldsymbol{\theta})$ from (4.30) and corresponding $\widehat{\text{SDIM}}_j$ for $j = 1, ..., m$.

4.2.3 Application of SDIM to the waiting time process in a M/M/1 queue

An M/M/1 queueing system is the simplest non-trivial queuing model where the requests arrive according to a Poisson process with rate λ. Then, interarrival times are independent, exponentially distributed random variables with parameter λ. The service times are also assumed to be independent and exponentially distributed with parameter μ. Moreover, all the involved random variables are supposed to be independent of each other. We are interested to assess the sensitivity of the arrival and service rates on the mean waiting time of the system for a given values of λ and μ. This kind of analysis can be used to answer queuing problems such as what happens to the waiting time of the system if we improve the service rate by some percentage.

The waiting time process in a M/M/1 queue is driven by sequences of inter arrival times $\{A_t\}$ and service times $\{S_t\}$ via the Lindley equation

$$Y_t = \max\{Y_{t-1} + S_t - A_t, 0\}, t = 1, 2, ... \tag{4.31}$$

with $Y_0 = 0$. Writing $\boldsymbol{X}_t = (A_t, S_t)$, the $\{\boldsymbol{X}_t, t = 1, 2, ...\}$ are iid random variables with

$S \sim \text{Exp}(\mu)$ and $A \sim \text{Exp}(\lambda)$; S and A independent. The process $\{Y_t, t = 0, 1, ...\}$ is a regenerative process, which regenerates every time $Y_t = 0$. Let $T > 0$ denote the first such time, and let Y denote the steady -state (refer Sztrik [2010] about the steady state of queuing systems) waiting time in the M/M/1 queue. Then the steady state performance is

$$l(\boldsymbol{\theta}) = \mathbb{E}_{\boldsymbol{\theta}}[Y] = \frac{\mathbb{E}[\sum_{t=1}^{T} Y_t]}{\mathbb{E}[T]} \tag{4.32}$$

with $\mathbb{E}(Y) = \lambda/(\mu(\mu - \lambda))$ for $\mu > \lambda$ and $\boldsymbol{\theta} = (\lambda, \mu)$. Hence the analytical expressions of SDIM_μ and SDIM_λ are $(\lambda^2 - 2\mu\lambda)/(\mu - \lambda)^2$ and $\mu^2/(\mu - \lambda)^2$, respectively. We carried out the simulation for two scenarios, first using service rate $\tilde{\mu} = 2$ and fixed $\lambda = 1$ and estimated $\partial l(\boldsymbol{\theta})/\partial\mu$ for different values of μ and secondly using arrival rate $\tilde{\lambda} = 1.5$ and fixed $\mu = 2.5$ and estimated $\partial l(\boldsymbol{\theta})/\partial\lambda$ for different values of λ . Let $(S_1, A_1), ..., (S_T, A_T)$ denote the service and inter arrival times in the first cycle, respectively. Then, for the first cycle

$$\Lambda_t^\mu = \Lambda_{t-1}^\mu \frac{\mu \exp(-\mu S_t)}{\tilde{\mu} \exp(-\tilde{\mu} S_t)} \qquad t = 1, 2, ..., T \quad (\Lambda_0^\mu = 1)$$

$$\Lambda_t^\lambda = \Lambda_{t-1}^\lambda \frac{\lambda \exp(-\lambda A_t)}{\tilde{\lambda} \exp(-\tilde{\lambda} A_t)} \qquad t = 1, 2, ..., T \quad (\Lambda_0^\lambda = 1)$$

are likelihood ratios when λ and μ are fixed. Moreover the corresponding score functions are

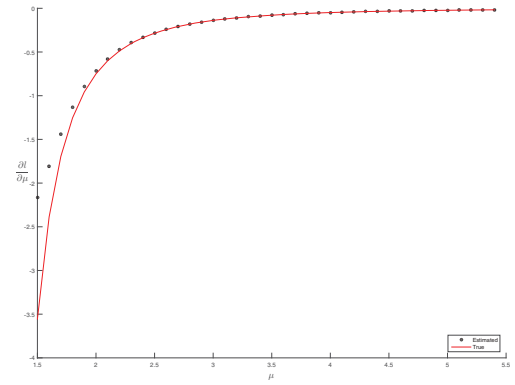
$$\mathcal{S}_t^\mu = \mathcal{S}_{t-1}^\mu + \frac{1}{\mu} - S_t \qquad t = 1, 2, ..., T \quad (\mathcal{S}_0^\mu = 0) \tag{4.33}$$

$$\mathcal{S}_t^\lambda = \mathcal{S}_{t-1}^\lambda + \frac{1}{\lambda} - A_t \qquad t = 1, 2, ..., T \quad (\mathcal{S}_0^\lambda = 0) \tag{4.34}$$

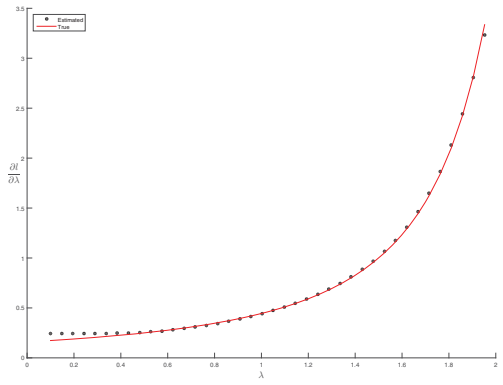
From these quantities, the sums $\sum_{t=1}^{T} Y_t \Lambda_t$, $\sum_{t=1}^{T} \Lambda_t$, $\sum_{t=1}^{T} \Lambda_t \mathcal{S}_t$, and $\sum_{t=1}^{T} Y_t \Lambda_t \mathcal{S}_t$ are computed. Repeating this for the subsequent cycles, we estimated SDIM_μ and SDIM_λ, first by estimating $\nabla l(\boldsymbol{\theta})$ for $\boldsymbol{\theta} = (\mu = 2.5, \lambda = 1)$ and then using equation (4.13). The graph in the top of figure (4.11) show the estimated $\partial l/\partial\mu$ and $\partial l/\partial\lambda$ with $N = 10^5$ for different values of μ and λ, respectively. The red line corresponds to the analytical value. The bottom part of the figure (4.11) show the estimated SDIM_μ and SDIM_λ when $\mu = 2.5$ and $\lambda = 1$ across different sample sizes. The red lines correspond to the analytical values of SDIM_μ and SDIM_λ and we observe that as the sample size increases the estimated quantities reach their analytical values.

4.3 Summary

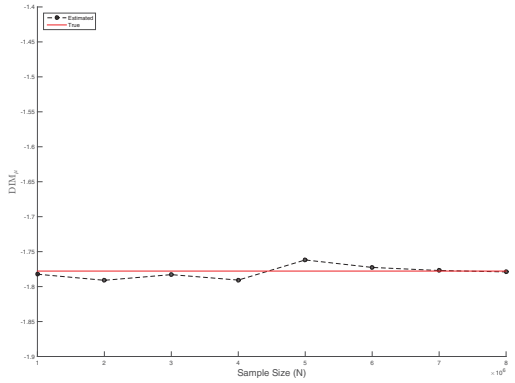
We have proposed a local sensitivity measure, SDIM in the presence of uncertainty on the model inputs. Specifically, the output of interest is deterministic given the input value but stochastic given the distributional parameters of the model inputs. The uncertainty



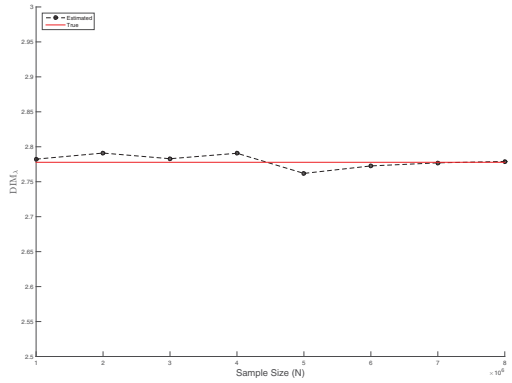
(a) Estimated and true values of $\partial l/\partial \mu$



(b) Estimated and true values of $\partial l/\partial \lambda$



(c) Estimated and true values of $\text{SDIM}_\mu = -1.778$



(d) Estimated and true values of $\text{SDIM}_\lambda = 2.778$

Figure 4.11: Estimated and true values for the expected steady-state waiting time derivatives and its SDIM for $\boldsymbol{\theta} = (\mu, \lambda) = (2.5, 1)$

about the model inputs is expressed through a probability distribution through a fixed and known parametric family. The sensitivity analysis is carried out using SDIM with respect to parameters on the expected value of a model seen as a deterministic function of the parameters. Further a simulation study has been carried out to illustrate the performance of the estimator of SDIM in applications of discrete event static and dynamic systems. The estimation method is associated with the score function of the underlying probability density function $f(\boldsymbol{x}; \boldsymbol{\theta})$ and a realization of the output process $g(\boldsymbol{X})$. Hence, one is capable of reducing computational burden. Further, one can generalize SDIM to a global sensitivity measure using importance sampling to obtain SDIM at several random points in the distributional parameter space, Θ. This intuition coincides with that of RDIM introduced in the previous chapter. Further, the additivity property of SDIM plays an important role in evaluating the importance of the system components, especially in reliability analysis applications.

Chapter 5

Sensitivity Analysis of Stochastic Models

There are situations in which the model produces different values each time it is run with a fixed set of inputs. In this case, we treat the simulation model as a process mapping input values to output distributions. Performing sensitivity analysis in this context is challenging. This chapter takes the initial step of introducing a novel methodology to perform sensitivity analysis of such models.

5.1 Motivation

For the purpose of this thesis, we take in to account only the models with scalar outputs. In chapter 3 we presented RDIM, a global sensitivity measure for deterministic outputs constructed as the expected value of DIM. Moreover, in chapter 4, we proposed a local sensitivity measure SDIM with respect to input distributional parameters. So in this case the unobservable variables are integrated out. Aside of these mentioned sensitivity measures, in this chapter we are interested to evaluate the sensitivities with respect to unobservable variables in a fully stochastic framework. This chapter introduces a new class of density based measures for stochastic models while it is looking to future research of implementing more efficient estimation methods.

In this context, a stochastic model is a computer program, for which the output value produced is *random* or *non deterministic* once all model inputs are fixed at a given value. That is, for a fixed set of inputs, the stochastic model will produce different output values each time it is run. Hence, the output presents an inherent uncertainty not necessarily induced by uncertainty on the model inputs. Since a stochastic model does not map a set of input values to a single output value, we cannot use the methods presented in the previous sections to address its sensitivity. Formally, a stochastic model, g is a process mapping a set of inputs, $\boldsymbol{X} = (X_1, X_2, \cdots, X_j, \cdots, X_n)$ to a distribution for the output

values. We let Y denote the output of this model for a given $\boldsymbol{X}$ and we write $Y|\boldsymbol{X} \sim g(\boldsymbol{X})$ to indicate both the randomness in Y and the role of g as the process mapping the inputs, $\boldsymbol{X}$, to the distribution governing $Y|\boldsymbol{X}$. When there is no ambiguity about g(x), we omit g and refer to $f_{Y|\boldsymbol{X}}$ as the output distribution (see figure 5.1).

Specially, we are interested to quantify how much changing one or more of the model inputs changes the distribution of the output, i.e., how sensitive the output distribution is to changes in the inputs.

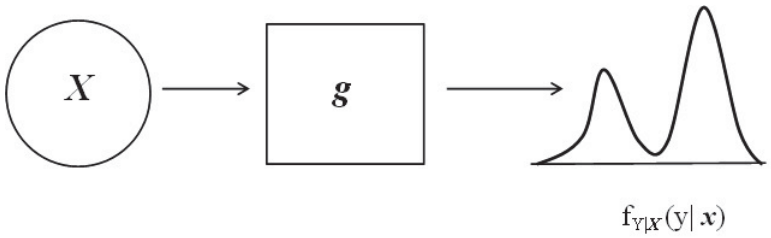


Figure 5.1: Diagram illustrating the structure of a stochastic model.

For a deterministic model, any output distribution is a result of input uncertainty. If the model inputs were known exactly, the output would not be random. Formally, let $\mathcal{G}_{\boldsymbol{X}}$ be some uncertainty distribution on the inputs $\boldsymbol{X}$, that is, $\boldsymbol{X} \sim \mathcal{G}_{\boldsymbol{X}}$. Then this input uncertainty induces a distribution on the output $Y = g(\boldsymbol{X})$. If the form of g is known, then the distribution of Y can be derived analytically in many cases. However, if the model g is stochastic then it is inherently random by definition, thus certainty in the model inputs would still result in a distribution for the output Y which means that uncertainty in the model inputs is not the only factor inducing uncertainty on Y. Formally, if $\boldsymbol{X} \sim \mathcal{G}_{\boldsymbol{X}}$, then $\mathcal{G}_{\boldsymbol{X}}$ induces a distribution over distributions for the output Y, and $f_{Y|\boldsymbol{X}}$ denotes one potential realization from those possible distributions.

5.2 Sensitivity Analysis of Stochastic Models

In the case of global climate models for example climatologist would be interested in the effect of the humidity on the long term weather forecast. In most of these applications the provided model is *stochastic*. Our goal is to perform sensitivity analysis by characterizing the relationship between the model inputs and the output distribution in the presence of randomness in the model. Particularly, we want to measure how much changing one or more inputs changes the output distribution.

Quantifying the effect of the model inputs on the output distribution requires a good way to characterize distributions. A basic approach would be to summarize the distribution with a mean and a variance. That is, for a given output distribution $f_{Y|\boldsymbol{X}}$, we would calculate

$$M(\boldsymbol{x}) = E(Y|\boldsymbol{X} = \boldsymbol{x}) = \int_{\mathcal{Y}} y f_{Y|\boldsymbol{X}}(y|\boldsymbol{x}) \mathrm{d}y$$

$$V(\boldsymbol{x}) = V(Y|\boldsymbol{X} = \boldsymbol{x}) = \int_{\mathcal{Y}} (y - M(\boldsymbol{x})) f_{Y|\boldsymbol{X}}(y|\boldsymbol{x}) \mathrm{d}y.$$

The effect of the model inputs on the output distribution can then be measured by calculating some sensitivity measures on these two functions. In fact, since M and V are deterministic functions, one can apply any sensitivity measure for deterministic models, i.e., Variance based measures, differential based measures etc. However, there are a few problems to this approach. First, sensitivity measures calculated in this manner only quantify the effects of $\boldsymbol{X}$ on two moments of the output distribution. Whether conclusions drawn from these effects translate back to the output distribution depends entirely on how adequately the distribution of Y is characterised by these moments. For output distributions like a normal distribution, this may not be much of a problem. If the form of the output distribution is unknown or has a complex behaviour (e.g. asymmetry, multi-modality), then conclusions about the impact of the inputs on M and V may not necessarily apply to the output distribution.

Moreover, it is not always clear how to simultaneously interpret the results of a sensitivity analysis on the two functions $M(\boldsymbol{x})$ and $V(\boldsymbol{x})$. For instance, suppose the model has two inputs X_1 and X_2. After calculating $M(x_1, x_2)$ and $V(x_1, x_2)$ and performing a sensitivity analysis, one finds that X_1 has a large impact on the mean function, but a low impact on the variance. Conversely, X_2 has a low impact on the mean function and a high impact on the variance function. Even though in most cases, sensitivity analysis may provide some insights on the importance of these two factors, it is often difficult to interpret these two different summaries simultaneously. While having both the mean and variance provides more information about the process than a single number, situations possibly arise where a single number is desired.

Instead of relying on the mean and the variance of the distribution of a stochastic output to quantify the relationship between the model inputs and the output distribution, we propose the use of a sensitivity measure (η_ϕ) associated with "*Csiszár f-divergences*" which belongs to the family of density based sensitivity measures introduced in chapter 2. This approach permits the evaluation of the model input importance by measuring the discrepancy between the conditional and the unconditional distribution of Y. In the stochastic model framework, the f-divergence between f_Y and $f_{Y|X_j}$ quantifies how much learning the value of $f_{Y|X_j}$ reduces the uncertainty about the output f_Y. If an input has a large effect on the output distribution, be it through an effect on the mean or the variance, η_ϕ between f_Y and $f_{Y|X_j}$ will be high.

5.2.1 Csiszár's f-divergences as Sensitivity Measures for Stochastic Models

Assuming that (Y,X_j) has an absolutely continuous distribution with respect to the Lebesgue measure on $\mathbb{R}^2$ for all $j = 1, 2, ..., n$, an f-divergence (Csiszár [1972]) between f_Y and $f_{Y|X_j}$ is given by

$$d_\phi(f_Y||f_{Y|X_j}) = \int_{\mathbb{R}} \phi\left(\frac{f_Y(y)}{f_{Y|X_j}(y)}\right) f_{Y|X_j}(y)\mathrm{d}y \tag{5.1}$$

where ϕ is a convex function such that $\phi(1) = 0$ and f_Y and $f_{Y|X_j}$ are the marginal and conditional probability density functions of Y and $Y|X_j$, respectively. Potential choices of ϕ lead to well known divergences found in the literature (see table (5.1)) [Da Veiga, 2013].

Table 5.1: Standard choices of ϕ in f-divergences

Choice of ϕ	Name
$\phi(x) = -ln(x)$ or $\phi(x) = xlnx$	Kullback-Leibler divergence (ϕ_{KL})
$\phi(x) = (\sqrt{x} - 1)^2$	Hellinger distance (ϕ_H)
$\phi(x) = \lvert x - 1\rvert$	Total variation distance (ϕ_{TV})
$\phi(x) = (x-1)^2$ or $\phi(x) = x^2 - 1$	Pearson χ^2 divergence (ϕ_P)

Formally, the sensitivity index of X_j is obtained by taking the expectation of $d_\phi(f_Y||f_{Y|X_j})$ with respect to X_j. i.e.,

$$\eta_\phi(X_j, Y) = \mathbb{E}_{X_j}[d_\phi(f_Y||f_{Y|X_j})] \tag{5.2}$$

Plugging equation (5.1) into (5.2) yields the following sensitivity index:

$$\eta_\phi(X_j, Y) = \int_{\mathbb{R}^2} \phi\left(\frac{f_Y(y)f_{X_j}(x)}{f_{X_j,Y}(x,y)}\right) f_{X_j,Y}(x,y)\mathrm{d}x\mathrm{d}y. \tag{5.3}$$

η_ϕ measures the average divergence between Y and X_j. It quantifies the probabilistic dependence between Y and X_j. The stronger the statistical dependence, the higher the value of $\eta_\phi(X_j, Y)$.

It is not difficult to see that $\eta_\phi(X_j, Y)$ possesses the following properties:

- $\eta_\phi(X_j, Y) \geq 0$ (due to Jensen's inequality).
- $\eta_\phi(X_j, Y) = 0$ if Y and X_j are independent.
- For any given standard choice of ϕ, $\eta_\phi(X_j, Y)$ is *invariant under any smooth and uniquely invertible* (homeomorphism) transformation of the variables X_j and Y (see

the following lemma). This is a main advantage over variance-based sensitivity indices, which are only invariant under linear transformations.

Note that similar results were found in Borgonovo et al. [2013] where families of transformation invariant sensitivity indices are discussed.

Lemma

If $X_j' = \mathrm{F}(X_j)$ and $Y' = \mathrm{Z}(Y)$ are homeomorphisms with corresponding realizations $x_j \in \mathcal{X}_j$ and $y \in \mathcal{Y}$, and $\mathrm{J}_{X_j} = ||\partial X_j/\partial X_j'||, \mathrm{J}_Y = ||\partial Y/\partial Y'||$ are the corresponding Jacobi determinants, then $\eta_\phi(X_j', Y') = \eta_\phi(X_j, Y)$

Proof. $f_{X_j',Y'}(x_j', y') = \mathrm{J}_{X_j}(x_j')\mathrm{J}_Y(y')f_{X_j,Y}(x_j, y)$

$$\begin{aligned}\eta_\phi(X_j', Y') &= \int_{\boldsymbol{\mathcal{X}_j'}}\int_{\boldsymbol{\mathcal{Y}'}} \phi\left(\frac{f_{Y'}(y')f_{X_j'}(x_j')}{f_{Y',X_j'}(y', x_j')}\right) f_{Y',X_j'}(y', x_j')\mathrm{d}x_j'\mathrm{d}y' \\ &= \int_{\boldsymbol{\mathcal{X}_j'}}\int_{\boldsymbol{\mathcal{Y}'}} \phi\left(\frac{f_{Y'}(y')f_{X_j'}(x_j')}{f_{Y',X_j'}(y', x_j')}\right) \mathrm{J}_{X_j}(x_j')\mathrm{J}_Y(y')f_{Y,X_j}(y, x_j)\mathrm{d}x_j'\mathrm{d}y'\end{aligned}$$

$$f_{Y'}(y') = \mathrm{J}_Y(y')f_Y(y) \tag{i}$$

$$f_{X'}(x_j') = \mathrm{J}_{X_j}(x_j')f_{X_j}(x_j) \tag{ii}$$

$$f_{Y',X_j'}(y', x_j') = \mathrm{J}_{X_j}(x_j')\mathrm{J}_Y(y')f_{Y,X_j}(y, x_j) \tag{iii}$$

By (i),(ii) and (iii), we obtain

$$\phi\left(\frac{f_{Y'}(y')f_{X_j'}(x_j')}{f_{Y',X_j'}(y', x_j')}\right) = \phi\left(\frac{f_Y(y)f_{X_j}(x_j)}{f_{Y,X_j}(y, x_j)}\right)$$

Thus,

$$\eta_\phi(X_j', Y') = \int_{\mathcal{X}_j}\int_{\mathcal{Y}} \phi\left(\frac{f_Y(y)f_{X_j}(x_j)}{f_{Y,X_j}(y, x_j)}\right) f_{Y,X_j}(y, x_j)\mathrm{d}x_j\mathrm{d}y = \eta_\phi(X_j, Y) \tag{5.4}$$

□

When ϕ is the total variation distance, $\eta_{\phi_{TV}}$ gives [Da Veiga, 2013] a sensitivity index which is equal to the one proposed by Borgonovo [2007] and it is a symmetric sensitivity measure, i.e., $\eta_{\phi_{TV}}(X_j, Y) = \eta_{\phi_{TV}}(Y, X_j)$. In addition, the Kullback-Leibler divergence

with $\phi(x) = -\ln(x)$ gives the mutual information $I(X_j,\mathrm{Y})$ between X_j and Y. Similarly the sensitivity index given by, the Neyman χ^2 divergence with $\phi(x) = (1-x)^2/x$ is the same as the so-called squared-loss mutual information between X_j and Y. This concludes that some previously proposed sensitivity indices are actually some special cases of the expected value of the Csiszár's f-divergence between f_Y and $f_{Y|\boldsymbol{X}}$. However, we are interested to see how sensitivity measures based on f-divergences perform in a stochastic model frame work. Depending on the choice of ϕ, the importance of the model inputs may differ. The following example illustrates of obtaining analytical expression for $\eta_{\phi_{KL}}$.

5.2.2 An Example

Let X be a normal random variable with mean μ and variance σ^2. Given X, let Y be a Gaussian random variable, with mean X and variance τ^2.

$$Y|X \sim N(X, \tau^2)$$
$$X \sim N(\mu, \sigma^2)$$

Let us obtain the analytical expression for $\eta_{\phi_{KL}}(X,Y)$ where $\phi(x) = -\ln(x)$ which corresponds to the Kullback-Leibler sensitivity index, i.e., mutual information.

$$\eta_{\phi_{KL}}(X,Y) = \mathbb{E}_X(d_{\phi_{KL}}(f_{\mathrm{Y}}||f_{\mathrm{Y}|X})) = \int_{\boldsymbol{\mathcal{X}}}\int_{\boldsymbol{\mathcal{Y}}} f_{X,Y}(x,y)\ln\left(\frac{f_{X,Y}(x,y)}{f_X(x)f_Y(y)}\right)\mathrm{d}y\,\mathrm{d}x$$

A result known in information theory tells us that

$$\eta_{\phi_{KL}}(X,Y) = H(X) + H(Y) - H(X,Y). \tag{5.5}$$

$H(X) = -\mathbb{E}_X\left(\log f_X(x)\right)$ called the differential entropy of X is a measure of the uncertainty or randomness of the variable X. If the entropy is large, then a realization of X is unpredictable. Analogously, for $H(Y)$ and $H(X,Y)$. The entropy of X in this example

is given by

$$\begin{aligned}
H(X) &= -\int_{\mathcal{X}} \log\{f_X(x)\} f_X(x)\mathrm{d}x \\
&= -\int_{\mathcal{X}} \log\left(\frac{1}{(2\pi\sigma^2)^{1/2}}\ e^{\frac{-(x-\mu)^2}{2\sigma^2}}\right)\frac{1}{(2\pi\sigma^2)^{1/2}}\ e^{\frac{-(x-\mu)^2}{2\sigma^2}}\mathrm{d}x \\
&= -\int_{\mathcal{X}} \left[\log\left(\frac{1}{2\pi\sigma^2)^{1/2}}\right) - \frac{(x-\mu)^2}{2\sigma^2}\right]\left[\frac{1}{(2\pi\sigma^2)^{1/2}}\ e^{\frac{-(x-\mu)^2}{2\sigma^2}}\right]\mathrm{d}x \\
&= -\log\left(\frac{1}{2\pi\sigma^2}\right) + \int_{\mathcal{X}} \frac{(x-\mu)^2}{2\sigma^2}\frac{1}{(2\pi\sigma^2)^{1/2}}\ e^{\frac{-(x-\mu)^2}{2\sigma^2}}\mathrm{d}x \\
&= \frac{1}{2}\log\big(2\pi\sigma^2\big) + \frac{1}{2\sigma^2}\underbrace{\int_{\mathcal{X}} (x-\mu)^2\ \frac{1}{(2\pi\sigma^2)^{1/2}}\ e^{\frac{-(x-\mu)^2}{2\sigma^2}}\mathrm{d}x}_{\mathrm{E}(X-\mu)^2=\sigma^2} \\
&= \frac{1}{2}\log\big(2\pi\sigma^2\big) + \frac{\sigma^2}{2\sigma^2} \\
&= \frac{1}{2}\log\left(2\pi\sigma^2 e\right).
\end{aligned}$$

In order to find $H(Y)$, first we need to find the marginal distribution of Y which can be obtained by integrating out X from the conditional distribution $Y|X$.

$$f_Y(y) = \int_{\mathcal{X}} f_{Y|X}(y) f_X(x)\mathrm{d}x \propto \int_{\mathcal{X}} \exp\left(\frac{-(y-x)^2}{2\tau^2}\right)\ \exp\left(\frac{-(x-\mu)^2}{2\sigma^2}\right)\mathrm{d}x$$

Therefore, Y has a Gaussian distribution with mean

$$\mathbb{E}_Y[Y] = \mathbb{E}_X[\mathbb{E}_{Y|X}[Y|X]] = \mathbb{E}_X[X] = \mu$$

and a variance

$$\begin{aligned}
\mathbb{V}_Y(Y) &= \mathbb{V}_X(\mathbb{E}_{Y|X}[Y|X]) + \mathbb{E}_X(\mathbb{V}_{Y|X}(Y|X)) \\
&= \mathbb{V}_X[X] + \mathbb{E}_X[\tau^2] \\
&= \sigma^2 + \tau^2
\end{aligned}$$

Thus, $H(Y) = \frac{1}{2}\log\left(2\pi e(\sigma^2+\tau^2)\right)$. Since the dependence between Y and X is specified by the conditional distribution, it is straightforward to obtain the conditional entropy $H(Y|X)$

$$H(Y|X) = -\int_{\mathcal{X}}\int_{\mathcal{Y}} \log\{f_{Y|X}(y|x)\} f_{X,Y}(x,y)\mathrm{d}x\mathrm{d}y$$

$$\begin{aligned} H(Y|X) &= -\int_{\mathcal{X}} \left[\int_{\mathcal{Y}} \log\{f_{Y|X}(y|x)\} f_{Y|X}(y|x) \mathrm{d}y \right] f_X(x) \mathrm{d}x \\ &= -\mathbb{E}_X[\mathbb{E}_{Y|X}\left[\log\{f_{Y|X}(Y|X)\}\right]] \\ &= \mathbb{E}_X\left[\frac{1}{2}\log\left(2\pi\tau^2 e\right)\right] \\ &= \frac{1}{2}\log\left(2\pi\tau^2 e\right) \end{aligned}$$

Note that from the chain rule,

$$H(X,Y) = H(Y|X) + H(X) = H(Y) + H(X|Y)$$

Thus,

$$H(X,Y) = \frac{1}{2}\log\left(2\pi\tau^2 e\right) + \frac{1}{2}\log\left(2\pi\sigma^2 e\right) = \frac{1}{2}\log\{(2\pi e)^2\sigma^2\tau^2)\}$$

Returning to equation (5.5),

$$\eta_{\phi_{KL}}(X,Y) = \frac{1}{2}\log\left(2\pi\sigma^2 e\right) + \frac{1}{2}\log\left(2\pi e(\sigma^2+\tau^2) - \frac{1}{2}\log\{(2\pi e)^2\sigma^2\tau^2)\}\right.$$

$$\eta_{\phi_{KL}}(X,Y) = \frac{1}{2}\log\left(\frac{\sigma^2+\tau^2}{\tau^2}\right) \tag{5.6}$$

If the variance of X, σ^2, is fixed, increasing the conditional variance of Y (τ^2) decreases the mutual information. As τ^2 tends to be higher, the mutual information approaches 0. Of course, this is true since increasing the conditional variance should decrease the effect of the uncertainty in X. On the other hand, if τ^2 is fixed, increasing σ^2, the prior variance of the mean, increases the mutual information. Increasing σ^2, increases $H(Y) = \frac{1}{2}\log\left(2\pi e(\sigma^2+\tau^2)\right.$, which means that, it increases the marginal randomness of Y. Thus, it increases the importance of learning the value of X. This is exactly what we expect from the mutual information.

The above example clearly demonstrates how mutual information can be a tool for conducting sensitivity analysis. Thus, we would expect $\eta_{\phi_H}, \eta_{\phi_{TV}}$ and η_{ϕ_P} to give the same conclusions as $\eta_{\phi_{KL}}$. Due to intractable integrals, it is not efficient to obtain closed form expressions for $\eta_{\phi_H}, \eta_{\phi_{TV}}$ and η_{ϕ_P}. Thus, a naive approach is to estimate these indices numerically. The next section is devoted to the estimation of η_ϕ in a general framework.

5.3 Estimation of Csiszár's f-divergence Sensitivity Indices

Our goal is to estimate

$$\eta_\phi(X_j, Y) = \int_{\mathbb{R}^2} \phi\left(\frac{1}{r(X_j, \mathrm{Y})}\right) f_{X_j,\mathrm{Y}}(x, y)\mathrm{d}x\mathrm{d}y = \mathbb{E}_{(X_j,\mathrm{Y})}\left[\phi\left(\frac{1}{r(X_j, \mathrm{Y})}\right)\right]$$

where $r(X_j, \mathrm{Y}) = f_{X_j,Y}(x, y)/f_{X_j}(x)f_Y(y)$. In the literature, different methods have been proposed for estimating $\eta_{\phi_{KL}}$ such as nearest neighbor strategy (Kraskov et al. [2008]) and maximum likelihood estimation (Suzuki et al. [2008]). There are also estimation methods proposed for ϕ_{TV} [Liu and Homma, 2009]. However, a general approach to estimate sensitivity indices associated with f-divergence would be to use *re-substitution estimates* of the form

$$\hat{\eta}_\phi(X_j, \mathrm{Y}) = \frac{1}{N}\sum_{i=1}^{N} \phi\left(\frac{1}{\hat{r}(X_{ji}, \mathrm{Y}_i)}\right) \tag{5.7}$$

where

$$\hat{r}(X_j, \mathrm{Y}) = \frac{\hat{f}_{X_j,\mathrm{Y}}(x, y)}{\hat{f}_Y(y)\hat{f}_{X_j}(x)}$$

where $\hat{f}$ denotes an estimate of the corresponding density based on a sample $(\boldsymbol{X}_i, \mathrm{Y}_i)_{i=1,...,N}$, where, $\boldsymbol{X}_i = (X_{1,i}, X_{2,i}, ..., X_{j,i}, ..., X_{n,i})$, n is the number of model inputs and N is the sample size. This type of estimator goes through two approximations: a Monte Carlo approximation for η_ϕ and approximation of the density. This Monte Carlo integral can be viewed as an application of the law of large numbers as discussed in Chapter 3. A potential choice of $\hat{f}$ is a non-parametric density estimator such as kernel density estimator (KDE) or histogram estimator.

Let us focus on KDE in this setting. The kernel density estimator of $f_{X_j,Y}(x, y)$ is given by

$$\hat{f}_{X_j,Y}(x, y) = \frac{1}{N}\sum_{i=1}^{N} K_L(\boldsymbol{x} - \boldsymbol{X}_i) \tag{5.8}$$

where $\boldsymbol{x} = (x, y)$ and $K_L = |L|^{-1/2}K(L^{-1/2}\boldsymbol{x})$ where K is a multivariate kernel and L is the bandwidth matrix. In a similar manner, $\hat{f}_Y(y)$ and $\hat{f}_{X_j}(x)$ can be also obtained. By plugging these estimators in equation (5.7), we obtain a point estimator of the sensitivity index η_ϕ between X_j and Y.

5.3.1 Methodology for Conducting Sensitivity Analysis of Stochastic Models

In this section we discuss the methodology for conducting a sensitivity analysis of a stochastic model leaving the application for future work. Our main focus is on calculating the sensitivity indices ($\eta_\phi(X_j, Y)$).

Let $\mathcal{X} \subseteq \mathbb{R}^n$ be the model input space. An input $\boldsymbol{X} \subseteq \mathcal{X}$ is considered as a vector containing all model inputs such that $\boldsymbol{X} = \{X_1, ..., X_j, ..., X_n\}$. Hence, a *collection* of inputs is denoted as $\{\boldsymbol{X}_1, \boldsymbol{X}_2, \cdots, \boldsymbol{X}_N\} \subseteq \mathcal{X}$ where $\boldsymbol{X}_i = \{X_{1,i}, X_{2,i}, \cdots, X_{n,i}\}$.

To estimate the sensitivity index on the model g, we shall quantify the impact of one of the input dimensions, say X_j on the output distribution $f_{Y|\boldsymbol{X}}$. Note that we shall consider the definition of η_ϕ in equation (5.3) which is associated with the joint and the marginal density functions of X_j and Y. Formally,

$$\begin{aligned} f_Y(y) &= \int_{\mathcal{X}} f(y|x) f(x) \mathrm{d}x \\ f_{Y|X_j}(y|x_j) &= \int_{\mathcal{X}_{-j}} f(y|x) f_{-j|j}(x_{-j}|x_j) \mathrm{d}x_{-j} \\ f_{Y,X_j}(y,x) &= \int_{\mathcal{X}_{-j}} f(y|x) f(x) \mathrm{d}x_{-j} \end{aligned} \tag{5.9}$$

$f_{\boldsymbol{X}}$ is the marginal probability density of the model inputs and $f_{-j|j}$ is the conditional probability density of the model inputs $X_{-j} = (X_1, X_2, ..., X_{j-1}, X_{j+1}, ..., X_n)$ when conditioning on the value of X_j. Similarly $\mathcal{X}_{-j} = \mathcal{X}_1 \times \mathcal{X}_2 \times ... \times \mathcal{X}_{j-1} \times \mathcal{X}_{j+1} \times ... \times \mathcal{X}_n$.

The stochastic model maps the model inputs $\boldsymbol{X}$ to conditional densities. For a deterministic value of $\boldsymbol{X}$, $Y|\boldsymbol{X}$ is random. Together with the input distribution, these conditional densities define the joint marginal densities $f_{Y,X_j}(y, x)$ as shown in the last expression of the equation (5.9). In most practical applications, we don't know these densities, so $\eta_\phi(X_j, Y)$ can not be calculated directly. However, if a sample from the joint distribution $f_{Y,X_j}(y, x)$ was given, kernel density estimation would produce an estimate of $\eta_\phi(X_j, Y)$.

In order to conduct a meaningful form of inference, a variance or some other measure of uncertainty in the estimated sensitivity index is required. Based on the functional forms given in the equation (5.9), it is not easy to derive expressions of the variance of the point estimate of $\eta_\phi(X_j, Y)$. To overcome such situations, a common approach is to estimate the variance of $\hat{\eta_\phi}$ through re-sampling of the data. However, since $\hat{\eta}_\phi(X_j, Y)$ are based on kernel density estimation, it is unclear what the effect of having replicates in the re-sampled datasets is on the desired variance estimates.

5.4 Simulation Study

We first evaluate the performance of $\hat{\eta}_{KL}$ (given in equation (5.7)) as an estimator of the true value $\eta_{\phi_{KL}}(X,Y) = \frac{1}{2}\log\left(\frac{\sigma^2+\tau^2}{\tau^2}\right)$ for the example discussed in section (5.2.2) focusing on the overall accuracy of the estimator obtained with different sample sizes and how well the kernel density approximates the true density. For density estimation, we use Gaussian kernels. The two cases considered are (i) $\sigma^2 = 3$ and $\tau^2 = 3$ and (ii) $\sigma^2 = 4$ and $\tau^2 = 2$. Note that, in both cases the marginal variance of Y is equal to 6 ($\sigma^2 + \tau^2 = 6$). The analytical values for case (i) are

$$\begin{aligned}\eta_{\phi_{KL}} &= 0.3466\\ \eta_{\phi_H} &= 0.2021 \approx 0.20\\ \eta_{\phi_{TV}} &= 0.199135 \approx 0.2\end{aligned}$$

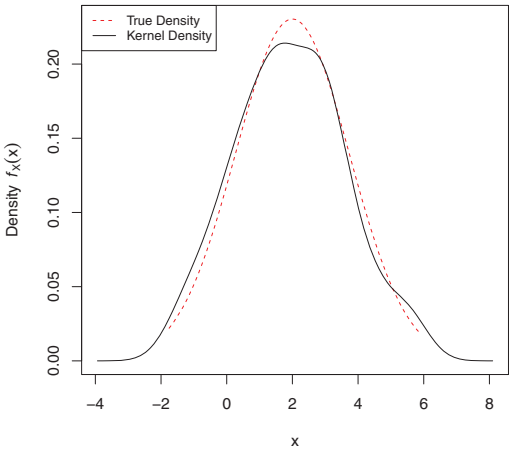
The analytical values for case (ii) are

$$\begin{aligned}\eta_{\phi_{KL}} &= 0.8959\\ \eta_{\phi_H} &= 0.56378\\ \eta_{\phi_{TV}} &= 0.508474\end{aligned}$$

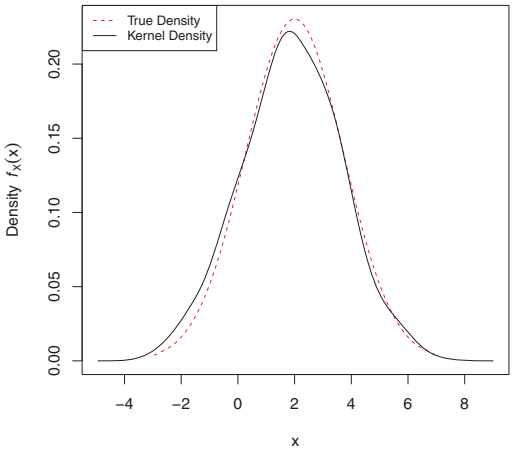
Figures (5.2), (5.3) and (5.4) show the kernel density estimates (for case (ii)) obtained for different sample sizes. It is clear that as the sample size increases, the kernel density estimates approximate well the true densities. However, we note that convergence is obtained only at a large sample size (N=4000) for this simple example. Therefore, an alternative would be to explore more density estimation methods that can approximate the true density from a reasonable sample size.

Moreover, figure (5.5) shows the behaviour of the estimators of $\hat{\eta}_{\phi_{KL}}$, $\hat{\eta}_{\phi_H}$ and $\hat{\eta}_{\phi_{TV}}$ as the sample size increases for the case $\sigma^2 = 3$, $\tau^2 = 3$ with their corresponding theoretical values denoted by red lines. The convergence of the estimator of the mutual information is obtained at a large sample size $N = 4000$. On the other hand, the convergence of $\hat{\eta}_{\phi_{TV}}$ is obtained at a small sample size and $\hat{\eta}_{\phi_H}$ becomes stable after $N = 5000$.

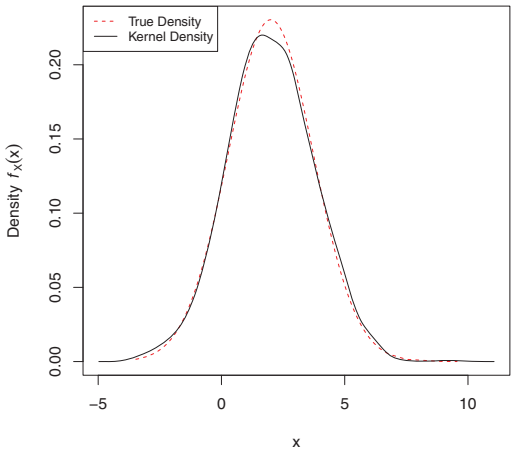
Figure (5.6) illustrates the estimated sensitivity indices for both case (i) and (ii). $\hat{\eta}_{\phi_{KL}}$ converges fast to its true value whereas $\hat{\eta}_{\phi_{TV}}$ behaves well for small sample sizes. Further the behaviour of $\hat{\eta}_{\phi_H}$ becomes stable after $N = 5000$. We observed that the estimator of η_{ϕ_P} did not reach to a specific value as the sample size increased.



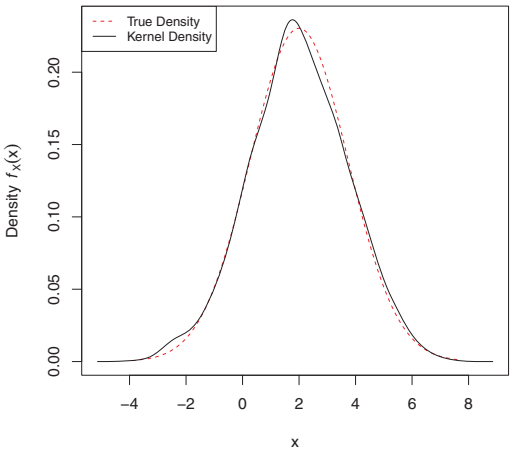
(a) Kernel density estimation of $f_X(x)$ with $N = 250$



(b) Kernel density estimation of $f_X(x)$ with $N = 500$

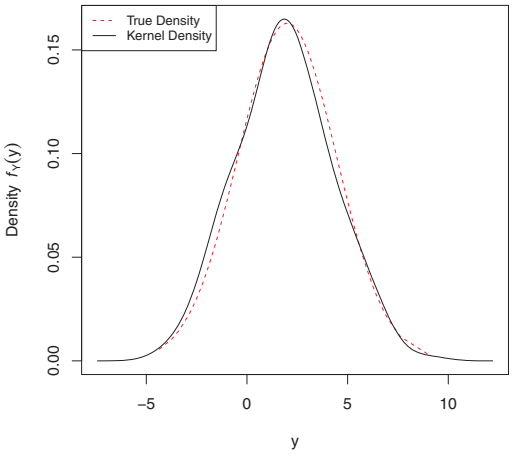


(c) Kernel density estimation of $f_X(x)$ with $N = 2000$

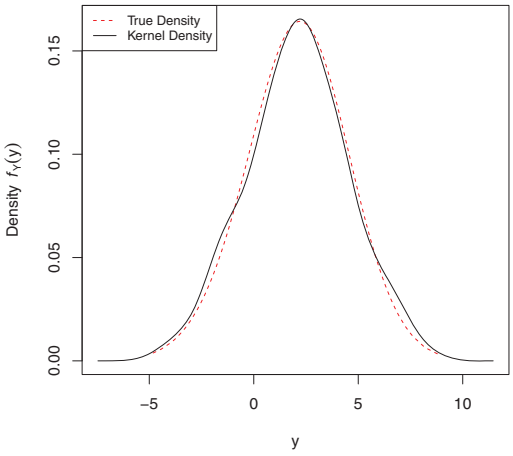


(d) Kernel density estimation of $f_X(x)$ with $N = 4000$

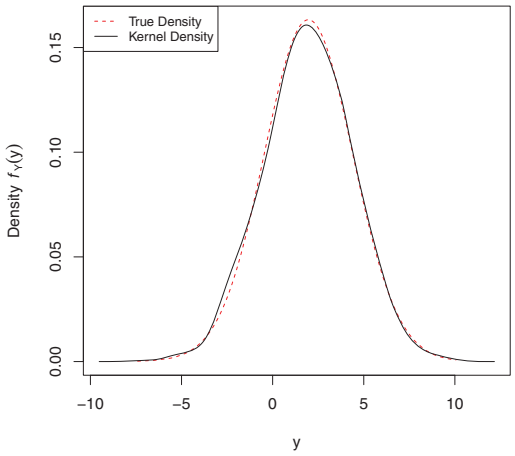
Figure 5.2: Kernel density estimation of $f_X(x)$ with different sample sizes



(a) Kernel density estimation of $f_Y(y)$ with $N = 250$

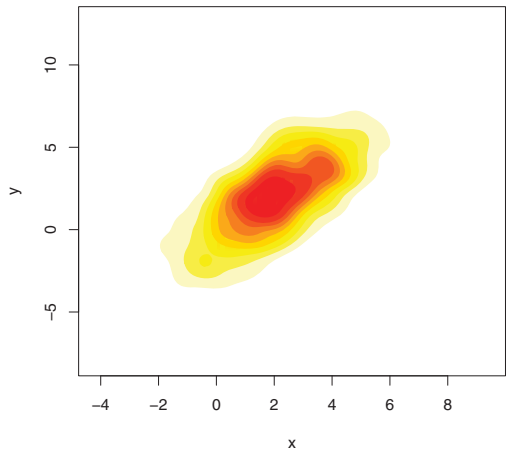


(b) Kernel density estimation of $f_Y(y)$ with $N = 500$

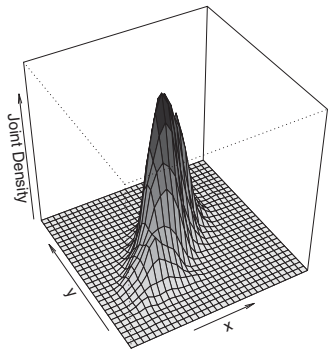


(c) Kernel density estimation of $f_Y(y)$ with $N = 2000$

Figure 5.3: Kernel density estimation of $f_Y(y)$ with different sample sizes



(a) Contour plot of $f_{X,Y}(x, y)$ with $N = 2000$

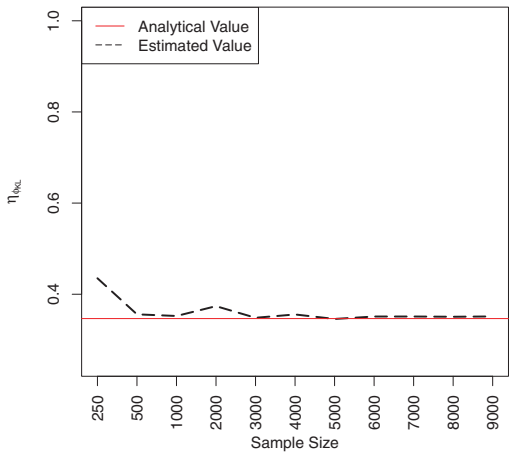


(b) Density plot of $f_{X,Y}(x, y)$ with $N = 2000$

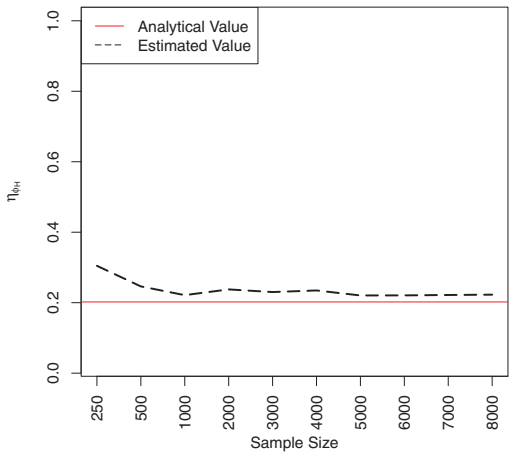
Figure 5.4: Kernel density estimation of $f_{X,Y}(x, y)$ with different sample sizes

5.5 Summary

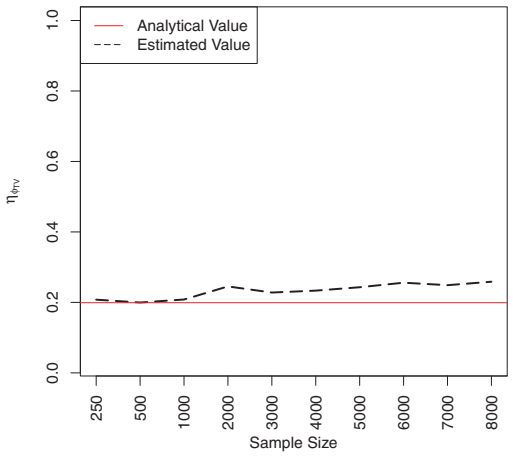
In this chapter, we considered sensitivity analysis for stochastic models where the output is purely stochastic. In this case, even for known and fixed model input value, the output is random, hence the sensitivity analysis was carried out by considering the conditional distribution of the output given an input vector. Density based sensitivity measures were proposed based on Cziszár f-divergences between the marginal density and the conditional density of the output when a known fixed input distribution is available. We showed that many existing sensitivity measures are particular cases of sensitivity measures associated with Cziszár f-divergences. Further, as for estimation of the sensitivity indices we proposed the use of kernel density estimation of the marginal and joint densities of model input and output avoiding the estimation of conditional density. A small simulation was carried out to illustrate performance of the proposed estimation method and different behaviour of the resulting measure when different divergences were used. However, the results showed that due to the complexity of the problem, large sample sizes are required to estimate such density based sensitivity indices. Therefore, the study of more efficient algorithms is in need in this framework. Hence, this chapter opens a future research to implement sensitivity analysis of purely stochastic outputs by using density based sensitivity measures.



(a) Behaviour of $\hat{\eta}_{\phi_{KL}}$ across varying sample sizes.

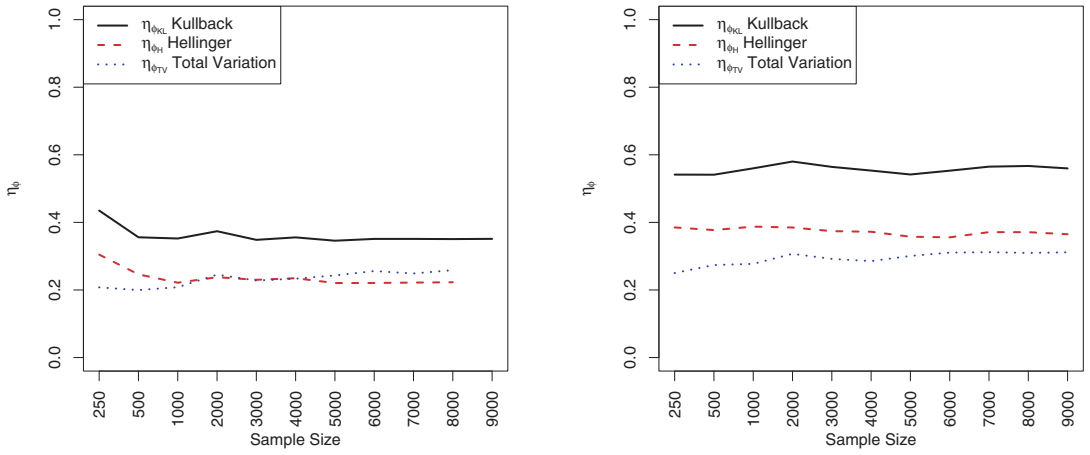


(b) Behaviour of $\hat{\eta}_{\phi_H}$ across varying sample sizes.



(c) Behaviour of $\hat{\eta}_{\phi_{TV}}$ across varying sample sizes.

Figure 5.5: Behaviour of sensitivity measures across varying sample sizes for $\sigma^2 = 3, \tau^2 = 3$.



(a) $\sigma^2 = 3, \tau^2 = 3$ (b) $\sigma^2 = 4, \tau^2 = 2$

Figure 5.6: Behaviour of sensitivity measures across varying sample sizes

Chapter 6

Discussion

6.1 Summary and Future Work

In this thesis we introduced two new sensitivity measures, RDIM and SDIM and studied their properties and their applications. In particular, we defined RDIM in a deterministic framework and SDIM in a stochastic framework. Additionally, we discussed a new importance measure based on Csiszár's f-divergences for the estimation of global sensitivity measures using kernel density estimation for models with purely stochastic outputs.

In chapter 2, we investigated thoroughly the relevant literature on sensitivity analysis. We grouped sensitivity analysis techniques into the classes of local, global and screening methods. We presented the details of the one at a time approach and differential based sensitivity methods for local sensitivity analysis, as well as regression based, variance based, density based and transformation invariant methods for global sensitivity analysis.

In chapter 3, we proposed a new bridge between local and global sensitivity analyses. The bridge was created by evaluating DIM at multiple points in the model input space defining what we called the randomized differential importance measure (RDIM). We showed that this new bridge, RDIM, helps the decision maker to identify the importance of different model inputs without relying on many assumptions such as independence among model inputs. In addition we showed that one can evaluate the joint sensitivity of any subsets of the model inputs in a single simulation run, which is computationally efficient. We presented an estimator for RDIM, $\widehat{\text{RDIM}}$ and it was consistent across sample sizes. We have studied the convergence rate of the estimator and provided a closed form expression for the convergence rate under some assumptions. We compared the ranking induced by the new sensitivity measure with the ranking of global sensitivity indices for the PSA model. DELSA has particularly been considered because it follows the same intuition of evaluating a local measure at random points in the model input space. Note that our proposed method can only be implemented if the model is differentiable. Therefore, future work is needed to develop a bridge that can work when the model is not differentiable.

In chapter 4 we generalized DIM to evaluate the sensitivity of an expectation of a stochastic model output with respect to its distributional parameters and we named this measure as Stochastic Differential Importance Measure (SDIM). We applied the LRM (Score function method) to estimate the derivatives of the expected value of the output with respect to model input distributional parameters. Moreover, we estimated SDIM simultaneously for different values of the parameters. A simulation study was carried out to illustrate the performance of the estimator of SDIM in real life applications paying special attention to discrete event static and dynamic systems. The implementation of the score function method for estimation is very simple. It is associated with the computation of the score function of the underlying probability density function $f_{\boldsymbol{X}}(\boldsymbol{x};\boldsymbol{\theta})$ only. In summary, all we need to have at our disposal is a realization of the output process $g(\boldsymbol{X})$ and a realization of the score function. Note that SDIM is a local sensitivity measure. However, one can generalize SDIM to a global sensitivity measure using importance sampling to obtain SDIM of several random points in the distributional parameter space, Θ. This intuition coincides with that of RDIM introduced in chapter 3 and its application is left for future work.

In chapter 5, we considered sensitivity analysis for stochastic models. In this context, the sensitivity analysis was carried out by considering the conditional distribution of the output paying special attention to sensitivity measures associated with Cziszár f-divergences between such conditional distribution and the marginal distribution of the output. The proposed index encompasses several existing global sensitivity measures. We have studied the analytical properties of the new sensitivity index. We have performed preliminary experiments concerning convergence. Results show that, due to the problem complexity, large sample sizes may be required to obtain accurate estimate. The study of more efficient estimation algorithms is a future research avenue opened by this thesis.

In order to perform a meaningful form of inference on η_ϕ the need of many sample data from the model is required. This becomes challenging specially for extremely slow models. Hence, we propose using original data to estimate the model. In other words, we propose to replace an emulator for g. If the emulator for g given the data produces a good fit for the model, any quantity of dependence or sensitivity can be calculated from data produced by the emulator.

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