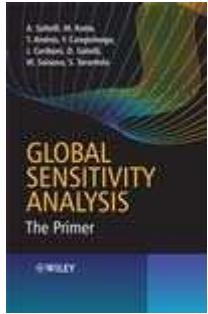


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## Global Sensitivity Analysis: The Primer



### Global Sensitivity Analysis: The Primer

[Andrea Saltelli](#), [Marco Ratto](#), [Terry Andres](#), [Francesca Campolongo](#), [Jessica Cariboni](#), [Debora Gatelli](#), [Michaela Saisana](#), [Dr. Stefano Tarantola](#)

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Written by the leading names in the field, *Global Sensitivity Analysis: The Primer* offers an accessible summary of the essential concepts involved in a sound sensitivity analysis. It is a self-contained book allowing the reader to learn about, and practice, sensitivity analysis through the use of many exercises and solved problems. This book brings the methodology and applications described in 'Sensitivity Analysis' up-to-date. Includes a chapter on experimental design, a topic neglected by the sensitivity analysis literature to date.

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# GLOBAL SENSITIVITY ANALYSIS

## The Primer

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The Primer

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11 In the field of modelling it is easier to find academic papers, guidelines  
12 tailored to specific disciplines and handbooks of numerical simulation rather  
13 than plain textbooks of broad appeal. The various academic communities  
14 go about modelling largely independently of each other. Is this an indication  
15 that modelling is not a science but a craft, as argued by epistemologists? In  
16 other words, is it because it is impossible to define a single set of rules to  
17 encode natural or man-made systems into sets of mathematical rules called  
18 models?

19 If modelling is in fact characterized by such heterogeneity and lack of  
20 systematization, it might seem overly ambitious to offer a set of good  
21 practices of universal application in sensitivity analysis. Furthermore, if  
22 one looks at the available literature, in most instances ‘sensitivities’ are  
23 understood as derivatives of a particular output versus a particular input  
24 (such as elasticities in economics). This is not surprising, as contemporary  
25 researchers – like the authors of the present volume – are likely to have  
26 received more training in calculus than in Monte Carlo methods and to  
27 have seen more Jacobians and Hessians than Russian roulettes. A minority  
28 of sensitivity analysis practitioners (mostly in statistics, risk analysis and  
29 reliability) actively use importance measures such as those described in this  
30 book, whereby the influence of factors on outputs is assessed by looking  
31 at the entire input space rather than at a point in that space. Slowly these  
32 methods are finding their way into more recent modelling guidelines in other  
33 disciplines (see, for example, those of the Environmental Protection Agency  
34 in the USA, EPA, 2001). The purpose of this book is to offer to students an  
35 easy-to-read manual for sensitivity analysis covering importance measures  
36 and to show how these global methods may help to produce more robust  
37 or parsimonious models as well as to make models more defensible in the  
38 face of scientific or technical controversy.

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# 1

# Introduction to Sensitivity Analysis

## 1.1 MODELS AND SENSITIVITY ANALYSIS

WHAT IS A MODEL? WHAT MODEL INPUT IS CONSIDERED IN A SENSITIVITY ANALYSIS? WHAT IS THE ROLE OF UNCERTAINTY AND SENSITIVITY ANALYSES IN MODEL BUILDING? MAIN APPROACHES TO THE PROPAGATION OF UNCERTAINTY WITHIN AND ACROSS MODELS. IMPLICATIONS FOR MODEL QUALITY.

### 1.1.1 Definition

A possible definition of sensitivity analysis is the following: *The study of how uncertainty in the output of a model (numerical or otherwise) can be apportioned to different sources of uncertainty in the model input* (Saltelli *et al.*, 2004). A related practice is ‘uncertainty analysis’, which focuses rather on *quantifying* uncertainty in model output. Ideally, uncertainty and sensitivity analyses should be run in tandem, with uncertainty analysis preceding in current practice.

For this definition of sensitivity analysis to be of use, it must first be made clear what is meant here by ‘model’, numerical or otherwise, as well as by the terms ‘input’ and ‘output’ which will be used throughout this book.

---

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### 1.1.2 Models

A view of modelling that may help to illustrate the role of sensitivity analysis in the scientific process is offered in Figure 1.1, taken from the work of biologist Robert Rosen (1991) (see also Saltelli *et al.*, 2000, pp. 3–4). On the left in Rosen’s diagram we have the ‘world’, that is the system which forms the subject of our investigation. We have reason to believe that the system, whether natural or artificial, is governed by rules which we have the ambition to uncover, or to use to our advantage. To this end we craft or hypothesize a set of structures in a model (depicted on the right-hand side of the figure). For example, a hypothesized growth mechanism for a species contained in the world can be translated into a differential equation in a model. While our species continues growing and dying quietly in the world, following the forces of its own systemic causality (which we aim to understand), our differential equation can be solved using the rules of mathematical calculus. The intuition of Rosen is that while the species in the world obeys rules, and the differential equation in the model has ‘rules’ as well, whether formal or mathematical, no ‘rule’ whatsoever can dictate how one should map the hypothesized rules in the world onto the rules in the model. In the words of Rosen, while the world and the model are each internally ‘entailed’, nothing entails the world with the model. Among the reasons for this paradox is the fact that the portion of the world captured by the model is an arbitrary ‘enclosure’ of an otherwise open, interconnected system.<sup>1</sup> This is the case when the world is part of a natural system, the main concern of Rosen’s inquiry. Yet experience has shown that even when the world is indeed a well-defined and closed system, for instance an artefact, an artificial device or a piece of machinery, different

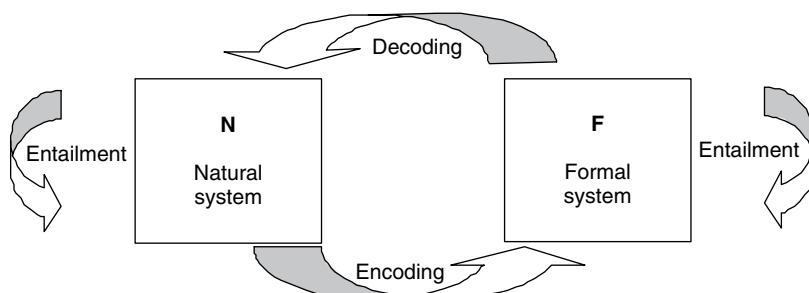


Figure 1.1 Modelling after Rosen (1991)

<sup>1</sup> Even more so when the purpose of a model is to learn about the nonobservable parts of a system.

01 modellers can generate different nonequivalent descriptions of it, that is,  
02 models whose outputs are compatible with the same set of observations but  
03 whose structures are not reconcilable with one another.

04 While this may be disturbing to a student accustomed to the beauty and  
05 apparent self-evidence of physical laws, practitioners of modelling have  
06 come to live with the rather unpleasant reality that more than one model  
07 may be compatible with the same set of data or evidence. Some have gone  
08 so far as to coin a word for this paradox: equifinality – Beven (1993,  
09 2001), see also Saltelli *et al.* (2004, pp. 173–178) – meaning that different  
10 models can lead to the same end. Others refer to the phenomenon as model  
11 indeterminacy.

12 Since Galileo's time scientists have had to deal with the limited capacity  
13 of the human mind to create useful maps of 'world' into 'model'. The  
14 emergence of 'laws' can be seen in this context as the painful process  
15 of simplification, separation and identification which leads to a model of  
16 uncharacteristic simplicity and beauty.

17  
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19  
20 **1.1.3 Models and Uncertainty**  
21

22 What makes modelling and scientific inquiry in general so painful is uncer-  
23 tainty. Uncertainty is not an accident of the scientific method, but its  
24 substance.<sup>2</sup>

25 Modellers and philosophers of science have debated the issue of model  
26 indeterminacy at length (Oreskes *et al.*, 1994). Most modellers today would  
27 probably agree that a model cannot be validated, in the sense of 'be proven  
28 true'. Rather, it is more defensible and correct to say that a model has  
29 been extensively corroborated, meaning by this that the model has survived  
30 a series of tests – be they formal, of internal consistency, or relative to  
31 the model's capacity to explain or predict the 'world' in a convincing and  
32 parsimonious way.

33 When models fail publicly, the ensuing controversy can be devastating  
34 for the scientific parties involved.<sup>3</sup> Models are often used in highly polar-  
35 ized contexts and uncertainty may be used instrumentally. 'All parties deal  
36 with environmental information in a selective way, or even manipulate it',  
37 observed a Dutch environmental scientist (In 't Veld, 2000). Fabricated  
38

39  
40 <sup>2</sup> 'That is what we meant by science. That both question and answer are tied up with uncer-  
41 tainty, and that they are painful. But that there is no way around them. And that you hide  
42 nothing; instead, everything is brought out into the open' (Høeg, 1995).

43 <sup>3</sup> For the modelling credibility crisis in the Netherlands' RIVM Laboratories see Van der Sluijs  
44 (2002). See also Mac Lane (1988) for another example.

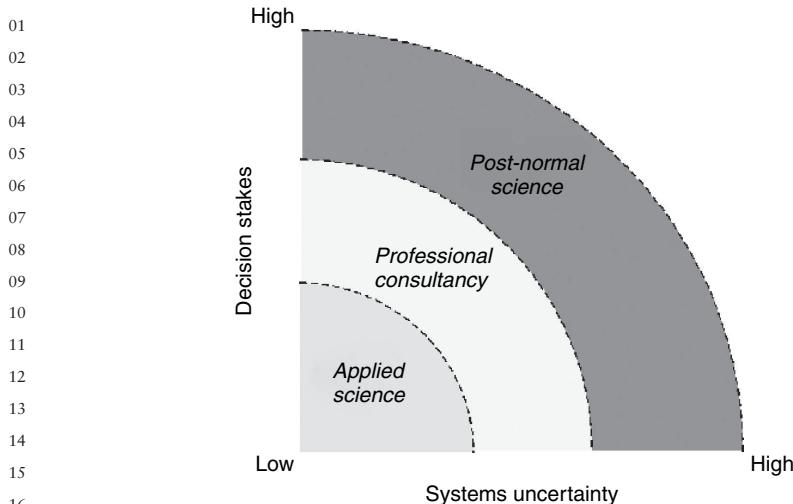


Figure 1.2 Uncertainty/stakes diagram after Funtowicz and Ravetz (1990)

uncertainty is a common concern in relation to important disputes over health or the environment (Michaels, 2005).

In short, models are part of the scientific method and hence subject to epistemological debate. A way of framing present-day debate on the scientific method is offered by Post-Normal Science (PNS, see Figure 1.2 and Funtowicz and Ravetz, 1990, 1993; Funtowicz *et al.*, 1996).

In PNS one distinguishes between three types of scientific production modes, depending on the system's uncertainties and the stakes involved. Applying this to modelling, different requirements and practices pertain:

- In applied science, when a model is written and employed within a closed consortium of experts who are the sole users of the model, e.g. when this is used to solve a circumscribed chemical kinetics problem;
- In 'consultancy' when the model is more likely to be scrutinized, e.g. as part of a cost–benefit analysis for the construction of a new road or bridge that will affect a community;
- When computing climate sensitivity in the context of global change. In this latter case we are in the domain of PNS, where science (and its models) is called on to provide evidence under circumstances of conflicting stakes and beliefs.

Like scientific theories, models may be given pedigrees which help us to judge their quality. Pedigrees take account of past usage of the model, status of its proponents, degree of acceptance by peers and so on (Van der Sluijs, 2002; Craye *et al.*, 2005). In pedigrees, model quality is more closely

01 associated with ‘fitness for purpose’ – that is, with a specific purpose – than  
02 with the model’s intrinsic fabric.

03 A post-normal view of the modes of scientific production in relation to  
04 policy is given in Funtowicz (2004). Models as metaphors are discussed in  
05 Ravetz (2006).

#### 06

#### 07 1.1.4 How to Set Up Uncertainty and Sensitivity Analyses

#### 08

09 As mentioned at the beginning of the chapter, our definition of sensitivity  
10 analysis involves models, model input and model output. We now try to  
11 define model input in relation to the nature and purpose of the model, as  
12 well as to the set-up of the uncertainty and sensitivity analyses. A model  
13 can be:

14

- 15 • *Diagnostic or prognostic.* In other words, we try to distinguish between  
16 models used to understand a law and models used to predict the  
17 behaviour of a system given a supposedly understood law. Models can  
18 thus range from wild speculations used to play what-if games (e.g. models  
19 for the existence of extraterrestrial intelligence) to models which can be  
20 considered accurate and trusted predictors of a system (e.g. a control  
21 system for a chemical plant).

- 22 • *Data-driven or law-driven.* A law-driven model tries to put together  
23 accepted laws which have been attributed to the system, in order to  
24 predict its behaviour. For example, we use Darcy’s and Ficks’ laws to  
25 understand the motion of a solute in water flowing through a porous  
26 medium. A data-driven model tries to treat the solute as a signal and to  
27 derive its properties statistically. Advocates of data-driven models like to  
28 point out that these can be built so as to be parsimonious, i.e. to describe  
29 reality with a minimum of adjustable parameters (Young *et al.*, 1996).  
30 Law-driven models, by contrast, are customarily overparametrized, as  
31 they may include more relevant laws than the amount of available data  
32 would support. For the same reason, law-driven models may have a  
33 greater capacity to describe the system under unobserved circumstances,  
34 while data-driven models tend to adhere to the behaviour associated with  
35 the data used in their estimation. Statistical models (such as hierarchical  
36 or multilevel models) are another example of data-driven models.

37

38 Many other categorizations of models are possible,<sup>4</sup> and the definition of  
39 model input depends on the particular model under study. For the purpose  
40

41

42 <sup>4</sup> Bell *et al.* (1988) distinguish between formal (axiomatic), descriptive and normative models  
43 (rules an agent should follow to reach a target). The examples in this book are descriptive  
44 models.

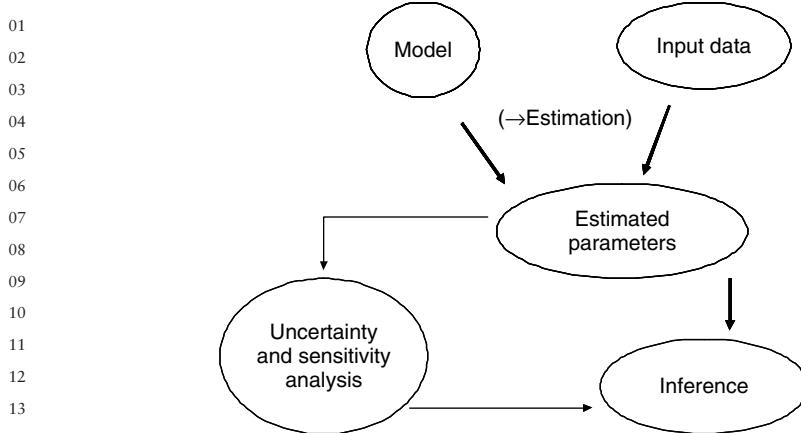


Figure 1.3 Parametric bootstrap version of uncertainty and sensitivity analyses

of uncertainty and sensitivity analyses we could liberally classify as input everything that can drive a variation in the output of the model.

Consider the scheme in Figure 1.3. Here we have observations (assumed error-free for simplicity's sake) and a model whose parameters are estimated from the data. Estimation can take different courses. Usually it is achieved by minimizing, e.g. by least squares, some measure of distance between the model's prediction and the data. At the end of the estimation step, 'best' parameter values as well as their errors are known. At this point we might consider the model 'true' and run an uncertainty analysis by propagating the uncertainty in the parameters through the model, all the way to the model output. In this case the estimated parameters become our factors.

One way of doing this is through Monte Carlo analysis, in which we look at the distribution functions of the input parameters, as derived from the estimation. For example, we may have the following scheme:

- We start from a factor  $\alpha \sim N(\bar{\alpha}, \sigma_\alpha)$ , which reads: after estimation  $\alpha$  is known to be normally distributed with mean  $\bar{\alpha}$  and standard deviation  $\sigma_\alpha$ .
- Likewise for factors  $\beta, \gamma$  and so on. Contrary to what logic would suggest, and for the sake of simplicity, we assume that the factors are independent of each other. This issue is discussed later in the chapter.
- For each of these factors, we draw a sample from the respective distributions, i.e. we produce a set of row vectors  $(\alpha^{(j)}, \beta^{(j)}, \dots)$  with  $j = 1, 2, \dots, N$  in such a way that  $(\alpha^{(1)}, \alpha^{(2)}, \dots, \alpha^{(N)})$  is a sample

01 from  $N(\bar{\alpha}, \sigma_\alpha)$  and likewise for the distribution function of the other  
02 factors.

$$03 \quad \begin{bmatrix} \alpha^{(1)} & \beta^{(1)} & \gamma^{(1)} & \dots \\ 04 & \alpha^{(2)} & \beta^{(2)} & \gamma^{(2)} & \dots \\ 05 & \dots & \dots & \dots & \dots \\ 06 & \alpha^{(N-1)} & \beta^{(N-1)} & \gamma^{(N-1)} & \dots \\ 07 & \alpha^{(N)} & \beta^{(N)} & \gamma^{(N)} & \dots \end{bmatrix} \quad (1.1)$$

- 09 • We can then compute ('run' is the conventional term) the model for all  
10 vectors  $(\alpha^{(j)}, \beta^{(j)}, \dots)$  thereby producing a set of  $N$  values of a model  
11 output  $Y_j$ .<sup>5</sup>

$$13 \quad \begin{bmatrix} y^{(1)} \\ 14 & y^{(2)} \\ 15 & \dots \\ 16 & y^{(N-1)} \\ 17 & y^{(N)} \end{bmatrix} \quad (1.2)$$

18 These steps constitute our uncertainty analysis. From these we can  
19 compute the average output, its standard deviation, the quantiles of its  
20 distribution, confidence bounds, plot the distribution itself and so on. It is  
21 clear that in this analysis, sometimes called a 'parametric bootstrap',<sup>6</sup> our  
22 inputs are the model's parameters. Having performed this uncertainty anal-  
23 ysis we can then move on to a sensitivity analysis, in order to determine  
24 which of the input parameters are more important in influencing the uncer-  
25 tainty in the model output. However, we defer this step in order to continue  
26 our discussion of model input.

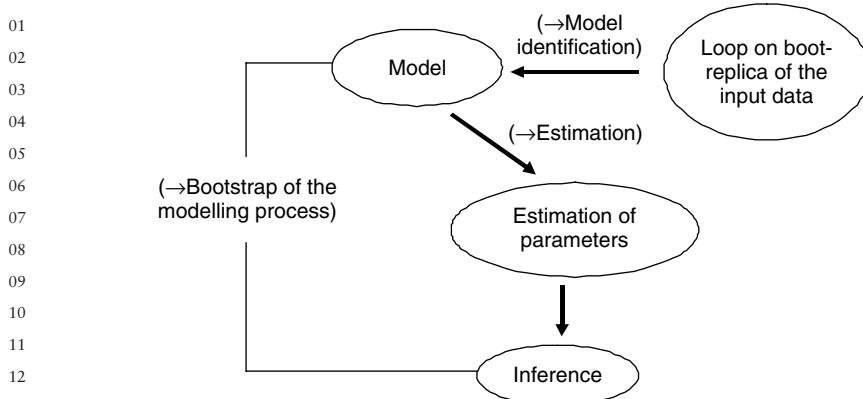
27 Note that for the purpose of the uncertainty analysis just described we  
28 consider as relevant inputs only our estimated parameters. All other types  
29 of information fed into the model, e.g. the observations, physical or math-  
30 ematical constants, internal model variables (e.g. number of grid points if  
31 the model needs a mesh), are disregarded – that is, we do not allow them  
32 to vary and hence they cannot cause variation in the output.

33 In Figure 1.4 we have played the uncertainty analysis game differently by  
34 sampling the observations rather than the parameters. We have a limited  
35 set of observations, and we are aware that different subsets of these could

---

38  
39 <sup>5</sup> Note that this model output  $Y_j$  may be different from the model output used in the estimation  
40 step.

41 <sup>6</sup> Bootstrapping is the process of repeatedly sampling 'with replacements'. For example, if we  
42 want to estimate the average sum of three Bingo chips, we could do this by extracting three  
43 random chips from the Bingo bag, computing their average, putting the chips back into the  
44 bag and extracting again. With a sufficiently large number of extractions we could determine  
the average sum being sought, and this strategy would be called a bootstrap of the Bingo chips.



**Figure 1.4** Bootstrapping of the modelling process (Chatfield, 1993)

potentially lead us to try one model rather than another to fit the data. What we can do in order to be fair to the data is to select a subset of the observations, choose a model based on these data using a pre-established model selection rule, estimate the corresponding parameters using the same sampled data, and run the model to compute  $Y_j$ . We have drawn the sample with replacement, and we can now repeat the process, identifying a potentially different (or indeed the same) model, estimating the parameters (which may differ in number from those of the previous run if the model is different), and so on for a total of  $N$  times, until we yield our desired sample for the uncertainty analysis. This approach can be called ‘bootstrapping of the modelling process’ (Chatfield, 1993).

The input for this uncertainty analysis is the data which have been bootstrapped, since we have assumed that all the rest (from model selection to parametric estimation) is done automatically given the data and hence adds no variation to model output.

Finally in Figure 1.5 we compare a set of plausible models with the data. Using Bayesian analysis it is possible to derive posterior probabilities for the models as well as distributions of the related parameters (Saltelli *et al.*, 2004). Once this model update and parameter estimation step is complete, a model averaging can be used in uncertainty analysis. This is done by propagating the uncertainty through the system by sampling both the model and the parameters according to their distributions, to produce a sample of model outcome  $Y_j$ . This procedure is known as Bayesian model averaging,<sup>7</sup> and the inputs in this case are both models and parameters, or

---

<sup>7</sup> For a thorough account of this approach see Kass and Raftery (1995) and Hoeting *et al.* (1999). See Saltelli *et al.* (2004, pp. 151–192) for related sensitivity issues.

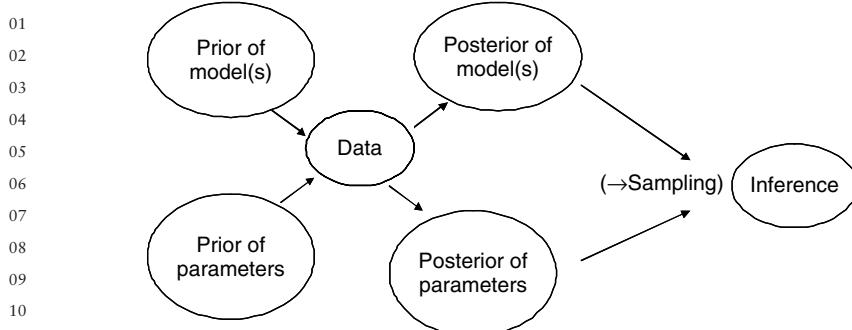


Figure 1.5 Bayesian model averaging

more precisely the probabilities of the different model representations and the distributions of the parameters. In a Monte Carlo framework, a trigger variable would be sampled to select a model according to its posterior probability, while the parameters would also be sampled and the model outcome determined. A sensitivity analysis could be executed at this point, and a question that it might address is the following: how much of the uncertainty is due to the model selection and how much to the estimation of the parameters?

### 1.1.5 Implications for Model Quality

The superficial illustration given above of approaches to uncertainty and sensitivity analyses has shown that what constitutes an input for the analysis depends upon how the analysis is set up. The input is that which is allowed to vary in order to study its effect on the output. A sensitivity analysis will in turn instruct the modellers as to the relative importance of the inputs in determining the output. An obvious consequence of this is that the modeller will remain ignorant of the importance of those variables which have been kept fixed. This is of course a hazard for the modeller, as a variable deemed noninfluential and kept fixed could haunt the results of the analysis at a later stage. For example, it would be unfortunate for the modeller to discover a posteriori that the mesh size had been too large, and that the number of grid points had had a dramatic effect on the model output.

It seems, therefore, that one should be as careful and objective as possible in deciding on the input for uncertainty and sensitivity analyses. Clearly, the more variables we promote to the rank of input, and allow to vary, the greater the variance to be expected in the model prediction. This could lead to a situation in which we discover that, having incorporated all uncertainties, the model prediction varies so wildly as to be of no practical use. This

01 trade-off has been brilliantly summarized by the econometrician Edward  
02 E. Leamer (1990):

03 I have proposed a form of organized sensitivity analysis that I call ‘global sensi-  
04 tivity analysis’ in which a neighborhood of alternative assumptions is selected and  
05 the corresponding interval of inferences is identified. Conclusions are judged to  
06 be sturdy only if the neighborhood of assumptions is wide enough to be credible  
07 and the corresponding interval of inferences is narrow enough to be useful.

08  
09 Note Leamer’s emphasis on the need for ‘credibility’ in the selection of  
10 assumptions. The easiest way to invalidate a model is to demonstrate it  
11 fragile with respect to shaky assumptions. Note, however, that the trade-off  
12 may not be as dramatic as one might expect, and that increasing the number  
13 of input factors does not necessarily lead to an increased variance in model  
14 output. Practitioners have recorded that in most uncertainty and sensitivity  
15 analyses the input factors’ importance is distributed similarly to wealth  
16 in nations, with a few factors creating almost all the uncertainty and the  
17 majority making only a negligible contribution. Hence, if the ‘key’ factors  
18 have been judiciously chosen, adding further variables to the analysis may  
19 add to its completeness and defensibility without adversely increasing the  
20 variance in the output.  
21

22 As mentioned, the quality of a model is largely a function of its fitness for  
23 purpose. If modelling is a craft and models cannot be proven true (because  
24 of the pervasive nature of uncertainty and the difficulty of separating obser-  
25 vation from observer and facts from values),<sup>8</sup> then the modeller has a  
26 moral obligation, and indeed it is in the modeller’s own practical interest,  
27 to be as rigorous as possible when assessing the robustness of model infer-  
28 ence. Doing so should produce better and more parsimonious models, and  
29 will strengthen the analyst’s defence of the results in the case of scientific  
30 controversy or public policy debate.  
31

## 32 33 1.2 METHODS AND SETTINGS FOR SENSITIVITY 34 ANALYSIS – AN INTRODUCTION 35

36 **WHAT METHODS ARE AVAILABLE? HOW CAN A PARTICULAR METHOD BE  
37 RELATED TO A PROBLEM-SPECIFIC QUESTION? HOW CAN WE DEFINE A FACTOR’S  
38 IMPORTANCE UNAMBIGUOUSLY? SUGGESTED PRACTICES.**  
39

40  
41 <sup>8</sup> ‘Values’ here mean ethical judgements. Cases in which the separation of facts and values  
42 becomes arduous are many, e.g. when models try to assess the impact of the adoption of new  
43 technologies, the relevance of environmental threats, distributional issues in economics and so on.  
44

01           1.2.1 Local versus Global  
02

03           As we shall learn in the following chapters, sensitivity analysis can serve a  
04           number of useful purposes in the economy of modelling. It can surprise the  
05           analyst, uncover technical errors in the model, identify critical regions in  
06           the space of the inputs, establish priorities for research, simplify models and  
07           defend against falsifications of the analysis. In the context of models used  
08           for policy assessment, sensitivity analysis can verify whether policy options  
09           can be distinguished from one another given the uncertainties in the system,  
10           and so on. What methods would one choose to perform sensitivity analysis  
11           for any or all of the above?

12           It is not by chance that most of the sensitivity analyses met in the literature  
13           are based on derivatives. Indeed the derivative  $\partial Y_j / \partial X_i$  of an output  $Y_j$   
14           versus an input  $X_i$  can be thought of as a mathematical definition of the  
15           sensitivity of  $Y_j$  versus  $X_i$ .

16           Sometimes computer programs that implement complex physical, chem-  
17           ical or genetic models are augmented by special routines that allow the  
18           efficient computation of large arrays of system derivatives, which are subse-  
19           quently used for model calibration, model reduction or verification and  
20           model inversion (Rabitz, 1989; Turanyi, 1990; Varma *et al.*, 1999; Cacuci,  
21           2003; Saltelli *et al.*, 2000, pp. 81–101).

22           The derivative-based approach has the attraction of being very efficient in  
23           computer time. The model needs to be executed few times compared to the  
24           dimension of the array of derivatives to be computed. However, it is inef-  
25           ficient in terms of the analyst's time. One has to intervene in the computer  
26           program, inserting ad hoc coding, to perform this operation efficiently. Yet  
27           the fatal limitation of a derivative-based approach is that it is unwarranted  
28           when the model input is uncertain and when the model is of unknown  
29           linearity. In other words, derivatives are only informative at the base point  
30           where they are computed and do not provide for an exploration of the rest  
31           of the space of the input factors. This would matter relatively little for linear  
32           systems, in which the property at a point away from the baseline can be  
33           computed quickly by linear extrapolation using first-order point derivatives,  
34           but it would matter greatly for nonlinear ones. The focus of this book is on  
35           quantitative uncertainty and sensitivity analysis in the presence of uncer-  
36           tain inputs. We shall therefore make use of methods based on exploring  
37           the space of the input factors, based on the consideration that a handful  
38           of data points judiciously thrown into that space is far more effective, in  
39           the sense of being informative and robust, than estimating derivatives at  
40           a single data point in the centre of the space. In this book, when we use  
41           derivatives, or rather incremental ratios such as  $(Y_j(X_i + \Delta X_i) - Y_j(X_i)) / \Delta X_i$ ,  
42           we will normally compute them at a set of different points in the space of  
43           the input factors, in order to obtain an average response of  $Y_j$  when moving

44

01 a factor  $X_i$  of a step  $\Delta X_i$  at different points in the input space, i.e. for  
 02 different values of  $\mathbf{X}_{\sim i}$ .<sup>9</sup>

03 However, in order to introduce the methods of sensitivity analysis, we  
 04 shall start from derivatives, taking a very simple test case.

07 **1.2.2 A Test Model**

09 Imagine the model has a linear error-free form

$$11 \quad 12 \quad Y = \sum_{i=1}^r \Omega_i Z_i \quad (1.3)$$

14 where the input factors are  $\mathbf{X} = (\Omega_1, \Omega_2, \dots, \Omega_r, Z_1, Z_2, \dots, Z_r)$ .

15 We have dropped the subscript  $j$  of the model output  $Y$  for simplicity.  
 16 Model equation (1.3) has just a single output variable. Let us assume first  
 17 that the  $\Omega$ 's are fixed coefficients, so that the true (active) factors for model  
 18 (1.3) are just the  $Z_1, Z_2, \dots, Z_r$ .  $Y$  could be a composite indicator, for  
 19 example a sustainability index or a greenhouse gas emission index, in which  
 20 the  $\Omega$ 's are the weights attached by experts to the individual  $Z$ -variables. For  
 21 the sake of the example we consider the weights fixed, while the individual  
 22 variables have been characterized as independent and distributed normally  
 23 with mean zero, i.e.

$$25 \quad 26 \quad Z_i \sim N(0, \sigma_{Z_i}) \quad i = 1, 2, \dots, r. \quad (1.4)$$

28 If the model were indeed a composite indicator with ‘standardized’ vari-  
 29 ables<sup>10</sup> all  $\sigma_{Z_i}$ 's would be equally one.

30 It is easy to verify (see the Exercises) that, given the Equations (1.3, and  
 31 1.4),  $Y$  will also be normally distributed with parameters

$$33 \quad 34 \quad \bar{y} = \sum_{i=1}^r \Omega_i \bar{z}_i \quad (1.5)$$

$$37 \quad 38 \quad \sigma_Y = \sqrt{\sum_{i=1}^r \Omega_i^2 \sigma_{Z_i}^2}. \quad (1.6)$$

---

42 <sup>9</sup> Here, and in the following,  $\mathbf{X}_{\sim i}$  denotes the vector of all factors but  $X_i$ .

43 <sup>10</sup> Standardization of a variable is achieved by subtracting from the variable its sample mean  
 44 and dividing the result by its standard deviation.

For the sake of the example we would also like to assume that for this particular index the variables have been ordered from the less uncertain to the most uncertain, i.e.

$$\sigma_{Z_1} < \sigma_{Z_2} < \dots < \sigma_{Z_r},$$

and that the weights  $\Omega$ 's are all equal and constant:

$$\Omega_1 = \Omega_2 = \dots = \Omega_r = \text{constant}. \quad (1.7)$$

### 1.2.3 Scatterplots versus Derivatives

Figure 1.6 shows the scatterplots  $Y, Z_i$  that we obtain by performing a Monte Carlo experiment with our model. As already mentioned (and described in more detail in Chapter 2), Monte Carlo methods are based on sampling factors' values from their distribution. In most cases factors are assumed independent so that the samples are taken from the marginal distribution of each factor. An input sample is thus produced:

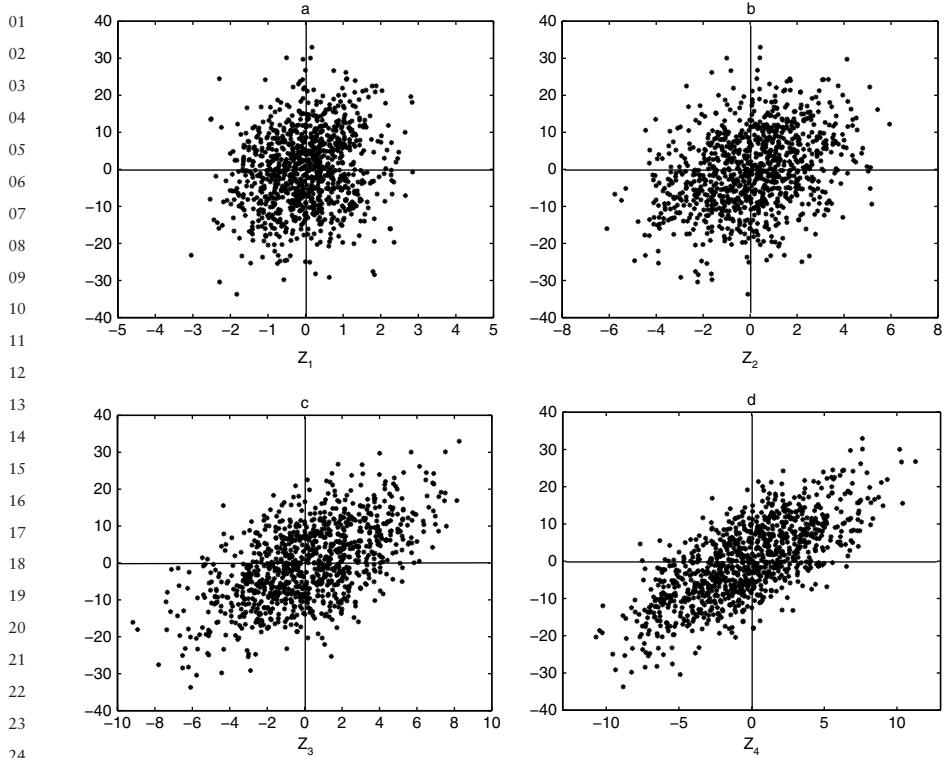
$$M = \begin{bmatrix} z_1^{(1)} & z_2^{(1)} & \dots & z_r^{(1)} \\ z_1^{(2)} & z_2^{(2)} & \dots & z_r^{(2)} \\ \dots & \dots & \dots & \dots \\ z_1^{(N-1)} & z_2^{(N-1)} & \dots & z_r^{(N-1)} \\ z_1^{(N)} & z_2^{(N)} & \dots & z_r^{(N)} \end{bmatrix} \quad (1.8)$$

Computing  $Y$  for each row of matrix (1.8) using model (1.3) produces the desired output vector

$$Y = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \dots \\ y^{(N-1)} \\ y^{(N)} \end{bmatrix} \quad (1.9)$$

where  $y^{(1)}$  is the value obtained by running Equation (1.3) with the input given by the row vector  $z_1^{(1)}, z_2^{(1)}, \dots, z_r^{(1)}$ , and so on for the other rows of matrix (1.8).

With this sample of model input and output one can produce  $r$  scatterplots by projecting in turn the  $N$  values of the selected output  $Y$  (assumed here to be a scalar) against the  $N$  values of each of the  $r$  input factors. These scatterplots can be used to investigate the behaviour of models.



**Figure 1.6** Scatterplots of  $Y$  versus  $Z_1, \dots, Z_4$ . Which is the most influential factor? One can compare occupancy of quadrants I and III versus that of II and IV to decide where the positive linear relationship is stronger

The scatterplots show that  $Y$  is more sensitive to  $Z_4$  than it is to  $Z_3$ , and that the ordering of the input factors by their influence on  $Y$  is

$$Z_4 > Z_3 > Z_2 > Z_1. \quad (1.10)$$

Such a conclusion can be drawn from Figure 1.6, as there is more shape (or a better pattern) in the plot for  $Z_4$  than for  $Z_3$ , and so on.

However, if we used the straightforward derivative of  $Y$  versus  $Z_i$  for the sensitivity analysis, i.e. if we decided upon the relative importance of the  $Z_i$ 's using the measure

$$S_{Z_i}^p = \frac{\partial Y}{\partial Z_i}, \quad (1.11)$$

which gives  $S_{Z_i}^p = \Omega_i$  for Equation (1.3), we would have to conclude that all factors are equally important, based on Equation (1.7), irrespective of

the values in  $\sigma$ . This is clearly not reasonable. Note that we have used the superscript  $p$  for ‘partial derivative’ in Equation (1.11), and that the derivative is nonnormalized, i.e. it is based on the raw values of both input and output. Note also that the scatterplots in Figure 1.6 are more convincing than formula (1.11) as a sensitivity analysis tool. This is a rather general conclusion. Input/output scatterplots are in general a very simple and informative way of running a sensitivity analysis – we will use them often in this book, since they can provide an immediate visual depiction of the relative importance of the factors. For example, a scatterplot with little ‘shape’, e.g. plot  $Z_1$  in Figure 1.6, which presents a rather uniform cloud of points over the range of the input factor on the abscissa, is an almost sure sign that the parameter is less influential than factor  $Z_4$ . We say ‘almost’ because there are instances in which a bidimensional scatterplot can be deceiving, leading to type II errors (nonidentification of an influential factor).<sup>11</sup> These are, however, very special cases, see Saltelli *et al.* (2004, pp. 160–161).

Most sensitivity analysis measures developed by practitioners aim to preserve the rich information provided by scatterplots in condensed format. The challenge for sensitivity analysis, in situations with many input factors, is how to rank the factors rapidly and automatically without having to look at many separate scatterplots. Another problem with scatterplots is that some uncertain factors might be sets, that is, groups of factors, and while compact sensitivity measures can be defined for sets, the sensitivities of sets cannot be visualized via simple two-dimensional scatterplots.<sup>12</sup>

#### 1.2.4 Sigma-normalized Derivatives

Can we improve Equation (1.11) in such a way as to obtain a sensitivity measure that would rank the input factors consistently with Figure 1.6? A good possibility is

$$S_{Z_i}^\sigma = \frac{\sigma_{Z_i} \partial Y}{\sigma_Y \partial Z_i}. \quad (1.12)$$

<sup>11</sup> In sensitivity analysis, we refer to type I error when erroneously defining as important a noninfluential factor. Type II error occurs when we classify an important factor as noninfluential. It is nowadays common practice in modelling to include a third type of error: type III. This is typically a framing error, where right answers are sought for the wrong question. Sensitivity analysis is unable to help against type III errors. To make an example, if the range of plausible values for a factor taken as input for a sensitivity analysis is totally off the mark, the result of the sensitivity analysis will be of little help.

<sup>12</sup> In fact, one can force multidimensional scatterplots into a bidimensional plane by scanning the space of the input factors with a search curve. See Chapter 5.

This derivative is normalized by the input–output standard deviations (hence the  $\sigma$  in the superscript). Applied to model (1.3) this would give  $S_{Z_i}^\sigma = (\sigma_{Z_i}/\sigma_Y)\Omega_i$ . Squaring this and comparing with the square of  $\sigma_Y = \sqrt{\sum_{i=1}^r \Omega_i^2 \sigma_{Z_i}^2}$  (Equation (1.6) above) we obtain

$$\sigma_Y^2 = \sum_{i=1}^r \Omega_i^2 \sigma_{Z_i}^2 \quad \text{and} \quad (S_{Z_i}^\sigma)^2 = \left( \frac{\sigma_{Z_i}}{\sigma_Y} \Omega_i \right)^2 \quad (1.13)$$

which gives  $\sigma_Y^2 = \sigma_Y^2 \sum_{i=1}^r (S_{Z_i}^\sigma)^2$ , and finally

$$\sum_{i=1}^r (S_{Z_i}^\sigma)^2 = 1. \quad (1.14)$$

Measure (1.12) is more convincing than measure (1.11), see Table 1.1: first, because the relative ordering of the  $Z_i$ 's now depends on both vectors,  $\sigma$  and  $\Omega$ , just as it should; and second, because the sensitivity measures are neatly normalized to one.

Note that Equation (1.12) is a measure recommended for sensitivity analysis by a guideline of the Intergovernmental Panel for Climate Change (IPCC) (1999, 2000).

### 1.2.5 Monte Carlo and Linear Regression

Let us return briefly to the scatterplots of Figure 1.6. As mentioned, these are the result of a Monte Carlo simulation in which a matrix such as

$$\mathbf{M} = \begin{bmatrix} z_1^{(1)} & z_2^{(1)} & \dots & z_r^{(1)} \\ z_1^{(2)} & z_2^{(2)} & \dots & z_r^{(2)} \\ \dots & \dots & \dots & \dots \\ z_1^{(N-1)} & z_2^{(N-1)} & \dots & z_r^{(N-1)} \\ z_1^{(N)} & z_2^{(N)} & \dots & z_r^{(N)} \end{bmatrix} \quad (1.15)$$

**Table 1.1** Derivatives and normalized derivatives for the model (1.3, 1.4), where  $r = 4$ ,  $\Omega = (2, 2, 2, 2)$  and  $\sigma = (1, 2, 3, 4)$

	$S_{Z_i}^\sigma$	$(S_{Z_i}^\sigma)^2$
$Z_1$	2	0.036
$Z_2$	2	0.14
$Z_3$	2	0.31
$Z_4$	2	0.56

has been fed into model (1.3) to produce the desired output vector

$$\mathbf{Y} = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(N-1)} \\ y^{(N)} \end{bmatrix} \quad (1.16)$$

where  $y^{(1)}$  is the value obtained running Equation (1.3) with the input given by the row vector  $z_1^{(1)}, z_2^{(1)}, \dots, z_r^{(1)}$ , and so on for the other rows of the matrix.

Note that  $N$  is the size of the Monte Carlo experiment ( $N = 1000$  in Figure 1.6).  $N$  corresponds to the number of times we have computed Equation (1.3). In a sensitivity analysis experiment we shall have in general, instead of Equation (1.3), a computer program that calculates  $\mathbf{Y}$ . Running the program to obtain a vector as Equation (1.9) is customarily the most expensive part of the analysis in terms of computer time, as the model may be complicated, while the sensitivity analysis measures are easy to compute. Thus  $N$  is referred to as the cost of the analysis. Note that computer time is not to be confused with analysis time. A derivation of the factors' uncertainty distribution such as Equation (1.4) is in practice the most time-consuming and financially expensive part of an analysis, especially when this is based on formal elicitation of expert opinion (Helton *et al.*, 2006; see also Saltelli *et al.*, 2000, pp. 101–152).

Note also that care has to be taken so that each column

$$\begin{array}{c} z_1^{(1)} \\ z_1^{(2)} \\ \vdots \\ z_1^{(N)} \end{array}$$

in matrix (1.8) is a sample from the respective distribution  $Z_i \sim N(\bar{z}_i, \sigma_{Z_i})$ . In general, and unless otherwise specified, we assume that the input factors are independent of each other, so that each one can be independently sampled from its marginal distributions (Equation (1.4) in the present examples).

As mentioned above, analysts would like to summarize the results in plots such as Figure 1.6 with a single number per scatterplot. This is, after all, what a sensitivity measure is intended to do. The most popular method for this is to try a simple linear regression on the data of matrix (1.8) and vector (1.9), of the form

$$y(i) = b_0 + \sum_{j=1}^r b_{Z_j} z_j^{(i)}, \quad (1.17)$$

where the coefficients  $b_0, b_{Z_i}$  are determined by least-square computation, based on the squared differences between the  $y$ -values produced by the regression (meta)model<sup>13</sup> and the actual model output produced by the Monte Carlo simulation. Because the points have been generated using a linear model, we expect that the linear regression will re-discover it, i.e. we would expect that  $\hat{b}_0 \cong 0, \hat{b}_{Z_i} \cong \Omega_i, i = 1, 2, \dots, r$ , where the symbol  $\cong$  means that this is what we would obtain if  $N$  were large enough and the hat denotes estimates as in standard usage.

Results for the points in Figure 1.6 ( $N = 1000$ ) are given in Table 1.2.<sup>14</sup>

All available software for regression analysis will compute not only  $\hat{b}_0, \hat{b}_{Z_i}$ , but also their standardized equivalents  $\hat{\beta}_{Z_i} = \hat{b}_{Z_i} \sigma_{Z_i} / \sigma_Y$ . The  $\beta$ 's are known as standardized regression coefficients (sometime indicated with their initial as SRC), and are in general more widely used than the raw regression coefficients  $b$ 's. For our model (1.3), the regression coefficients, again for  $N$  tending to infinity, will tend to

$$\hat{\beta}_{Z_i} = \hat{b}_{Z_i} \sigma_{Z_i} / \sigma_Y \cong \Omega_i \sigma_{z_i} / \sigma_Y. \quad (1.18)$$

Comparing this formula with that previously obtained for the  $\sigma$ -normalized derivatives, i.e.  $S_{Z_i}^\sigma = (\sigma_{Z_i} / \sigma_Y) \Omega_i$ , we can conclude that in the special case of our model (1.3) the two measures of sensitivity coincide:

$$\hat{\beta}_{Z_i} = S_{Z_i}^\sigma \quad \text{for model (1.3).} \quad (1.19)$$

**Table 1.2** Linear regression coefficients and standardized coefficients for the model of Equations (1.3), (1.4), where  $r = 4$ ,  $\Omega = (4, 3, 2, 1)$  and  $\sigma = (2, 2, 2, 2)$ ,  $N = 1000$

	$b$	$\beta_{Z_i}^2$	$S_{Z_i}$ Analytic (see Exercises)
Intercept	0		
$Z_1$	2	0.034	0.03
$Z_2$	2	0.14	0.13
$Z_3$	2	0.31	0.3
$Z_4$	2	0.53	0.53

<sup>13</sup> Metamodels are surrogate models which are built to substitute for computationally intensive simulation models. Metamodels can be built with a variety of strategies (e.g. simple linear regression as discussed above) and purposes (e.g. to perform a sensitivity analysis). See Chapter 5.

<sup>14</sup> The results in Table 1.2 have been obtained with a simple piece of software for regression analysis. Yet, as explained in the next chapter, given that our model (1.3, 1.4) is linear, and the model does not contain any error term, we could have computed exact (analytic) values of the regression coefficients using only five runs and then applying the Kramer formula for a system of five equations (runs) in the five unknowns  $b_0, \dots, b_4$ .

01 As a result it will also be true for the  $\beta$ 's that

$$02 \quad 03 \quad 04 \quad \sum_{i=1}^r (\hat{\beta}_{Z_i})^2 = 1 \quad (1.20)$$

05 when the model is linear.

06 The fact that the two measures coincide for our model can be generalized  
 07 only to linear models and no further. If the model is nonlinear, the two  
 08 measures will be different. Yet the  $\beta$ 's will be a more robust and reliable  
 09 measure of sensitivity even for nonlinear models. First of all, the  $\beta$ 's are  
 10 multidimensionally averaged measures. Unlike  $S_{Z_i}^\sigma$ , which is computed at  
 11 the midpoint of the distribution of  $Z_i$  while keeping all other factors fixed at  
 12 their midpoint,  $\hat{\beta}_{Z_i}$  is the result of an exploration of the entire space of the  
 13 input factors – the limit being in the dimension  $N$  of the sample. For small  
 14  $N$  and large  $r$ , however, the  $\beta$ 's will be rather imprecise. Even in sensitivity  
 15 analysis there is no such thing as a free meal, and one cannot expect to have  
 16 explored a high-dimensionality space with a handful of points. Nevertheless  
 17 a handful is better than just one. Statistical significance tests are available  
 18 for the  $\beta$ 's, so that the analysts can at least know the extent of the problem.

19 Finally, by computing  $\sum_{i=1}^r (\hat{\beta}_{Z_i})^2$  or a related statistic, one will obtain a  
 20 number, in general less than one, equal to the fraction of linearity of the  
 21 model. More precisely, this number – known as the model coefficient of  
 22 determination, and written as  $R_Y^2$  – is equal to the fraction of the variance  
 23 of the original data which come from our model (Equations 1.3, 1.4, in  
 24 this case), which is explained by the regression model of Equation (1.17).  
 25 Again, this fraction should be equal to one for our model; however, to  
 26 give a different example, if  $R_Y^2$  were instead to be of the order of 0.9, then  
 27 the model would be 90% linear and one could use the  $\beta$ 's for sensitivity  
 28 analysis, at the risk of remaining ignorant of some 10% of the variance of  
 29 the problem.<sup>15</sup>

30 Note that

$$32 \quad 33 \quad 34 \quad \sum_{i=1}^r (\hat{\beta}_{Z_i})^2 = 1 = \sum_{i=1}^r (\hat{b}_{Z_i} \sigma_{Z_i} / \sigma_Y)^2, \quad (1.21)$$

35 so that

$$36 \quad 37 \quad 38 \quad \sum_{i=1}^r (\hat{b}_{Z_i} \sigma_{Z_i})^2 = \sigma_Y^2 = V(Y), \quad (1.22)$$

39 where  $V(Y)$  indicates the variance of  $Y$ . Equation (1.22) is to highlight that  
 40 both Equations (1.12) and (1.20) are variance decomposition formulas. As a

---

41  
 42  
 43 <sup>15</sup> This discussion holds for linear regression. More sophisticated metamodelling techniques  
 44 which can overcome these shortcomings are described in Chapter 5.

sensitivity analysis tool, these formulas allow us to decompose the variance of the model output, taken as a descriptor of output uncertainty. Although most practitioners tend to agree on this usage of variance as a proxy for uncertainty, one should remember that the two things are not identical. For example, a measure of uncertainty could be defined on the basis of entropy of model output (see Saltelli *et al.*, 2000, pp. 56–57). In this book we shall use variance decomposition schemes for sensitivity analysis whenever the setting of the analysis allows it.

Wrapping up the results so far, we have seen formulas for decomposing the variance of the model output of interest according to the input factors. Yet we would like to do this for all models, independently of their degree of linearity; that is, we would like to be able to decompose the variance of  $Y$  even for models with a low  $R^2_Y$ . We want to find what is referred to in the literature as a ‘model-free’ approach. One such ‘model-free’ sensitivity measure is based on averaged partial variances, which we now move on to describe along two separate lines.

### 1.2.6 Conditional Variances – First Path

We have a generic model

$$Y = f(X_1, X_2, \dots, X_k) \quad (1.23)$$

like model (1.3) above. Each  $X$  has a nonnull range of variation or uncertainty and we wish to determine what would happen to the uncertainty of  $Y$  if we could fix a factor. Imagine that we fix factor  $X_i$  at a particular value  $x_i^*$ . Let  $V_{X_{\sim i}}(Y | X_i = x_i^*)$  be the resulting variance of  $Y$ , taken over  $X_{\sim i}$  (all factors but  $X_i$ ). We call this a conditional variance, as it is conditional on  $X_i$  being fixed to  $x_i^*$ . We would imagine that, having frozen one potential source of variation ( $X_i$ ), the resulting variance  $V_{X_{\sim i}}(Y | X_i = x_i^*)$  will be less than the corresponding total or unconditional variance  $V(Y)$ . One could therefore conceive of using  $V_{X_{\sim i}}(Y | X_i = x_i^*)$  as a measure of the relative importance of  $X_i$ , reasoning that the smaller  $V_{X_{\sim i}}(Y | X_i = x_i^*)$ , the greater the influence of  $X_i$ . There are two problems with this approach. First, it makes the sensitivity measure dependent on the position of point  $x_i^*$  for each input factor, which is impractical. Second, one can design a model that for particular factors  $X_i$  and fixed point  $x_i^*$  yields  $V_{X_{\sim i}}(Y | X_i = x_i^*) > V(Y)$ , i.e. the conditional variance is in fact greater than the unconditional (see the Exercises at the end of this chapter). If we take instead the average of this measure over all possible points  $x_i^*$ , the dependence on  $x_i^*$  will disappear.

01 We write this as  $E_{X_i}(V_{X_{\sim i}}(Y | X_i))$ . This is always lower or equal to  $V(Y)$ ,  
 02 and in fact:

03

$$04 E_{X_i}(V_{X_{\sim i}}(Y | X_i)) + V_{X_i}(E_{X_{\sim i}}(Y | X_i)) = V(Y). \quad (1.24)$$

05

06 Hence a small  $E_{X_i}(V_{X_{\sim i}}(Y | X_i))$ , or a large  $V_{X_i}(E_{X_{\sim i}}(Y | X_i))$ , will  
 07 imply that  $X_i$  is an important factor. Note that, by Equation (1.24),  
 08  $V_{X_i}(E_{X_{\sim i}}(Y | X_i)) \leq V(Y)$ . The conditional variance  $V_{X_i}(E_{X_{\sim i}}(Y | X_i))$  is  
 09 called the first-order effect of  $X_i$  on  $Y$  and the sensitivity measure:  
 10

11

$$12 S_i = \frac{V_{X_i}(E_{X_{\sim i}}(Y | X_i))}{V(Y)} \quad (1.25)$$

13

14 is known as the first-order sensitivity index of  $X_i$  on  $Y$ .  $S_i$  is a number  
 15 always between 0 and 1.<sup>16</sup> A high value signals an important variable. And  
 16 vice versa? Does a small value of  $S_i$  flag a nonimportant variable? We leave  
 17 this question for later and move directly on to the second path for  $S_i$ .  
 18

20

### 21 1.2.7 Conditional Variances – Second Path

22

23 Let us go back to the scatterplots of Figure 1.6. We have said before that  
 24 what identifies an important factor is the existence of ‘shape’ or ‘pattern’  
 25 in the points, while a uniform cloud of points is a symptom (though not a  
 26 proof) of a noninfluential factor. What, then, constitutes shape? We could  
 27 say that we have a pattern when the distribution of  $Y$ -points over the  
 28 abscissa, i.e. over the factor  $X_i$ , is nonuniform. In other words, if the  $X_i$  axis  
 29 is cut into slices, does one see differences in the distribution of  $Y$ -points over  
 30 the slices (Figure 1.7)? Does the mean value of  $Y$  in each slice vary across  
 31 the slices (Figure 1.8)? From Figure 1.7 (which is the same as Figure 1.6,  
 32 with the addition of ‘slices’) and Figure 1.8 we can see that factor  $Z_4$  is  
 33 more influential than  $Z_1$ , and that the ordering of factors by importance  
 34 is  $Z_4 > Z_3 > Z_2 > Z_1$ , according to how much the mean value of  $Y$  varies  
 35 from one slice to another.

36 We thus suggest as a sensitivity measure the quantity:

37

38 Variation over the slices of the expected value of  $Y$  within each slice.

39

40

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41

42 <sup>16</sup> Here and in the following we shall tend to use the synthetic notation  $S_i$  when the factors  
 43 considered are labelled  $X$ , while we use the lengthier notation, e.g.  $S_{Z_i}$  or  $S_{\Omega_i}$ , when the factor  
 44 has a symbol different from  $X$ .

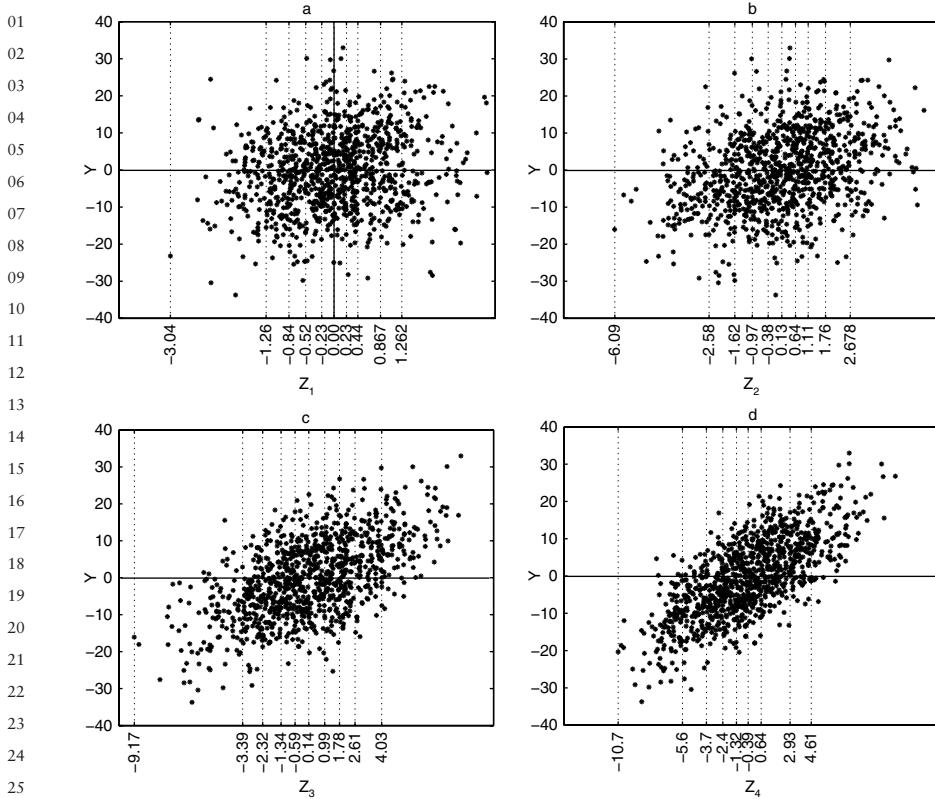


Figure 1.7 Cutting the scatterplots into slices . . .

Taking the limit of this for very thin slices we rediscover  $V_{X_i}(E_{X_{\sim i}}(Y | X_i))$ . Note indeed that the expected value of  $Y$  over a very thin slice corresponds to keeping  $X_i$  fixed while averaging over all-but- $X_i$ , which is exactly  $E_{X_{\sim i}}(Y | X_i)$ . The variance operator is also easily understood.

The issue of cutting the scatterplot into slices will be taken up again in Chapter 5 in the context of metamodelling, at which point a useful approximation of the function expectation value in the slices will be introduced. We anticipate here that  $E_{X_{\sim i}}(Y | X_i)$  will be the best predictor of  $Y$  based on  $X_i$ .

### 1.2.8 Application to Model (1.3)

Having defined the new sensitivity measure  $S_i$  we are eager to apply it to our model of Equation (1.3). It will come as no surprise that for our well-behaved, linear model we obtain

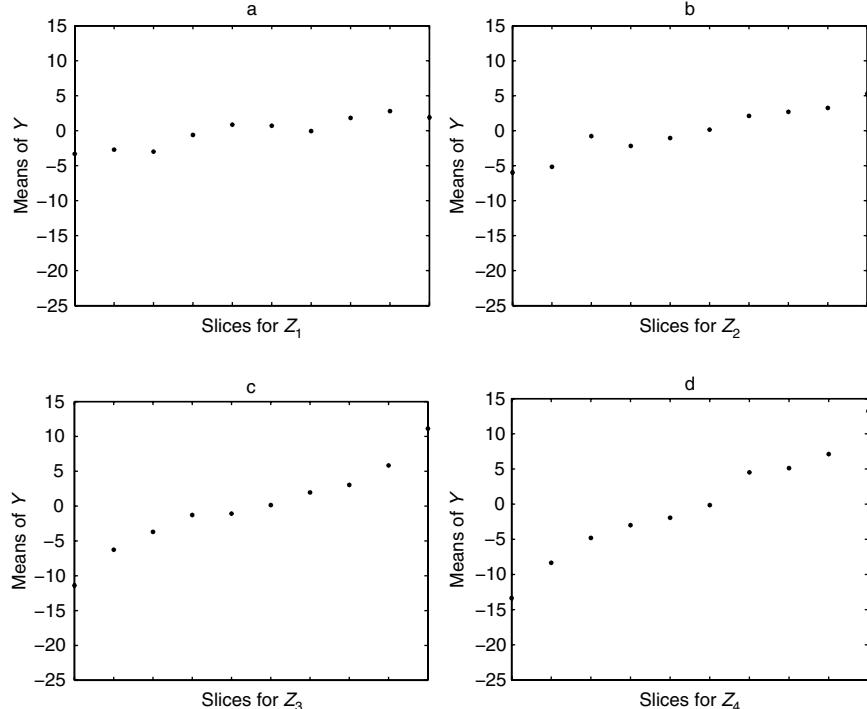


Figure 1.8 ... and taking the average within each slice. Looking at the ordinate, it is clear that  $Z_3$  and  $Z_4$  control more variation than  $Z_1$  and  $Z_2$

$$S_{Z_i} = \frac{V_{Z_i}(E_{Z_{-i}}(Y | Z_i))}{V(Y)} = \beta_{Z_i}^2 \quad (1.26)$$

(See Table 1.2 for a comparison between  $\beta_{Z_i}^2$  and the analytic value of  $S_{Z_i}$ .) The identity of Equation (1.26) holds for linear models, as we would expect given that  $S_{Z_i}$  is a model-free generalization of  $\beta_{Z_i}^2$ . For nonlinear models the two measures will differ, as we shall see in a moment. Another important difference between  $S_{Z_i}$  and  $\beta_{Z_i}^2$  is that while  $\sum_{i=1}^r \beta_{Z_i}^2 = 1$  only for linear models, the relationship  $\sum_{i=1}^r S_{Z_i} = 1$  holds for a larger class: that of additive models. By definition, a model is additive when it is possible to separate the effects of its input variables in a variance decomposition framework. For example,  $Y = \sum_i Z_i^2$  is a nonlinear, additive model in the  $Z$ 's;  $Y = \prod_i Z_i$  is nonlinear and nonadditive.

For nonadditive models the first-order terms do not add up to one, i.e.  $\sum_{i=1}^r S_{Z_i} \leq 1$ . This is also how nonadditive models are defined. We shall turn to this presently, after first discussing the need for 'settings' in sensitivity analysis.

### 01            1.2.9 A First Setting: 'Factor Prioritization'

02  
 03         Experience shows that a poor definition of the objective of the sensitivity  
 04         analysis (i.e. the reason we are investigating the importance of the factors,  
 05         and indeed what we mean by 'importance') can lead to confused or incon-  
 06         clusive results. There are many statistics which can be used for sensitivity  
 07         analysis, and one can easily imagine a table showing for each uncertain  
 08         factor a battery of statistical measures defining the factor's importance. In  
 09         general, each measure of sensitivity will produce its own ranking of factors  
 10         by importance. Since this is the case, how can we tell which factor is impor-  
 11         tant? To avoid this kind of confused result, it is in the analyst's best interests  
 12         to define beforehand what definition of a factor's importance is relevant  
 13         for the exercise in question. We call this a 'setting' (Saltelli *et al.*, 2004,  
 14         pp. 49–56). A setting is a way of framing the sensitivity quest in such a way  
 15         that the answer can be confidently entrusted to a well-identified measure.  
 16         By way of example, we describe here the Factor Prioritization (FP) setting.

17         In this setting one assumes that all factors, e.g. all  $Z$ 's in Equation (1.3),  
 18         have a true, albeit unknown value.<sup>17</sup> Ideally all factors could be 'discovered'  
 19         by the appropriate experiments. If all experiments have the same cost, our  
 20         quest or venture is to identify which factor, once 'discovered' and fixed at  
 21         its true value, would reduce  $V(Y)$  the most.

22         One way to answer this question would be to determine or discover the  
 23         value of the factors, for example, through more measurements. Yet if we  
 24         were to do this we would have gone beyond uncertainty and sensitivity  
 25         analyses. The challenge, therefore, is to identify the appropriate factors  
 26         before any of them are measured or discovered, i.e. when the value to  
 27         which each factor should be fixed is unknown. This suggests that a good  
 28         contender for the title of 'most influential factor' would be that factor which,  
 29         on average, once fixed, would cause the greatest reduction in variance.  
 30         'On average', in this case, means that we must average the fixing of the  
 31         factor over the distribution of the factor itself. It is straightforward to  
 32         see that in this setting  $E_{X_i}(V_{X_{-i}}(Y | X_i))$  is the measure to use. The lower  
 33          $E_{X_i}(V_{X_{-i}}(Y | X_i))$ , and hence the higher  $V_{X_i}(E_{X_{-i}}(Y | X_i))$ , the more probable  
 34         it is that factor  $X_i$  is the factor that one should measure first in order to  
 35         reduce the variance most. We have thus linked the FP setting to a measure,  
 36         the first-order sensitivity index  $S_i$ . This is a gamble, as we do not know  
 37  
 38

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39         <sup>17</sup> In most circumstances one will have factors susceptible of determination, for which  
 40         a true unknown value can be hypothesized (e.g. the failure rate of a component type,  
 41         the value of an activation energy for a chemical reaction), as well as factors intrinsically  
 42         uncertain (the time of failure of a specific component, the wind direction at a given time  
 43         and location). These are termed epistemic and stochastic uncertainties respectively. For  
 44         the purpose of illustrating the setting it is convenient to imagine all factors epistemically  
 45         uncertain.

the position of the true value of a factor over its distribution. Someone actually measuring a given factor could still beat our sensitivity analysis-based guess and reduce the variance by more than we have guessed, or reduce the variance using a factor other than the one we identified via sensitivity analysis.

### 1.2.10 Nonadditive Models

In order to gain confidence with nonadditivity in models, we return to the input for our elementary model (1.3),  $Y = \sum_{i=1}^r \Omega_i Z_i$ , and complicate it by allowing both the  $Z$ 's and the  $\Omega$ 's to become factors – the  $\Omega$ 's are no longer constants. We do this to generate a nonadditive model, as we shall see presently. The additivity of a model depends upon the characteristics of its input factors, so that it is sufficient to change a constant of the model into a factor in order to change the model from additive to nonadditive, although the model is left unchanged in the form (1.3). Our input description becomes

$$\begin{aligned} Z_i &\sim N(\bar{z}_i, \sigma_{Z_i}) & \bar{z}_i = 0 \\ \Omega_i &\sim N(\bar{\Omega}_i, \sigma_{\Omega_i}) & \bar{\Omega}_i = ic \end{aligned} \quad i = 1, 2, \dots, r. \quad (1.27)$$

The distribution of the  $Z$ 's remains unchanged, while the  $\Omega$ 's, so far constant, become input factors with normal distribution. Their mean is not zero as it is for the  $Z$ 's, but rather some number other than zero – we shall explain why in the Exercises at the end of this chapter. For the sake of the example we have made the means of the  $\Omega$ 's nonequivalent and equal in value to the product of the integer  $i$  (used as counter) and a positive constant  $c$ . This is simply a way to make the means of the  $\Omega$ 's increase, so that Equation (1.7) is no longer true. Instead

$$\bar{\Omega}_1 < \bar{\Omega}_2 < \dots < \bar{\Omega}_r. \quad (1.28)$$

The input factors for the analysis are

$$\mathbf{X} = (Z_1, Z_2, \dots, Z_r, \Omega_1, \Omega_2, \dots, \Omega_r) \quad (1.29)$$

and the total number of factors is  $k = 2r$ . We now perform another Monte Carlo experiment, sampling both the  $Z$ 's and the  $\Omega$ 's from their respective distributions in Equation (1.27). Remember that we assume all factors independent, so each factor is sampled from its marginal distribution with no consideration of where the other factors are sampled. How the Monte Carlo sample is used to produce estimates  $\hat{S}_i$  of the first-order sensitivity measures  $S_i$  is explained later in this book (see Chapter 4). We anticipate the results

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**Table 1.3** First-order indices  $S_i$  (analytic) and squared standardized regression coefficient  $\beta_i^2$  for model (1.3, 1.27), where  $r = 4$ ,  $c = 0.5$ ,  $\sigma = (1, 2, 3, 4)$  for both  $\Omega_i$  and  $Z_i$ , and  $N = 40.000$  for the regression analysis. Such a large sample was used to show the convergence between  $S_i$  and  $\beta_i^2$

	$S_i$	$\beta_i^2$
$Z_1$	0.0006	0
$Z_2$	0.009	0.01
$Z_3$	0.046	0.05
$Z_4$	0.145	0.14
$\Omega_1$	0	0
$\Omega_2$	0	0
$\Omega_3$	0	0
$\Omega_4$	0	0

in Table 1.3, where the squared standardized regression estimates  $\hat{\beta}^2$  are also reported for comparison.

It is evident from Table 1.3 that while  $\hat{S}_{Z_i}$  are still greater than zero, the  $\hat{S}_{\Omega_i}$  are practically zero. Furthermore

$$\sum_{i=1}^k \hat{S}_{X_i} = \sum_{i=1}^r \hat{S}_{Z_i} + \sum_{i=1}^r \hat{S}_{\Omega_i} < 1. \quad (1.30)$$

We had already anticipated that for a nonadditive model the sum of the first-order indices would be less than one.

However, it might seem puzzling that the  $\Omega$  input factors seem to have no influence. In fact, it is not difficult to understand why  $S_{\Omega_i}$  must be zero (Figure 1.9).

Let us go back to our definition of  $S_i$ , Equation (1.25):

$$S_i = \frac{V_{X_i}(E_{X_{-i}}(Y | X_i))}{V(Y)}, \quad (1.31)$$

and let us compute it for  $\Omega_i$ ,

$$S_{\Omega_i} = \frac{V_{\Omega_i}(E_{X_{-\Omega_i}}(Y | \Omega_i))}{V(Y)}. \quad (1.32)$$

We focus on the inner expectation  $E_{X_{-\Omega_i}}(Y | \Omega_i)$  which we now have to write explicitly as  $E_{X_{-\Omega_i}}(Y | \Omega_i = \omega_i^*)$  in order to remind ourselves that we have fixed  $\Omega_i$ .

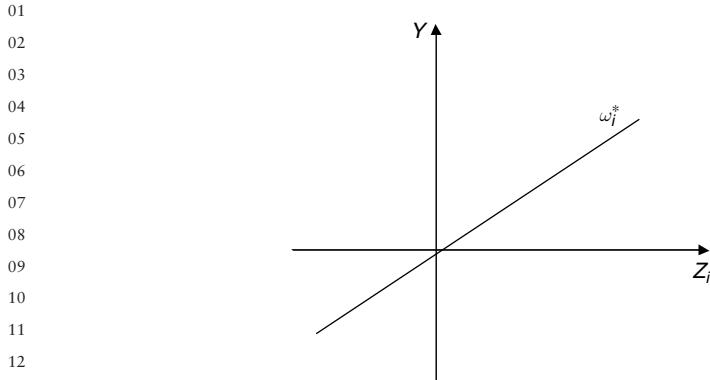


Figure 1.9  $Y$  versus  $Z_i$  for fixed values of  $X_{\sim Z_i}$

17 Note that  $E_{X_{\sim \Omega_i}}$  now means that the mean is taken over all  $Z_j$ 's, including  
18  $Z_i$ , and over all  $\Omega_j$ 's but  $\Omega_i$ .

19 Figure 1.9 shows the plot of  $Y$  versus  $Z_i$  for a fixed nonzero value of  $\omega_i^*$   
20 of input factor  $\Omega_i$  in the case that all the remaining  $\Omega_j$ 's, with  $j \neq i$ , are  
21 fixed to zero. This straight line will be shifted up or down vertically when  
22 the  $\Omega_j$ 's, with  $j \neq i$ , are fixed to values other than zero.

23 Positive and negative values of  $Y$  will hence be equally probable and  
24 equally distributed, so that  $E_{X_{\sim \Omega_i}}(Y | \Omega_i = \omega_i^*)$  will be zero. Figure 1.10  
25 shows how this emerges from Monte Carlo generated scatterplots of  $Y$   
26 versus  $Z_i$  and  $Y$  versus  $\Omega_i$ . It is clear that if  $E_{X_{\sim \Omega_i}}(Y | \Omega_i = \omega_i^*)$  is zero for  
27 any value  $\omega_i^*$ , its variance over all possible values of  $\omega_i^*$  will also be zero,  
28 so that both  $V_{\Omega_i}(E_{X_{\sim \Omega_i}}(Y | \Omega_i))$  and  $S_{\Omega_i}$  will be zero for all factors  $\Omega_i$ .

29 We now understand that the measure  $S_{\Omega_i}$  is zero, but we retain the belief  
30 that factors  $\Omega_i$  should have some influence, especially since this is suggested  
31 by the conical pattern evident in Figure 1.10. It seems therefore that there  
32 may be a problem with our sensitivity measure. A regression coefficient  
33  $\hat{\beta}_{\Omega_i}$  would produce a straight horizontal line through the horizontal conical  
34 plot of  $Y$  versus  $\Omega_i$  in Figure 1.10. However, it is clear from the shape of  
35 this plot that variable  $\Omega_i$  is influential. A possible interpretation is that  $\hat{\beta}_{\Omega_i}$   
36 fails as a sensitivity measure in this case. Does the fact that  $S_{\Omega_i}$  is zero imply  
37 that also  $\hat{\beta}_{\Omega_i}$  fails?

38 Indeed it is unfair to say that  $\beta_{\Omega_i}$  fails in Figure 1.10.  $\beta_{\Omega_i}$  is a linear  
39 measure, so clearly it should not be used on a nonlinear model.  $S_{\Omega_i}$ , however,  
40 is a model-free measure, and must be applicable to nonlinear models. Indeed  
41 this is the case, and we can say that if  $S_{\Omega_i}$  is zero, this means that  $\Omega_i$  has  
42 no effect on  $Y$  'at the first order' (recall that we have thus far discussed  
43 first-order sensitivity indices). The reader familiar with experimental design

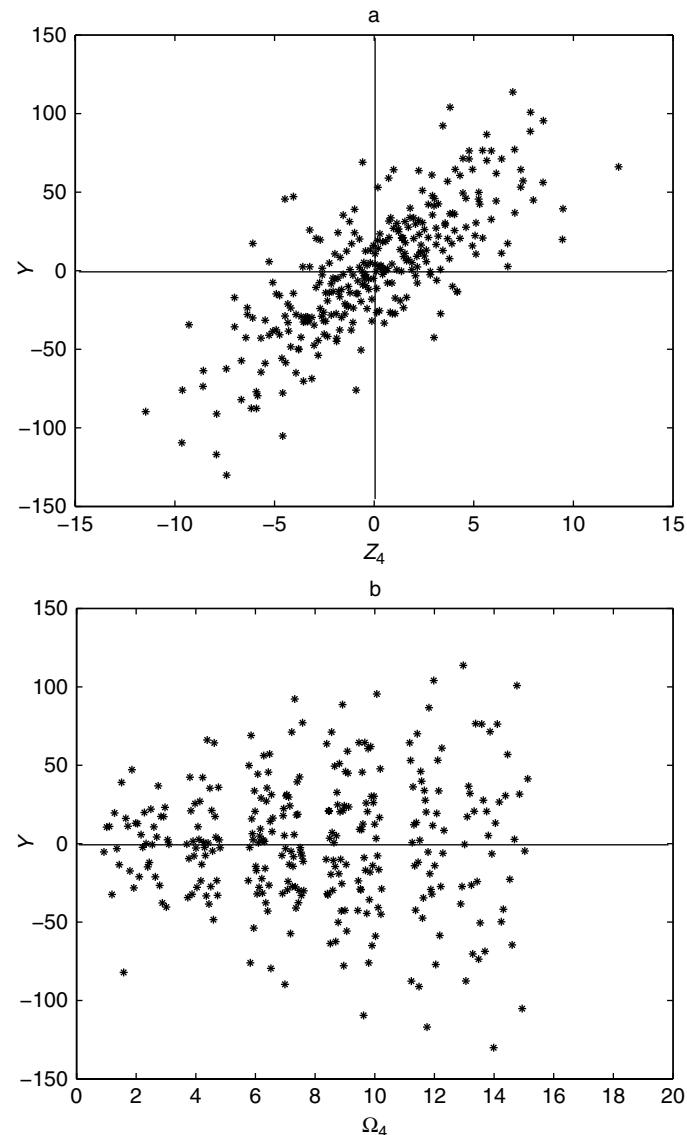


Figure 1.10 Scatterplots of  $Y$  versus  $Z_4$  and versus  $\Omega_4$  for model (1.3, 1.27), at sample size  $N = 1000$ . The first-order sensitivity index for  $Z_4$  is greater than zero while that for  $\Omega_4$  is zero

01 will already have guessed that the effect of  $\Omega_i$  must be captured by some  
 02 higher-order effect, as we now proceed to discuss.

03  
 04  
 05 **1.2.11 Higher-order Sensitivity Indices**

06  
 07 We continue our game with conditioned variances by playing with two  
 08 factors instead of one. Take for instance

09  
 10 
$$\frac{V(E(Y | Z_i, Z_j))}{V(Y)}, \quad (1.33)$$
  
 11  
 12

13 with  $i \neq j$ . We have dropped the indices of both the  $E$  and  $V$  operators.  
 14 Indeed we do not need them if we accept the convention that the argument  
 15 conditioning the inner operator,  $Z_i, Z_j$  in this case, is also the set over which  
 16 we apply the outer operator, i.e. the variance is taken over  $Z_i, Z_j$  (we should  
 17 have written  $V_{Z_i, Z_j}$ ). By default, the inner operator, the average  $E$ , must  
 18 be taken over all-but-( $Z_i, Z_j$ ). What would happen if we could compute  
 19 (1.33), with  $i \neq j$ , and compare it with the corresponding measure for the  
 20 individual factors  $Z_i, Z_j$ ? We would observe that  
 21

22  
 23 
$$\frac{V(E(Y | Z_i, Z_j))}{V(Y)} = S_{Z_i} + S_{Z_j} \quad \text{for } i \neq j, \quad (1.34)$$
  
 24

25 while  
 26

27  
 28 
$$\frac{V(E(Y | \Omega_i, \Omega_j))}{V(Y)} = 0, \quad (1.35)$$
  
 29

30 and  
 31

32 
$$\frac{V(E(Y | Z_i, \Omega_i))}{V(Y)} > S_{Z_i} + S_{\Omega_i}. \quad (1.36)$$
  
 33

34 We anticipate from Chapter 4 that, given two generic factors  $X_i, X_j$ , the  
 35 following result holds:

36  
 37 
$$V(E(Y | X_i, X_j)) = V_i + V_j + V_{ij}, \quad (1.37)$$
  
 38

39 where  
 40

41 
$$V_i = V(E(Y | X_i))$$
  
 42 
$$V_j = V(E(Y | X_j))$$
  
 43 
$$V_{ij} = V(E(Y | X_i, X_j)) - V_i - V_j. \quad (1.38)$$
  
 44

The term  $V_{ij}$  is the interaction term between factors  $X_i, X_j$ . It captures that part of the response of  $Y$  to  $X_i, X_j$  that cannot be written as a superposition of effects separately due to  $X_i$ , and  $X_j$ . Recalling our previous examples of  $Y = \sum_i Z_i^2$  (a nonlinear, additive model) and  $Y = \prod_i Z_i$  (nonlinear, nonadditive), the latter model will have nonzero second-order terms such as  $V_{ij}$ , while the former model will not.

Looking at Equations (1.37, 1.39) and remembering that for our model all  $S_{\Omega_i}$  are zero, we are now ready to grasp the results of Equations (1.34–1.36) (see also Table 1.4).

- Equation (1.34) holds because the interaction term between  $Z_i$  and  $Z_j$  is zero, which is evident from the form of Equation (1.3).
- Equation (1.35) holds because the  $S_{\Omega_i}$  and  $S_{\Omega_j}$  as well as their interaction term are zero.
- Equation (1.36) can be rewritten as

$$\frac{V(E(Y | Z_i, \Omega_j))}{V(Y)} = S_{Z_i} + S_{\Omega_i} + S_{Z_i, \Omega_i},$$

where  $S_{\Omega_i} = 0$ ,  $S_{Z_i, \Omega_i} = V_{Z_i, \Omega_i}/V(Y)$  and the term  $V_{Z_i, \Omega_i}$  is the only type of nonzero second-order term in model (1.3).

If we now sum all the nonzero first-order and second-order terms we get

**Table 1.4** First- and second-order indices for model (1.3, 1.27, analytic), where  $r = 4$ ,  $c = 0.5$ ,  $\sigma = (1, 2, 3, 4)$  for both  $\Omega_i$  and  $Z_i$

Factor	$S_i, S_{ij}$	Factor	$S_{ij}$	Factor	$S_{ij}$
$Z_1$	0.0006	$Z_1, \Omega_2$	0	$Z_3, \Omega_3$	0.183
$Z_2$	0.009	$Z_1, \Omega_3$	0	$Z_3, \Omega_4$	0
$Z_3$	0.046	$Z_1, \Omega_4$	0	$Z_4, \Omega_1$	0
$Z_4$	0.145	$Z_2, Z_3$	0	$Z_4, \Omega_2$	0
$\Omega_1$	0	$Z_2, Z_4$	0	$Z_4, \Omega_3$	0
$\Omega_2$	0	$Z_2, \Omega_1$	0	$Z_4, \Omega_4$	0.578
$\Omega_3$	0	$Z_2, \Omega_2$	0.036	$\Omega_1, \Omega_2$	0
$\Omega_4$	0	$Z_2, \Omega_3$	0	$\Omega_1, \Omega_3$	0
$Z_1, Z_2$	0	$Z_2, \Omega_4$	0	$\Omega_1, \Omega_4$	0
$Z_1, Z_3$	0	$Z_3, Z_4$	0	$\Omega_2, \Omega_3$	0
$Z_1, Z_4$	0	$Z_3, \Omega_1$	0	$\Omega_2, \Omega_4$	0
$Z_1, \Omega_1$	0.002	$Z_3, \Omega_2$	0	$\Omega_3, \Omega_4$	0

$$\sum_{i=1}^r (S_{Z_i} + S_{Z_i \Omega_i}) = 1. \quad (1.39)$$

This means that even for a nonadditive model we have found a way to recover (that is, to understand) 100% of the variance of  $Y$ . Thus variance-based sensitivity measures provide a theoretical framework whereby – provided one has the patience to compute all interaction terms – one can achieve a full understanding of the model's sensitivity pattern. Patience is indeed required, as in principle a model can have interactions of even higher order. Again anticipating one result from Chapter 4, a full analysis of a model with  $k$  factors is composed of

$$\sum_i S_i + \sum_i \sum_{j>i} S_{ij} + \sum_i \sum_{j>i} \sum_{l>j} S_{ijl} + \dots + S_{123\dots k} = 1. \quad (1.40)$$

Model (1.3) can only have nonzero terms up to the second order, and this can be seen ‘by inspection’, as the structure of the model is very simple. In practical applications the subject model of our analysis will be a computer program, and the only way to ascertain whether an interaction exists or not will be to estimate it numerically. The problem is that the series development of Equation (1.40) has as many as  $2^k - 1$  terms. For  $k = 3$  this gives just 7 terms, i.e.  $S_1, S_2, S_3, S_{12}, S_{23}, S_{13}, S_{123}$ ; for  $k = 10$  it gives 1023, too many to look at in practice.

In fact, the variance-based analysis can help us in these circumstances, by computing for each factor a ‘total effect’ term, which we describe next.

### 1.2.12 Total Effects

What is a total effect term? Let us again use our extended model (1.3, 1.27), and ask what we would obtain if we were to compute  $V(E(Y | X_{\sim \Omega_i})) / V(Y)$ . We are conditioning now on all factors but  $\Omega_i$ . In other words

$$\frac{V(E(Y | X_{\sim \Omega_i}))}{V(Y)} = \frac{V(E(Y | \Omega_1, \Omega_2, \dots, \Omega_{i-1}, \Omega_{i+1}, \dots, \Omega_r, Z_1, Z_2, \dots, Z_r))}{V(Y)}. \quad (1.41)$$

By analogy with our discussion of second-order terms, Equation (1.41) should include all terms of any order that do not include factor  $\Omega_i$ . As the sum of all possible sensitivity terms must be 1, the difference

$$\left(1 - \frac{V(E(Y|\mathbf{X}_{\sim\Omega_i}))}{V(Y)}\right)$$

must be made up of all terms of any order that include  $\omega_i$ . For our model, which has only first- and second-order terms, this gives

$$\left(1 - \frac{V(E(Y|\mathbf{X}_{\sim\Omega_i}))}{V(Y)}\right) = S_{\Omega_i} + S_{Z_i\Omega_i} \quad (\text{See Table 1.5}) \quad (1.42)$$

To consider a different example, for a generic three-factor model, one would have

$$S_{T1} = \left(1 - \frac{V(E(Y|\mathbf{X}_{-1}))}{V(Y)}\right) = S_1 + S_{12} + S_{13} + S_{123} \quad (1.43)$$

and

$$S_{T2} = S_2 + S_{12} + S_{23} + S_{123}$$

$$S_{T3} = S_3 + S_{13} + S_{23} + S_{123},$$

where  $S_{Ti}$  denotes the total effect of factor  $X_i$ . We recall that we tend to use the synthetic notation  $(S_i, S_{Ti}, V_i, S_{ij})$  when the factors considered are labelled  $X$ , while we use the lengthier notation  $(S_{Z_i}, S_{TZ_i}, V_{\Omega_i}, S_{Z_i\Omega_i})$  when the factor has a symbol other than  $X$ .

**Table 1.5** First-order and total effects for model (1.3, 1.27, analytic), where  $r = 4$ ,  $c = 0.5$ ,  $\sigma = (1, 2, 3, 4)$  for both  $\Omega_i$  and  $Z_i$

	$S_i$	$S_{Ti}$
$Z_1$	0.0006	$Z_1$ 0.003
$Z_2$	0.009	$Z_2$ 0.045
$Z_3$	0.046	$Z_3$ 0.229
$Z_4$	0.145	$Z_4$ 0.723
$\Omega_1$	0	$\Omega_1$ 0.002
$\Omega_2$	0	$\Omega_2$ 0.036
$\Omega_3$	0	$\Omega_3$ 0.183
$\Omega_4$	0	$\Omega_4$ 0.578

We have argued in a series of works (Saltelli *et al.*, 2004, and references therein) that a good, synthetic, though nonexhaustive characterization of the sensitivity pattern for a model with  $k$  factors is given by the total set of first-order terms plus the total effects. For a system with 10 factors this makes 20 terms rather than 1023.

One last observation about the total effect terms is the following. For the algebraic rule already mentioned in Equation (1.24) we have

$$E_{X_i}(V_{X_{\sim i}}(Y | X_i)) + V_{X_i}(E_{X_{\sim i}}(Y | X_i)) = V(Y),$$

and hence

$$S_{Ti} = 1 - \frac{V(E(Y | X_{\sim i}))}{V(Y)} = \frac{E(V(Y | X_{\sim i}))}{V(Y)}. \quad (1.44)$$

Equipped with this new sensitivity measure, the total effect, we are now ready to introduce another useful ‘setting’ for sensitivity analysis.

### 1.2.13 A Second Setting: ‘Factor Fixing’

One use of sensitivity analysis is to simplify models. If a model is used systematically in a Monte Carlo framework, so that input uncertainties are always propagated through the output, it might be useful to ascertain which of the input factors can be fixed anywhere in their range of variation without appreciably affecting a specific output of interest  $Y$ . This could help to simplify a model in a greater sense, since we might be able to condense (lump) an entire section of our model if all factors entering that section are noninfluential. From the preceding discussion it will be clear that  $S_i = 0$  is a necessary but insufficient condition for fixing factor  $X_i$ . This factor might be involved in interactions with other factors such that, although its first-order term is zero, there might be nonzero higher-order terms. This is exactly what happened with our factors  $\Omega_i$  in the model (1.3, 1.27).

Imagine now that a factor  $X_i$  is truly noninfluential. Let us compute  $V_{X_i}(Y | X_{\sim i} = \mathbf{x}_{\sim i}^*)$ , where we have fixed a point  $\mathbf{x}_{\sim i}^*$  in the multidimensional space  $\mathbf{X}_{\sim i}$ . If factor  $X_i$  is noninfluential, then  $V_{X_i}(Y | X_{\sim i} = \mathbf{x}_{\sim i}^*)$  must be zero, as the value of  $Y$  is totally determined by  $\mathbf{X}_{\sim i}$  and there will be no variance over  $X_i$ . Averaging over non- $X_i$  will not change the result, so that  $E_{X_{\sim i}}(V_{X_i}(Y | X_{\sim i}))$  must be zero as well. Based on our convention of not indicating the conditioning argument, we can also write this as  $E(V(Y | X_{\sim i})) = 0$ . These considerations prove that if  $X_i$  is noninfluential, then  $S_{Ti} = 0$  by Equation (1.44) above.

Conversely, if  $S_{Ti} = 0$  for factor  $X_i$ , then  $E(V(Y | \mathbf{X}_{\sim i})) = 0$ . As the variance can only be a positive number, the fact that the mean  $E(V(Y | \mathbf{X}_{\sim i}))$  is zero implies that  $V(Y | \mathbf{X}_{\sim i} = \mathbf{x}_{\sim i}^*)$  is identically zero for any value of  $\mathbf{x}_{\sim i}^*$ , which proves that  $X_i$  is noninfluential – there is no point in the hyperspace of  $\mathbf{X}$  where  $X_i$  has an effect. This demonstrates that  $S_{Ti} = 0$  is a necessary and sufficient condition for  $X_i$  being noninfluential.

Note that the model simplification underpinned by the ‘factor fixing’ setting can become very important when models need to be audited, for example in the face of a scientific controversy or for use in policy assessment. In these situations one might wish to optimize the ‘relevance’  $R$  of a model, defined as the ratio (Beck *et al.*, 1997):

$$R = \frac{\text{number of factors that truly induce variations in the output of interest}}{\text{total number of factors in the model}}.$$

This approach would guard against the criticism that an overly complex model was being used by one party to obfuscate or discourage investigation.

The concepts of parsimony or simplicity in the context of modelling are illustrated by the works of Peter C. Young (Young *et al.*, 1996; Young, 1999a), who recommends the use of data-driven models, in which a minimum of parameters are inferred directly from the data, as an alternative to law-driven, usually overparametrized models. To give an example, the hydrogeology of a catchment area can be modelled with a complex model based on Darcy’s laws or with a low-order model based on direct interpretation of precipitation and runoff time series. Such a parsimonious description of the system can also be thought of as a complement to a law-driven model. More generally, for models to be used in impact assessment or other regulatory settings, it might be advisable to have a back-of-the-envelope version of the general model for the purpose of negotiating assumptions and inferences with stakeholders. Sensitivity analysis may be instrumental in deriving such a simplified model.

The foregoing discussion of possible settings for sensitivity analysis allows us to make a few more observations on the rationale for sensitivity analysis.

### 1.2.14 Rationale for Sensitivity Analysis

Possible motivations for sensitivity analysis are:

- Model corroboration. Is the inference robust? Is the model overly dependent on fragile assumptions?

- 01 • Research prioritization. Which factor is most deserving of further analysis or measurement?  $\Rightarrow$  factor prioritization setting.
- 02 • Model simplification. Can some factors or compartments of the model be fixed or simplified?  $\Rightarrow$  factor fixing setting.
- 03 • Identifying critical or otherwise interesting regions in the space of the input factors. Identifying factors which interact and which may thus generate extreme values. This is important, for example in system reliability.
- 04 • Prior to parameter estimation, to help set up the (actual or numerical) experiment in those conditions in which the sensitivity of the output to the factor to be estimated is the greatest.

12 To illustrate the last point, imagine that one has actual measurements against which to compare model predictions. Ideally, predictions and measurements can feed into an estimation step. Yet before this is done, it is worth investigating what drives, for instance, the sum of the squared differences between model prediction and actual measurements. Only factors with this type of influence are good candidates for the estimation step. In this way the analyst can decide which experimental conditions are more interesting for the subsequent estimation (Saltelli *et al.*, 2004, pp.151–191).

21 We have already mentioned that uncertainty and sensitivity analyses can be run in tandem to ascertain whether different policies (e.g. strategies to alleviate an environmental problem) are indeed different from one another when compared in the overall space of the uncertainties. An example of such an analysis is found in Saltelli *et al.* (2000 pp. 385–397).

26 It is worth noting in this case that high uncertainty in the inference is not synonymous with low quality in the resulting assessment. Though uncertain, the assessment might still allow policy A to be distinguished from policy B (implying high quality) while the opposite is also possible, i.e. that the model might not allow these options to be distinguished even with only moderate uncertainties in the inference (implying a low-quality assessment). On a similar ground, when confronted with a plurality of stakeholders' views and beliefs as to how an issue should be tackled or framed, we may use sensitivity analysis to ascertain whether – within the latitude of the different framings and assumptions – we still can reach some robust inference, i.e. a high-quality assessment. We would call such an inference – or the resulting preferred policy – 'socially' robust, as it is compatible with such a plurality of viewpoints. On the contrary, we might find that the different framings give rise to such great latitude in the resulting inference that no robust policy can be identified.

41 Another general consideration with respect to the global, explorative nonparametric methods for the sensitivity analysis just described is that 42 these have a better chance of being resilient towards type II errors than 43 local (derivative-based) methods. The possibility of important factors 44

being overlooked or dangerous or critical combinations of input factors neglected decreases with the level of exploration of the space of the input factors (Farrell, 2007). The attention paid in global methods to interaction effects is also a protection against type II errors. In Saltelli *et al.* (2005) we show that, for even a relatively simple and well-studied chemical reactor system, global sensitivity analysis and attention to the interactions can lead to the identification of a larger ‘runaway’ portion in the space of the input factors than could previously be identified.

Some of the motivations just described would demand being able to apportion uncertainty not only among factors, but also among sets of factors, for example to distinguish data uncertainty from experts’ uncertainty, system uncertainty from policy option uncertainty and so on. We offer a few tools for this in the following.

### 1.2.15 Treating Sets

An additional interesting feature of variance-based methods is that they allow for a concise treatment of the sensitivity of sets of factors. Referring again to model (1.3, 1.27), we can imagine computing a variance measure conditioned on a subset of the input factors, e.g. on the set  $\Omega$ ,  $S_\Omega = V(E(Y | \Omega)) / V(Y)$ . From the description in the previous sections it is easy to understand that  $S_\Omega$  will include all first-order terms related to  $\Omega$  plus second- and higher-order product terms including only members of  $\Omega$ . We already know that these are all zero. We can likewise compute  $S_Z = V(E(Y | Z)) / V(Y)$  for the set  $Z$ . This similarly contains all nonzero first-order terms plus the null second- and higher-order terms internal to  $Z$ . Finally we can compute

$$S_{\Omega, Z} = V(Y) - S_\Omega - S_Z, \quad (1.45)$$

which will contain all cross-product terms not involved in  $S_\Omega, S_Z$ . Going back to our example of Equation (1.3) as a composite indicator with weights  $\Omega$  given by experts and variables  $Z$  coming from statistical offices, with Equation (1.45) we have apportioned variance between data and experts and an interaction between the two.

Similarly, we could share the uncertainty in  $Y$  among the couples  $A_i = (\Omega_i, Z_i)$  and apply

$$\sum_i S_{A_i} + \sum_i \sum_{j>i} S_{A_i A_j} + \sum_i \sum_{j>i} \sum_{l>j} S_{A_i A_j A_l} + \dots = 1. \quad (1.46)$$

01 As we already know that for our model all cross-product terms with  $i \neq j$   
 02 are zero, this can be reduced to the convenient

$$03 \quad 04 \quad 05 \quad \sum_i^r S_{A_i} = 1, \quad (1.47)$$

06 in which uncertainty is divided among ‘themes’, each theme comprising  
 07 an indicator and its weight. It is easy to imagine similar applications. For  
 08 example, one could divide uncertainty among observational data, estima-  
 09 tion, model assumptions, model resolution and so on.

### 11 12 1.2.16 Further Methods

13 So far we have discussed the following tools for sensitivity analysis:

- 14 • derivatives and sigma-normalized derivatives;
- 15 • regression coefficients (standardized);
- 16 • variance-based measures;
- 17 • scatterplots.

18 We have shown the equivalence of sigma-normalized coefficients  
 $S_i^\sigma = \sigma_{Z_i} \partial Y / \sigma_Y \partial X_i$ , regression coefficients  $\beta_i$  and variance-based first-order  
 19 sensitivity indices  $S_i$  for linear models, as well as how  $S_i$  is a model-free  
 20 extension of the variance decomposition scheme to models of unknown  
 21 linearity. We have discussed how nonadditive models can be treated in the  
 22 variance-based sensitivity framework. We have also indicated that scatter-  
 23 plots are a powerful tool for sensitivity analysis and shown how  $S_i$  can  
 24 be interpreted in relation to the existence of ‘shape’ in an  $X_i$  versus  $Y$   
 25 scatterplot.

26 At a greater level of detail (Ratto *et al.*, 2007) one can use modern regres-  
 27 sion tools (such as state-space filtering methods) to interpolate points in the  
 28 scatterplots, producing very reliable  $E(Y | X_i = x_i^*)$  curves. The curves can  
 29 then be used for sensitivity analysis. Their shape is more evident than that  
 30 of dense scatterplots (compare Figure 1.7 with Figure 1.8). Furthermore,  
 31 one can derive the first-order sensitivity indices directly from those curves,  
 32 so that an efficient way to estimate  $S_i$  is to use state-space regression on the  
 33 scatterplots and then take the variances of these.

34 In general, for a model of unknown linearity, monotonicity and additivity,  
 35 variance-based measures constitute a good means of tackling settings such  
 36 as factor fixing and factor prioritization. We shall discuss one further setting  
 37 before the end of this chapter, but let us first consider whether there are  
 38 alternatives to the use of variance-based methods for the settings so far  
 39 described.

01 Why might we need an alternative? The main problem with variance-based measures is computational cost. Estimating the sensitivity coefficients takes many model runs (see Chapter 4). Accelerating the computation of sensitivity indices of all orders – or even simply of the  $S_i, S_{Ti}$  couple – is the most intensely researched topic in sensitivity analysis (see the filtering approach just mentioned). It can reasonably be expected that the estimation of these measures will become more efficient over time.

08 At the same time, and if only for screening purposes, it would be useful to have methods to find approximate sensitivity information at lower sample sizes. One such method is the Elementary Effect Test.

### 12 1.2.17 Elementary Effect Test

15 The Elementary Effect Test is simply an average of derivatives over the space of factors. The method is very simple. Consider a model with  $k$  independent input factors  $X_i, i = 1, 2, \dots, k$ , which varies across  $p$  levels. The input space is the discretized  $p$ -level grid  $\Omega$ . For a given value of  $\mathbf{X}$ , the elementary effect of the  $i$ th input factor is defined as

$$21 EE_i = \frac{[Y(X_1, X_2, \dots, X_{i-1}, X_i + \Delta, \dots, X_k) - Y(X_1, X_2, \dots, X_k)]}{\Delta}, \quad (1.48)$$

24 where  $p$  is the number of levels,  $\Delta$  is a value in  $\{1/(p-1), \dots, 1-1/(p-1)\}$ ,  
 25  $\mathbf{X} = (X_1, X_2, \dots, X_k)$  is any selected value in  $\Omega$  such that the transformed  
 26 point  $(\mathbf{X} + \mathbf{e}_i \Delta)$  is still in  $\Omega$  for each index  $i = 1, \dots, k$ , and  $\mathbf{e}_i$  is a vector of  
 27 zeros but with a unit as its  $i$ th component. Then the absolute values of the  
 28  $EE_i$ , computed at  $r$  different grid points for each factor, are averaged

$$30 \mu_i^* = \frac{1}{r} \sum_{j=1}^r |EE_i^j| \quad (1.49)$$

33 and the factors ranked according to the obtained mean  $\mu_i^*$ .

35 In order to compute efficiently, a well-chosen strategy is needed for  
 36 moving from one effect to the next, so that the input space is explored with  
 37 a minimum of points (see Chapter 3).

38 Leaving aside computational issues for the moment,  $\mu^*$  is a useful measure  
 39 for the following reasons:

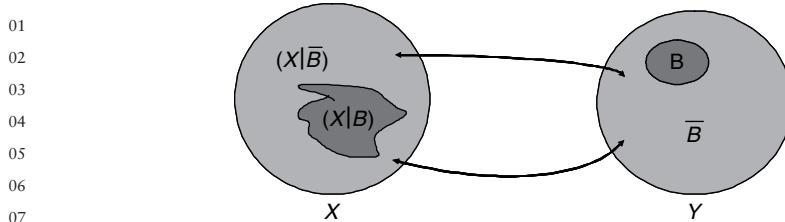
- 40 1. It is semi-quantitative – the factors are ranked on an interval scale;
- 41 2. It is numerically efficient;
- 42 3. It is very good for factor fixing – it is indeed a good proxy for  $S_{Ti}$ ;
- 43 4. It can be applied to sets of factors.

01 Due to its semi-quantitative nature the  $\mu^*$  can be considered a screening  
02 method, especially useful for investigating models with many (from a few  
03 dozen to 100) uncertain factors. It can also be used before applying a  
04 variance-based measure to prune the number of factors to be considered.  
05 As far as point (3) above is concerned,  $\mu^*$  is rather resilient against type  
06 II errors, i.e. if a factor is deemed noninfluential by  $\mu^*$  it is unlikely to be  
07 identified as influential by another measure.

### 08 1.2.18 Monte Carlo Filtering

10 While  $\mu^*$  is a method of tackling factor fixing at lower sample size, the next  
11 method we present is linked to an altogether different setting for sensitivity  
12 analysis. We call this ‘factor mapping’ and it relates to situations in which  
13 we are especially concerned with a particular portion of the distribution of  
14 output  $Y$ . For example, we are often interested in  $Y$  being above or below  
15 a given threshold. If  $Y$  were a dose of contaminant, we might be interested  
16 in how much (how often) a threshold level for this contaminant is being  
17 exceeded. Or  $Y$  could be a loss (e.g. financial) and we might be interested in  
18 how often a maximum admissible loss is being exceeded. In these settings  
19 we tend to divide the realization of  $Y$  into ‘good’ and ‘bad’. This leads to  
20 Monte Carlo filtering (MCF, see Saltelli *et al.*, 2004, pp. 151–191 for a  
21 review). In MCF one runs a Monte Carlo experiment producing realizations  
22 of the output of interest corresponding to different sampled points in the  
23 input factor space, as for variance-based or regression analysis. Having  
24 done this, one ‘filters’ the realizations, e.g. elements of the  $Y$ -vector. This  
25 may entail comparing them with some sort of evidence or for plausibility  
26 (e.g. one may have good reason to reject all negative values of  $Y$ ). Or one  
27 might simply compare  $Y$  against thresholds, as just mentioned. This will  
28 divide the vector  $Y$  into two subsets: that of the well-behaved realizations  
29 and that of the ‘misbehaving’ ones. The same will apply to the (marginal)  
30 distributions of each of the input factors. Note that in this context one is  
31 not interested in the variance of  $Y$  as much as in that part of the distribution  
32 of  $Y$  that matters – for example, the lower-end tail of the distribution may  
33 be irrelevant compared to the upper-end tail or vice versa, depending on  
34 the problem. Thus the analysis is not concerned with which factor drives  
35 the variance of  $Y$  as much as with which factor produces realizations of  $Y$   
36 in the forbidden zone. Clearly, if a factor has been judged noninfluential by  
37 either  $\mu^*$  or  $S_{Ti}$ , it will be unlikely to show up in an MCF. Steps for MCF  
38 are as follows:

- 40
- 41 • A simulation is classified as either  $B$ , for behavioural, or  $\bar{B}$ , for nonbe-  
42 havioural (Figure 1.11).
  - 43 • Thus a set of binary elements is defined, allowing for the identification of  
44 two subsets for each  $X_i$ : one containing a number  $n$  of elements denoted

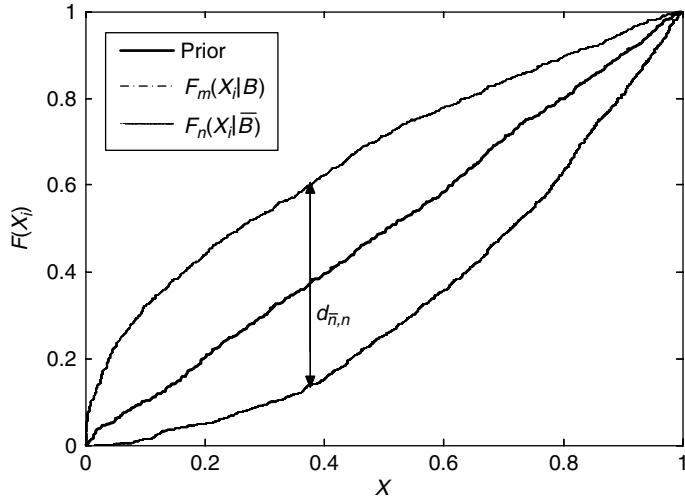


**Figure 1.11** Mapping behavioural and nonbehavioural realizations with Monte Carlo filtering

$(X | B)$  and a complementary set  $(X | \bar{B})$  containing the remaining  $\bar{n} = N - n$  simulations (Figure 1.11).

- A statistical test can be performed for each factor independently, analysing the maximum distance between the cumulative distributions of the  $(X | B)$  and  $(X | \bar{B})$  sets (Figure 1.12).

If the two sets are visually and statistically<sup>18</sup> different, then  $X_i$  is an influential factor in the factor mapping setting.



**Figure 1.12** Distinguishing between the two sets using a test statistic

<sup>18</sup> Smirnov two-sample test (two-sided version) is used in Figure 1.12 (see Saltelli *et al.*, 2004, pp. 38–39).

### 01           1.3 NONINDEPENDENT INPUT FACTORS

02  
03     Throughout this introductory chapter we have systematically assumed that  
04     input factors are independent of one another. The main reason for this  
05     assumption is of a very practical nature: dependent input samples are more  
06     laborious to generate (although methods are available for this; see Saltelli  
07     *et al.*, 2000) and, even worse, the sample size needed to compute sensi-  
08     tivity measures for nonindependent samples is much higher than in the case  
09     of uncorrelated samples.<sup>19</sup> For this reason we advise the analyst to work  
10     on uncorrelated samples as much as possible, e.g. by treating dependen-  
11     cies as explicit relationships with a noise term.<sup>20</sup> Note that when working  
12     with the MCF just described a dependency structure is generated by the  
13     filtering itself. The filtered factors will probably correlate with one another  
14     even if they were independent in the original unfiltered sample. This could  
15     be a useful strategy to circumvent the use of correlated samples in sensi-  
16     tivity analysis. Still there might be very particular instances where the use  
17     of correlated factors is unavoidable. A case could occur with the para-  
18     metric bootstrap approach described in Figure 1.3. After the estimation  
19     step the factors will in general be correlated with one another, and if a  
20     sample is to be drawn from these, it will have to respect the correlation  
21     structure.

22     Another special instance when one has to take factors' dependence into  
23     consideration is when analyst A tries to demonstrate the falsity of an uncer-  
24     tainty analysis produced by analyst B. In such an adversarial context, A  
25     needs to show that B's analysis is wrong (e.g. nonconservative) even when  
26     taking due consideration of the covariance of the input factors as explicitly  
27     or implicitly framed by B.

### 31           1.4 POSSIBLE PITFALLS FOR A SENSITIVITY 32           ANALYSIS

33  
34     As mentioned when discussing the need for settings, a sensitivity analysis  
35     can fail if its underlying purpose is left undefined; diverse statistical tests  
36     and measures may be thrown at a problem, producing a range of different  
37     factor rankings but leaving the researcher none the wiser as to which

38  
39  
40     <sup>19</sup> Dependence and correlation are not synonymous. Correlation implies dependence, while  
41     the opposite is not true. Dependencies are nevertheless described via correlations for practical  
42     numerical computations.

43     <sup>20</sup> Instead of entering  $X_1$  and  $X_2$  as correlated factors one can enter  $X_1$  and  $X_3$ , with  $X_3$  being  
44     a factor describing noise, and model  $X_2$  as a function of  $X_1$  and  $X_3$ .

ranking to believe or privilege. Another potential danger is to present sensitivity measures for too many output variables  $Y$ . Although exploring the sensitivity of several model outputs is sound practice for testing the quality of the model, it is better, when presenting the results of the sensitivity analysis, to focus on the key inference suggested by the model, rather than to confuse the reader with arrays of sensitivity indices relating to intermediate output variables. Piecewise sensitivity analysis, such as when investigating one model compartment at a time, can lead to type II errors if interactions among factors of different compartments are neglected. It is also worth noting that, once a model-based analysis has been produced, most modellers will not willingly submit it to a revision via sensitivity analysis by a third party.

This anticipation of criticism by sensitivity analysis is also one of the 10 commandments of applied econometrics according to Peter Kennedy:

Thou shall confess in the presence of sensitivity. Corollary: Thou shall anticipate criticism [...] When reporting a sensitivity analysis, researchers should explain fully their specification search so that the readers can judge for themselves how the results may have been affected. This is basically an ‘honesty is the best policy’ approach, advocated by Leamer, (1978, p. vi) (Kennedy, 2007).

To avoid this pitfall, an analyst should implement uncertainty and sensitivity analyses routinely, both in the process of modelling and in the operational use of the model to produce useful inferences.

Finally the danger of type III error should be kept in mind. Framing error can occur commonly. If a sensitivity analysis is jointly implemented by the owner of the problem (which may coincide with the modeller) and a practitioner (who could again be a modeller or a statistician or a practitioner of sensitivity analysis), it is important to avoid the former asking for just some ‘technical help’ from the latter upon a predefined framing of the problem. Most often than not the practitioner will challenge the framing before anything else.

## 1.5 CONCLUDING REMARKS

1. We have just shown different settings for sensitivity analysis, such as:

- factor prioritization, linked to  $S_i$ ;
- factor fixing, linked to  $S_{Ti}$  or  $\mu^*$ ;
- factor mapping, linked to MCF;
- metamodelling (hints).

- 01       The authors have found these settings useful in a number of applications.  
02       This does not mean that other settings cannot be defined and usefully  
03       applied.
- 04       2. We have discussed fitness for purpose as a key element of model quality.  
05       If the purpose is well defined, the output of interest will also be well  
06       identified. In the context of a controversy, this is where attention will be  
07       focused and where sensitivity analysis should be concentrated.
- 08       3. As discussed, a few factors often account for most of the variation.  
09       Advantage should be taken of this feature to simplify the results of  
10       a sensitivity analysis. Group sensitivities are also useful for presenting  
11       results in a concise fashion.
- 12       4. Assuming models to be true is always dangerous. An uncer-  
13       tainty/sensitivity analysis is always more convincing when uncertainty  
14       has been propagated through more than just one model. Using a pars-  
15       imonious data-driven and a less parsimonious law-driven model for the  
16       same application can be especially effective and compelling.
- 17       5. When communicating scientific results transparency is an asset. As the  
18       assumptions of a parsimonious model are more easily assessed, sensitivity  
19       analysis should be followed by a model simplification.

20       The reader will find in this and the following chapters didactic examples  
21       for the purpose of familiarization with sensitivity measures. Most of the  
22       exercises will be based on models whose output (and possibly the associ-  
23       ated sensitivity measures) can be computed analytically. In most practical  
24       instances the model under analysis or development will be a computational  
25       one, without a closed analytic formula.

26       Typically, models will involve differential equations or optimization algo-  
27       rithms involving numerical solutions. For this reason the best available prac-  
28       tices for numerical computations will be presented in the following chapters.  
29       For the Elementary Effects Test, we shall offer numerical procedures devel-  
30       oped by Campolongo *et al.* (1999b, 2000, 2007). For the variance-based  
31       measures we shall present the Monte Carlo based design developed by Saltelli  
32       (2002) as well as the Random Balance Designs based on Fourier Amplitude  
33       Sensitivity Test (FAST-RBD, Tarantola *et al.*, 2006, see Chapter 4). All these  
34       methods are based on true points in the space of the input factors, i.e. on actual  
35       computations of the model at these points. An important and powerful class  
36       of methods will be presented in Chapter 5; such techniques are based on meta-  
37       modelling, e.g. on estimates of the model at untried points. Metamodelling  
38       allows for a great reduction in the cost of the analysis and becomes in fact the  
39       only option when the model is expensive to run, e.g. when a single simulation  
40       of the model takes tens of minutes or hours or more. The drawback is that  
41       metamodelling tools such as those developed by Ratto *et al.* (2007) are less  
42       straightforward to encode than plain Monte Carlo. Where possible, pointers  
43       will be given to available software.

## 01 1.6 EXERCISES

02 1. Prove that

$$03 V(Y) = E(Y^2) - E^2(Y).$$

- 04 2. Prove that for an additive model of two independent variables  $X_1$  and  
05  $X_2$ , fixing one variable can only decrease the variance of the model.
- 06 3. Why in  $\mu^*$  are absolute differences used rather than simple differences?
- 07 4. If the variance of  $Y$  as results from an uncertainty analysis is too large,  
08 and the objective is to reduce it, sensitivity analysis can be used to suggest  
09 how many and which factors should be better determined. Is this a new  
10 setting? Would you be inclined to fix factors with a larger first-order  
11 term or rather those with a larger total effect term?
- 12 5. Suppose  $X_1$  and  $X_2$  are uniform variates on the interval  $[0, 1]$ . What is  
13 the mean? What is the variance? What is the mean of  $X_1 + X_2$ ? What is  
14 the variance of  $X_1 + X_2$ ?
- 15 6. Compute  $S_i$  analytically for model (1.3, 1.4) with the following values:  
16  $r = 2$ ,  $\sigma = \{1, 2\}$  and  $\Omega = \{2, 1\}$ .
- 17 7. Write a model (an analytic function and the factor distribution functions)  
18 in which fixing an uncertain factor increases the variance.
- 19 8. What would have been the result of using zero-centred distributions for  
20 the  $\Omega$ 's in Equation (1.27)?

## 25 1.7 ANSWERS

- 26 1. Given a function  $Y = f(\mathbf{X})$  where  $\mathbf{X} = (X_1, X_2, \dots, X_k)$  and  $\mathbf{X} \sim p(\mathbf{X})$   
27 where  $p(\mathbf{X})$  is the joint distribution of  $\mathbf{X}$  with  $\int p(\mathbf{X}) d\mathbf{X} = 1$ , then the  
28 function mean can be defined as

$$31 E(Y) = \int f(\mathbf{X}) p(\mathbf{X}) d\mathbf{X},$$

33 and its variance as

$$35 \begin{aligned} \text{Var}(Y) &= \int (f(\mathbf{X}) - E(Y))^2 p(\mathbf{X}) d\mathbf{X} \\ 36 &= \int f^2(\mathbf{X}) p(\mathbf{X}) d\mathbf{X} + E^2(Y) - 2 \int E(Y) f(\mathbf{X}) p(\mathbf{X}) d\mathbf{X} \\ 37 &= E(Y^2) + E^2(Y) - 2E^2(Y) \\ 38 &= E(Y^2) - E^2(Y). \end{aligned}$$

42 Using this formula it can easily be proven that  $\text{Var}(Y) = \text{Var}(Y + c)$ ,  
43 with  $c$  an arbitrary constant. This result is used in Monte Carlo-based

01 variance (and conditional variance) computation by rescaling all values  
 02 of  $Y$  subtracting  $E(Y)$ . This is done because the numerical error in the  
 03 variance estimate increases with the value of  $Y$ .

- 04 2. We can write the additive model of two variables  $X_1$  and  $X_2$  as  
 05  $Y = f_1(X_1) + f_2(X_2)$ , where  $f_1$  is only a function of  $X_1$  and  $f_2$  is only a  
 06 function of  $X_2$ .

07 Recalling that the variance of  $(Y)$  can be written as  $V(Y) = E(Y^2) -$   
 08  $E^2(Y)$ , where  $E$  stands for the expectation value, and applying it to  $Y$   
 09 we obtain

$$10 \quad 11 \quad V(Y) = E(f_1^2 + f_2^2 + 2f_1f_2) - E^2(f_1 + f_2).$$

12 Given that  $E(f_1f_2) = E(f_1)E(f_2)$  for independent variables, then the above  
 13 can be reduced to

$$14 \quad 15 \quad V(Y) = E(f_1^2) + E(f_2^2) - E^2(f_1) - E^2(f_2),$$

17 which can be rewritten as

$$19 \quad 20 \quad V(Y) = V(f_1) + V(f_2),$$

21 which proves that fixing either  $X_1$  or  $X_2$  can only reduce the variance of  $Y$ .

- 22 3. Modulus incremental ratios are used in order to avoid positive and  
 23 negative values cancelling each other out when calculating the average.  
 24 4. It is a new setting. In Saltelli *et al.* (2004) we called it the variance  
 25 cutting setting, when the objective of sensitivity analysis is the reduction  
 26 of the output variance to a lower level by fixing the smallest number of  
 27 input factors. This setting can be considered as relevant in, for example,  
 28 risk assessment studies. Fixing the factors with the highest total effect  
 29 term increases our chances of fixing, besides the first-order terms, some  
 30 interaction terms possibly enclosed in the totals, thus maximizing our  
 31 chances of reducing the variance (see Saltelli *et al.*, 2004).  
 32 5. Both  $X_1$  and  $X_2$  are uniformly distributed in  $[0, 1]$ , i.e.

$$34 \quad p(X_1) = p(X_2) = U(0, 1).$$

36 This means that  $p(X_i)$  is 1 for  $X_i \in [0, 1]$  and zero otherwise. Thus

$$38 \quad 39 \quad E(X_1) = E(X_2) = \int_{x=0}^1 p(x)x dx = \left[ \frac{x^2}{2} \right]_0^1 = \frac{1}{2}.$$

41 Further:

$$43 \quad 44 \quad Var(X_1) = Var(X_2) = \int_{x=0}^1 p(x) \left( x - \frac{1}{2} \right)^2 dx = \int_{x=0}^1 \left( x^2 - x + \frac{1}{4} \right) dx$$

$$\begin{aligned} &= \left[ \frac{x^3}{3} - \frac{x^2}{2} + \frac{1}{4}x \right]_0^1 = \frac{1}{3} - \frac{1}{2} + \frac{1}{4} = \frac{1}{12} \\ &E(X_1 + X_2) = E(X_1) + E(X_2) = 1, \end{aligned}$$

as the variables are separable in the integral.

Given that  $X_1 + X_2$  is an additive model (see Exercise 1) it is also true that

$$Var(X_1 + X_2) = Var(X_1) + Var(X_2) = \frac{1}{6}.$$

The same result is obtained integrating explicitly

$$Var(X_1 + X_2) = \int_{x_1=0}^1 \int_{x_2=0}^1 p(\mathbf{x}) (x_1 + x_2 - 1)^2 dx_1 dx_2.$$

Note that the model (1.3, 1.4) is linear and additive. Further, its probability density function can be written as the product of the factors' marginal distributions (independent factors). Writing the model for  $r = 2$  we have

$$Y(Z_1, Z_2) = \Omega_1 Z_1 + \Omega_2 Z_2$$

with

$$Z_1 \sim N(0, 1) \quad \text{or equivalently } p(Z_1) = \frac{1}{\sigma_{Z_1} \sqrt{2\pi}} e^{-\frac{(Z_1)^2}{2\sigma_{Z_1}^2}}$$

and a similar equation for  $p(Z_2)$ . Note that by definition the distributions are normalized, i.e. the integral of each  $p(Z_i)$  over its own variable  $Z_1$  is 1, so that the mean of  $Y$  can be reduced to

$$E(Y) = \Omega_1 \int_{-\infty}^{+\infty} Z_1 p(Z_1) dZ_1 + \Omega_2 \int_{-\infty}^{+\infty} Z_2 p(Z_2) dZ_2.$$

These integrals are of the type  $\int x e^{-x^2} dx$ , whose primitive  $-e^{-x^2}/2$  vanishes at the extremes of integration, so that  $E(Y) = 0$ . Given that the model is additive, the variance will be

$$V(Y) = V_{Z_1} + V_{Z_2} = V(\Omega_1 Z_1) + V(\Omega_2 Z_2).$$

For either  $Z_1$  or  $Z_2$  it will be

$$V_{Z_i} = V(\Omega_i Z_i) = \Omega_i^2 V(Z_i).$$

We write

$$V(Z_i) = E(Z_i^2) - E^2(Z_i) = E(Z_i^2)$$

01           and

02           03           04

$$E(Z_i^2) = \frac{1}{\sqrt{2\pi}\sigma_{Z_i}} \int_{-\infty}^{\infty} z_i^2 e^{-z_i^2/2\sigma_{Z_i}^2} dz_i.$$

05           The tabulated form is

06           07           08

$$\int_{-\infty}^{+\infty} t^2 e^{-at^2} dt = \frac{\sqrt{\pi}}{4},$$

09           10           which gives with an easy transformation

11           12

$$E(Z_i^2) = \sigma_{Z_i}^2$$

13           so that

14           15

$$V_{Z_i} = \Omega_i^2 \sigma_{Z_i}^2$$

16           17           and

18           19           20

$$V(Y) = \Omega_1^2 \sigma_{Z_1}^2 + \Omega_2^2 \sigma_{Z_2}^2$$

21           22           and

23           24           25

$$S_{Z_i} = \frac{\Omega_i^2 \sigma_{Z_i}^2}{V(Y)}.$$

26           Inserting the values  $\sigma = \{1, 2\}$  and  $\Omega = \{2, 1\}$  we obtain  $V(Y) = 8$  and  
27            $S_{Z_1} = S_{Z_2} = \frac{1}{2}$ .

28           The result above can be obtained by explicitly applying the formula  
29           for  $S_i$  to our model:

30           31           32

$$S_{Z_i} = \frac{V(E(Y | Z_i))}{V(Y)},$$

33           which entails computing first  $E(Y | Z_i = z_i^*)$ . Applying this to our model  
34            $Y = \Omega_1 Z_1 + \Omega_2 Z_2$  we obtain, for example, for factor  $Z_1$ :

35           36           37           38

$$E(Y | Z_1 = z_1^*) = \int_{-\infty}^{+\infty} p(z_1) p(z_2) (\Omega_1 z_1^* + \Omega_2 z_2) dz_1 dz_2 = \Omega_1 z_1^*.$$

39           40           Hence  $V_{Z_1}$  – the variance over  $z_1^*$  of  $\Omega_1 z_1^*$  – is, as before, equal to  $\Omega_1^2 \sigma_{Z_1}^2$   
41           and

42           43           44

$$S_{Z_i} = \frac{\Omega_i^2 \sigma_{Z_i}^2}{\Omega_1^2 \sigma_{Z_1}^2 + \Omega_2^2 \sigma_{Z_2}^2}.$$

01     7. We consider the model  $Y = X_1 \cdot X_2$ , with the factors identically  
02     distributed as

$$03 \quad X_1, X_2 \sim N(0, \sigma).$$

05     Based on the previous exercise it is easy to see that  
06

$$07 \quad E(Y) = E(X_1 X_2) = E(X_1)E(X_2) = 0,$$

09     so that

$$11 \quad V(Y) = E(X_1^2 X_2^2) = E(X_1^2) E(X_2^2) = \sigma^4.$$

12     If  $X_2$  is fixed to a generic value  $x_2^*$ , then  
13

$$14 \quad E(X_1 x_2^*) = x_2^* E(X_1) = 0$$

16     as in a previous exercise, and  
17

$$18 \quad V(Y | X_2 = x_2^*) = V(X_1 x_2^*) = E(X_1^2 (x_2^*)^2) = (x_2^*)^2 E(X_1^2) = (x_2^*)^2 \sigma^2.$$

20     It is easy to see that  $V(X_1 x_2^*)$  becomes bigger than  $V(Y)$  whenever the  
21     modulus of  $x_2^*$  is bigger than  $\sigma$ .

23     Further, from the relation

$$24 \quad V(Y | X_2 = x_2^*) = (x_2^*)^2 \sigma^2$$

26     one gets

$$28 \quad E(V(Y | X_2)) = \sigma^4 = V(Y).$$

30     Given that

$$32 \quad E(V(Y | X_2)) + V(E(Y | X_2)) = V(Y)$$

33     it must be that  
34

$$35 \quad V(E(Y | X_2)) = 0,$$

37     i.e. the first-order sensitivity index is null for both  $X_1$  and  $X_2$ . These  
38     results are illustrated in the two figures which follow.

39     Figure 1.13 shows a plot of  $V_{X_{-2}}(Y | X_2 = x_2^*)$ , i.e.  $V_{X_1}(Y | X_2 = x_2^*)$  at  
40     different values of  $x_2^*$  for  $\sigma = 1$ . The horizontal line is the unconditional  
41     variance of  $Y$ . The ordinate is zero for  $x_2^* = 0$ , and becomes higher than  
42      $V(Y)$  for  $x_2^* \sim 1$ .

43     Figure 1.14 shows a scatterplot of  $Y$  versus  $x_1^*$  (the same shape would  
44     appear for  $x_2^*$ ). It is clear from the plot that whatever the value of

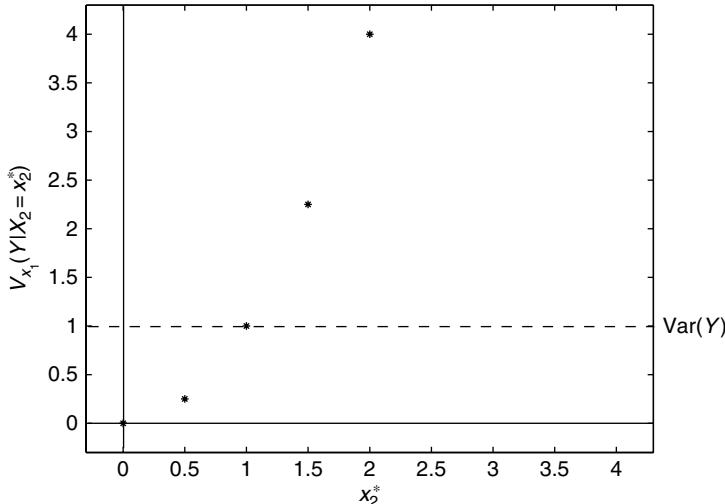


Figure 1.13  $V_{X_1}(Y | X_2 = x_2^*)$  at different values of  $x_2^*$

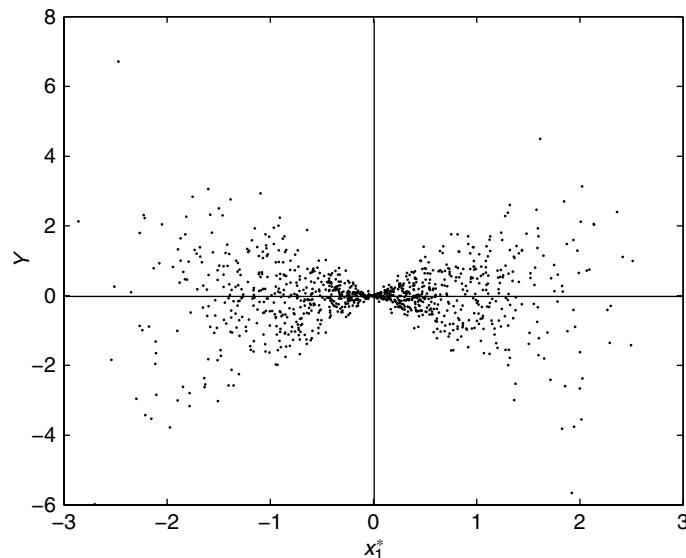


Figure 1.14 Scatterplot of  $Y$  versus  $x_1^*$

the abscissa, the average of the points on the ordinate is zero, i.e.  $E_{X_1}(Y | X_1) = E_{X_2}(Y | X_1) = 0$ . It is also clear from Figure 1.14 that even  $V_{X_1}(E_{X_2}(Y | X_1))$  will be zero, such that both  $S_1$  and  $S_2$  are zero for this model and all variance is captured by the second-order term, i.e.  $S_{12} = 1$ .

- 01        8. Referring to the previous exercise it is clear that if both  $Z_i$  and  
 02         $\Omega_i$  are centred in zero, all first-order terms will be zero and the  
 03        model will be purely interactive. In this case the only nonzero  
 04        terms are the four interactions (second order) relative to the couples  
 05         $(Z_1, \Omega_1), \dots (Z_4, \Omega_4)$ .

06  
 07        **1.8 ADDITIONAL EXERCISES**

- 08        1. Given the function

09  
 10        
$$f(x) = \sin(X_1 \sin(X_2 \sin(X_3)))$$

11  
 12        with  $X_1, X_2, X_3$  distributed normally with mean zero, can you guess  
 13        what the first-order indices will be?

- 14        2. Consider the model  $\Omega_1 Z_1 + \Omega_2 Z_2$  with  $\Omega_1, \Omega_2$  as fixed constants and

15  
 16        
$$Z_i \sim N(\mu_{Z_i}, \sigma_{Z_i}), \quad i = 1, 2$$

17  
 18        with

19  
 20        
$$\mu_{Z_i} \neq 0, \quad i = 1, 2$$

21        and compute the variance-based sensitivity indices  $S_1, S_2$ .

- 22        3. Consider the model  $Y = X_1 \cdot X_2$ , where the two factors are normally  
 23        distributed as

24  
 25        
$$X_i \sim N(\mu_i, \sigma_i), \quad i = 1, 2$$

26  
 27        with

28  
 29        
$$\mu_i \neq 0, \quad i = 1, 2$$

30        and compute the variance-based sensitivity indices  $S_1, S_2$ , and  $S_{12}$ .

- 31        4. Given a set of standardized variables  $X_1, X_2, \dots, X_k$  (all variables have  
 32        thus zero mean and unit standard deviation), and a linear polynomial  
 33        of the form  $f(X_1, X_2, \dots, X_k) = a_0 + \sum_{i=1}^k a_i X_i$ , where  $a_0, a_1, \dots, a_k$  are  
 34        constants, write the formula for the first-order indices  $S_i$ .
- 35        5. Repeat the previous exercise, for the case where both the  $a_0, a_1, \dots, a_k$   
 36        and the  $X_1, X_2, \dots, X_k$  are normally distributed:

37  
 38        
$$X_i \sim N(\mu_{X_i}, \sigma_{X_i})$$

39  
 40        and

41  
 42        
$$a_i \sim N(\mu_{a_i}, \sigma_{a_i}).$$

01      **1.9 SOLUTIONS TO ADDITIONAL EXERCISES**

- 02      1. The first-order indices will be zero.  
 03      2. The solution is

04      
$$S_{Z_i} = \frac{\Omega_i^2 \sigma_{Z_i}^2}{V(Y)}$$

05      as for the case with

06      
$$\mu_{Z_i} = 0, \quad i = 1, 2$$

- 07      3. The solution is

08      
$$S_1 = \frac{\mu_2^2 \sigma_1^2}{(\mu_1^2 \sigma_2^2 + \mu_2^2 \sigma_1^2 + \sigma_1^2 \sigma_2^2)}$$

09      and analogous formula for  $S_2$ , while

10      
$$S_{12} = \frac{\sigma_1^2 \sigma_2^2}{(\mu_1^2 \sigma_2^2 + \mu_2^2 \sigma_1^2 + \sigma_1^2 \sigma_2^2)}.$$

- 11      4. It is simply

12      
$$S_i = \frac{a_i^2}{\sum_{i=1}^k a_i^2},$$

13      i.e. each sensitivity index is proportional to the square of its coefficient.

- 14      5. The problem is additive in  $a_0$  and in the  $k$  sets  $\{a_i, X_i\}$ . Using this and  
 15      the results from Exercise 3 it is easy to derive the solution.

16      
$$S_{a_i} = \frac{\mu_{X_i}^2 \sigma_{a_i}^2}{V}$$

17      
$$S_{X_i} = \frac{\mu_{a_i}^2 \sigma_{X_i}^2}{V}$$

18      
$$S_{a_i X_i} = \frac{\sigma_{a_i}^2 \sigma_{X_i}^2}{V}$$

19      
$$V = \sum_{i=1}^k (\mu_{a_i}^2 \sigma_{X_i}^2 + \mu_{X_i}^2 \sigma_{a_i}^2 + \sigma_{a_i}^2 \sigma_{X_i}^2).$$

20      By putting  $a_0 = 0$  the above solution can be used to compute the sensitivity indices for model (1.3, 1.27).

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## 2

# Experimental Designs

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WHEN HAVE RESEARCHERS DONE SIMILAR EXPERIMENTAL STUDIES IN THE PAST?  
HOW DOES SENSITIVITY ANALYSIS DIFFER FROM PREVIOUS STUDIES?

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### 2.1 INTRODUCTION

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In 1948, the National Heart Institute enlisted the help of over 5000 residents of the town of Framingham, Massachusetts. Researchers interviewed the volunteers and examined them physically, recording numerous details about their health and lifestyles; they subsequently revisited Framingham every two years for follow-up examinations. The purpose of the study was to investigate the incidence of heart disease and to determine the circumstances that gave rise to it. The pioneering Framingham Heart Study (NIH, 2002) revealed connections between lifestyle choices (smoking, physical activity), medical conditions (e.g. high blood pressure) and the contraction of heart disease.

The scale of the Framingham study doubled in 1971 when a new generation of descendants was incorporated into the investigation, and other health studies have used even larger groups of people. For instance, the Harvard Nurses Health Study (Hankinson, 2001) tracks over 100 000 women in an investigation of the effects of diet on the development of chronic diseases. Such large studies can screen many factors and many combinations of factors. They can also discriminate among factors (e.g. which is more effective in avoiding heart attacks: losing weight or taking up physical activity?).

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

01     However, even very large general studies are not appropriate to obtain  
02     certain kinds of information, such as the best treatment of very rare diseases or  
03     the effectiveness of experimental as opposed to standard treatments. In consider-  
04     ing rare diseases, a large study may not contain enough people suffering from  
05     the disease to get good statistical results. In determining the effectiveness of  
06     new treatments there are more powerful techniques available, such as pairing  
07     individuals with similar conditions and lifestyles. In a double-blind experi-  
08     ment, researchers give one of the pair the standard treatment, and the other the  
09     experimental treatment, without anyone knowing who has received which.  
10     A study of this kind may require only a few dozen individuals to determine  
11     whether the new treatment is promising enough to merit further study.

12     In carrying out sensitivity analysis of simulation models researchers are  
13     faced with similar choices. A large randomized study can answer most  
14     sensitivity analysis questions, but at a large cost in terms of computer execu-  
15     tion time and data management. In contrast, careful use of experimental  
16     designs can often answer more specific questions, with an investment of  
17     fewer resources.

18     In recent years, companies with large databases of customers and sales  
19     have often benefited from investigating possible connections among the  
20     fields of the database. A new discipline called *data mining* has emerged to  
21     organize research in this area. Data mining techniques can be applied to a  
22     simulation data set generated in a randomized fashion.

23     By contrast, sensitivity analysis tends to focus more on the application  
24     of a suitable experimental design to extract specific types of data. The  
25     strength of sensitivity analysis techniques is that they can be tuned to elicit  
26     information not readily available to data mining techniques.

27     Sensitivity analysis uses and extends experimental techniques originally  
28     developed for scientific research. By the early twentieth century, experi-  
29     mental research had become quantitative and comparative, teasing out  
30     experimental results from raw data using powerful statistical techniques. It  
31     was at this time that statisticians like Fisher and 'Student' (William Sealey  
32     Gosset) developed the theory of distributions like Student's-*t* and the chi-  
33     square distribution, useful in statistical testing.

34     In the design of experiments, a researcher has several variables that can  
35     be controlled (e.g. temperature, velocity, concentration, duration). There  
36     may be other variables that cannot be controlled but which can affect the  
37     results of an experiment (such as air pressure and humidity, genetic effects,  
38     unknown material defects). The goal is to determine how and how much  
39     each variable affects one or more measurements.

40     The set-up of simulation results for sensitivity analysis can be quite similar  
41     to the set-up for physical experimentation, so the results of the last century  
42     of experimental design are applicable. But there are also some differences  
43     that lead us into experimental regimes that would not be feasible for physical  
44     experimentation.

01      Experimental simulations allow us, for example, to explore the behaviour  
02      of complex systems. There may be many more variables involved than a  
03      physical experimenter would be able to handle, especially when exploring  
04      law-driven models. (For example, researchers could use simulations to inves-  
05      tigate possible environmental effects of toxic materials.) Complex systems  
06      can have physical, chemical, biological and environmental components, all  
07      acting in concert and influencing one another.

08      To understand the effect of parameters in complex systems, we must first  
09      examine their effects in simple systems.

## 13      2.2 DEPENDENCY ON A SINGLE PARAMETER

14  
15      **HOW DO WE CHARACTERIZE A SINGLE PARAMETER? WHAT STANDARDS SHOULD**  
16      **WE FOLLOW IN DESIGNATING ITS PROBABILITY DISTRIBUTION? HOW DO WE**  
17      **SAMPLE VALUES FOR PARAMETERS WITH DIFFERENT DISTRIBUTIONS? WHAT**  
18      **Possible EFFECTS COULD A SINGLE PARAMETER HAVE?**

19  
20      If an output variable depends on only a single parameter, one might  
21      think that a sensitivity analysis would be straightforward. It is true that  
22      identifying the influential parameter is a minor matter. In the notation of  
23      Chapter 1, there is only one sensitivity coefficient  $S_1 = 1$ , indicating that  
24       $X_1$  accounts for all the variance in the output. Nevertheless, characterizing  
25      the influence can still be a challenge. Some simple strategies for dealing  
26      with the single-parameter case can be generalized to sensitivity analysis of  
27      larger numbers of parameters. Conversely, sensitivity analysis of a complex  
28      model may degenerate to a study of the single dominant parameter. A  
29      multivariate approach should be able to generate useful information even  
30      in this constricted case.

31      Without loss of generality, call the single parameter  $X_1$ . In later sections  
32      we will expand the discussion to cover a set of  $k$  parameters  $\{X_r\}_{r=1,k}$  that  
33      can affect an output simultaneously.

34      Assume that  $X_1$  has a finite domain, from 0 to 1. This is one way  
35      of characterizing the domain of  $X_1$ , of several that have been used in  
36      the past. For instance, in cases where two-level designs are employed, it  
37      is traditional to designate the domain of a parameter to be  $[-1, 1]$ , and  
38      this convention will be followed in Section 2.4. The two discrete levels  
39      used in this type of design are designated  $\pm 1$ . If the design also uses a  
40      midpoint for  $X_1$ , 0 represents the midpoint. In other designs with  $s > 2$   
41      discrete levels, it is customary to designate the levels as  $0, 1, \dots, s - 1$ , and  
42      this approach will also be used in discussing Latin hypercube sampling.  
43      Eventually, however, samples for  $X_1$  will be transformed to the standard  
44      continuous domain  $[0, 1]$ .

If we begin the analysis with a variable that has a finite domain other than [0, 1], or even an infinite domain, we can normalize it by a transformation, so that the normalized value lies in this interval. The transformation can also remove a physical unit, like metres or degrees, converting the parameter to a standard form.

For instance, let parameter  $Z_1$  be a continuous random variable, with a probability density function (pdf)  $f_{Z_1}(z)$ , and a cumulative distribution function (cdf)  $F_{Z_1}(z) = \int_{-\infty}^z f_{Z_1}(z')dz'$ . Let  $X_1$  be a transformed variable based on  $Z_1$  according to the following equation:

$$X_1 = F_{Z_1}(Z_1). \quad (2.1)$$

Then the domain of  $X_1$  is the interval [0, 1], by the definition of cdf. While  $Z_1$  has an arbitrary domain and physical unit,  $X_1$  is restricted to [0, 1], and as a cumulative probability, is unitless. Moreover, we can assume that  $X_1$  is uniformly distributed across the interval, rather than concentrated in one part of the interval. This again follows from the transformation in Equation (2.1). Whatever distribution  $Z_1$  has, when  $X_1$  is defined as the value of  $Z_1$ 's cdf,  $X_1$  automatically acquires a uniform distribution from 0 to 1, since

$$F_{X_1}(x) = \Pr\{F_{Z_1}(Z_1) \leq x\} = x \quad (2.2)$$

in this interval.

Given a normalized parameter value  $X_1$  between 0 and 1, an analyst can determine the associated value for  $Z_1$  through the inverse transformation

$$Z_1 = F_{Z_1}^{-1}(X_1). \quad (2.3)$$

If  $X_1$  is uniformly distributed over [0, 1], then  $Z_1$  will follow the distribution specified by  $F_{Z_1}(z)$ . For many standard distributions, the mapping between  $Z_1$  and  $X_1$  can be inverted in this way without ambiguity. Therefore, since we can use normalized variables in an analysis if necessary, we will simply assume that our single parameter  $X_1$  is uniformly distributed in the unitless interval [0, 1].

To analyse the effect of this single, uniformly distributed parameter  $X_1$ , an analyst chooses an experimental design that will extract the maximum information about the influence of  $X_1$  on a simulation outcome  $Y$ . Standard strategies assume the model is a black box, and that the only way of extracting information is through simulations. If other sources of information are available (e.g. the slope of the response curve, found by taking derivatives), then they may be used to modify the strategy.

What possible types of influence could  $X_1$  have on  $Y$ ? Consider Figure 2.1. It shows a few of the infinite possibilities. In each panel of the figure,  $Y$  is plotted as a function of  $X_1$ . Figure 2.1(a) shows the influence of a

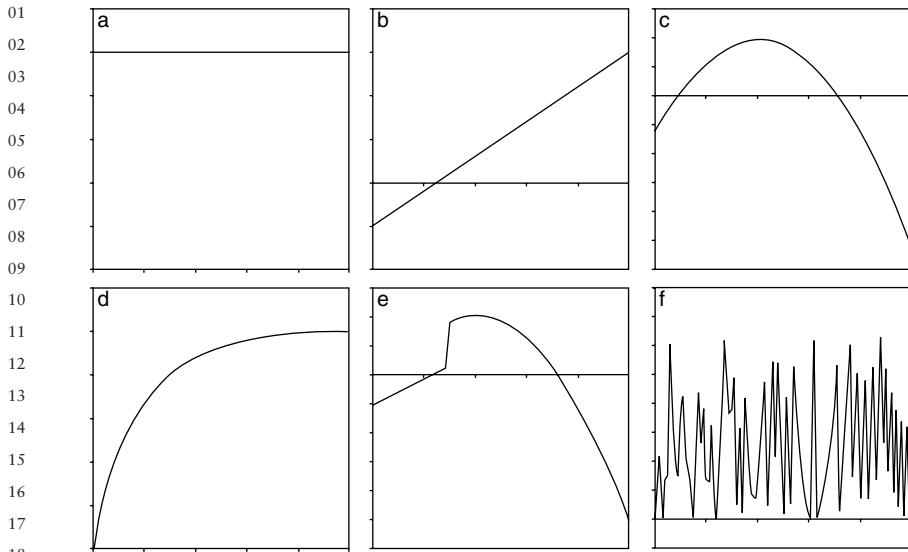


Figure 2.1 Examples of single-variable functions

parameter that has no effect at all on  $Y$ . In large models, there may be many parameters like this. They appear in a model for completeness, and they may affect some other output, but not the output of interest. Alternatively, the parameter's distribution may be so narrow that its possible variation, if any, has little effect on the output of interest. The variable  $X_1$  could even be the transformed representation of a constant parameter  $Z_1$ , so that all values of  $X_1$  between 0 and 1 correspond to a single fixed value of  $Z_1$ .

Figures 2.1(b)–(d) show common forms of smooth dependencies. Figures 2.1(b) and (c) are respectively linear and quadratic polynomials. The former is completely determined by two points, and its extreme values occur at the endpoints of the interval. The quadratic polynomial is completely determined by three points. Extreme values of a nonlinear curve may occur as a local extremum within the interval, like the maximum in Figure 2.1(c), or at an endpoint, like the minimum value in the same figure. Note that in Figure 2.1(c), the initial slope of the curve is opposite in sign to the average slope one would deduce from the two endpoints alone. In contrast to these two polynomials, Figure 2.1(d) shows an asymptotic curve that cannot easily be represented by a low-order polynomial. It has endpoint extrema, and most of the variation occurs over the left half of its domain.

Figure 2.1(e) and (f) show discontinuous functional forms. Figure 2.1(f) is highly variable, and could represent a signal affected by a large amount of noise. In that case it would be worth repeating some of the simulations

with identical parameter values, to determine if the results vary from one simulation to another because of stochastic components of the model, implemented with a pseudo-random number generator. If the variations are repeatable, arising from small changes in  $X_1$ , the sensitivity analyst will face a significant challenge in characterizing the nature of this dependence.

Any of these functional forms can be easily implemented in a computer model. Some features of a function, such as the discontinuity in Figure 2.1(e) or the oscillations in 2.1(f), could be caused either by design or by accident, possibly as a result of a software defect. One of the main roles of sensitivity analysis is to ‘stress’ a model, by subjecting it to unusual parameter values or combinations of values. The benefit of stressing the code is to determine whether it can handle such inputs without failing, and to see if the results produced remain plausible and realistic.

In the analysis to follow, we shall assume that the analyst will be simulating quantities that behave like most physical quantities, and therefore that the function  $Y = Y(X_1)$  is mostly continuous and may have at most a small, finite number of jump discontinuities.

### 2.3 SENSITIVITY ANALYSIS OF A SINGLE PARAMETER

HOW DO WE PERFORM SENSITIVITY ANALYSIS ON A SINGLE PARAMETER? HOW SHOULD PARAMETER VALUES BE SELECTED? WHAT IS STRATIFIED SAMPLING? HOW DO DIFFERENT SAMPLING METHODS AFFECT THE ESTIMATION OF OUTPUT MEAN AND VARIANCE?

How much information a sensitivity analysis will reveal about a parameter’s influence depends on the number of sample points that are simulated and where they are located.

#### 2.3.1 Random Values

If the data come from a random source (e.g. random samples from a database or a pseudo-random number generator), they will be scattered in an uncontrolled manner across the domain of  $X_1$ . Suppose the data points are  $\{(x_{i1}, y_i)\}_{i=1,N}$ , where  $N$  is the number of points in the sample. There is a problem with such data, which can readily be corrected by experimental design. In particular, the values for  $X_1$  are not evenly distributed across the interval  $[0, 1]$ . The density of points in one part of the interval can differ from that in another. In fact, if examined closely, the values for  $X_1$  exhibit *clusters* and *gaps*. Clusters occur when several values are quite close together. Gaps are regions without any points at all.

As  $N$  grows large the density evens out and larger gaps will be filled in, while smaller gaps remain. For this reason, random samples for  $X_1$  give rise to unbiased estimates of the mean and variance of  $Y$ :

$$\bar{Y} = \frac{1}{N} \sum_{i=1}^N y_i$$

$$\hat{V}_Y = \frac{1}{N-1} \sum_{i=1}^N (y_i - \bar{Y})^2. \quad (2.4)$$

However, a mean and variance estimated this way are uncertain. For instance, the uncertainty in the mean estimate  $\bar{Y}$  can be characterized by its standard error  $s_{\bar{Y}}$ :

$$s_{\bar{Y}} = \sqrt{\frac{1}{N^2} \sum_{i=1}^N \text{Var}\{y_i\}} \cong \sqrt{\frac{\hat{V}_Y}{N}}. \quad (2.5)$$

Because the standard error depends on the square root of  $N$ , the uncertainty shrinks slowly as  $N$  increases.

### 2.3.2 Stratified Sampling

Most designs use some sort of stratified sampling to improve the rate at which estimated quantities converge to the true quantities. In stratified sampling, the domain of  $X_1$  is divided into subintervals (often of equal length), and the sampling is constrained so that each subinterval contains the same number of sample points. The points themselves may be selected systematically to lie at particular locations within these subintervals, or they may be sampled randomly within each subinterval.

Figure 2.2 shows several number lines illustrating different ways of distributing 16 points across the interval from 0 to 1. The dashed vertical

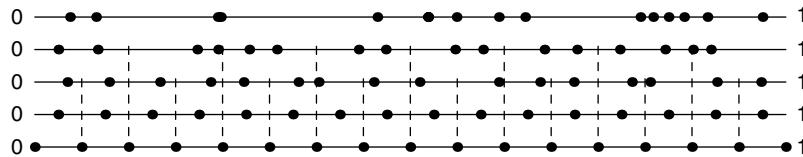


Figure 2.2 Different ways of distributing points from 0 to 1

lines show subinterval boundaries when the interval is subdivided. The distributions of points in the figure have the following properties:

- Top line: independently and identically distributed random points, with visible gaps and clusters. Some of the points overlap in the figure. This type of sample is easy to generate with a pseudo-random generator. By Equation (2.4), it yields unbiased estimates of the mean and variance of  $Y$ .
- Second line: a stratified sample, with eight subintervals, and two points randomly selected within each subinterval. Equation (2.4) can be applied to each subinterval to yield unbiased mean and variance estimates. These can be combined under the assumption that each subinterval has equal probability, yielding unbiased mean and variance estimates for  $Y$  covering the entire interval. It is also possible to compare variance *among* subintervals against variance *within* subintervals to determine if parameter  $X_1$  has a significant influence.
- Middle line: a stratified sample, with 16 subintervals, and one point randomly selected within each subinterval. Equation (2.4) can be applied to each subinterval to yield unbiased mean estimates. The variance among intervals can be estimated, but not the variance within intervals, as there is only one point per subinterval. (However, each pair of adjacent intervals can be combined to reduce the situation to the previous case.)
- Fourth line: a stratified sample, with 16 intervals, and one point at each interval's midpoint. Using a trapezoidal approximation (i.e. fitting a bar graph to the data), a good estimate of the area under the curve  $Y = Y(X_1)$  in each subinterval can be computed. From this area, a mean estimate can be produced, but it will be biased<sup>1</sup> by the selection of subinterval midpoints. A variance estimate among subintervals can be made, but it is also biased.
- Bottom line: a stratified sample, with 16 subintervals, and a point at the ends of each subinterval, for a total of 17 points instead of 16. By joining adjacent  $(x_{i1}, y)$  points with a straight line, an analyst can compute a good estimate of the area under the curve  $Y = Y(X_1)$  in each subinterval, yielding a (biased) mean estimate. By using a straight line approximation to the curve in each interval, (biased) variance estimates among and within subintervals can be obtained.

There are of course many other ways of generating points for a single parameter, and of computing mean and variance estimates, but this selection

---

<sup>1</sup> A *biased* estimator has an expected value that is potentially different from the true value. Redoing the analysis many times does not help to find the true value.

01 provides a good starting point. The following paragraphs describe how the  
02 computations can be done.

03

### 04 2.3.3 Mean and Variance Estimates for Stratified Sampling

05

06 Suppose the  $N$  points  $\{(x_{i1}, y_i)\}_{i=1,N}$  come from  $m \leq N$  subintervals of equal  
07 length, where  $m$  divides into  $N$ . Assume  $X_1$  is uniformly distributed, so  
08 that these subintervals have equal probability. Assume further that there  
09 may be another source of variation beside  $X_1$  affecting the output  $Y$ . For  
10 example, the model may include stochastic behaviour, or other parameters  
11 may change value from run to run in an unspecified manner.

12 By applying Equation (2.4) to each subinterval separately, we can devise  
13  $m$  mean and variance estimates  $\bar{Y}_j$  and  $\hat{V}_{Y_j}$

$$16 \quad \bar{Y}_j = \frac{1}{N/m} \sum_i y_i \quad \hat{V}_{Y_j} = \frac{1}{(N/m)-1} \sum_i (y_i - \bar{Y}_j)^2 \quad (2.6)$$

17 where in each summation,  $i$  varies over points belonging to subinterval  $j$ .

18 The variance estimate in Equation (2.6) applies only when  $m < N$ .  
19 When these quantities are equal,  $N/m$  equals one point per subinterval,  
20 and the variance calculation is invalid as it would involve division by  
21 zero.

22 The global mean and variance when  $N/m$  parameter values are randomly  
23 sampled from each subinterval are calculated as shown in the following  
24 equations. Note that the mean estimator is still the overall sample mean.

$$27 \quad \bar{\bar{Y}} = \frac{1}{m} \sum_{j=1}^m \bar{Y}_j = \frac{1}{N} \sum_{i=1}^N y_i \quad (2.7)$$

$$31 \quad \tilde{V}_Y^a = \frac{N/m}{m-1} \sum_{j=1}^m (\bar{Y}_j - \bar{\bar{Y}})^2 \quad (2.8)$$

$$34 \quad \tilde{V}_Y^w = \frac{1}{m} \sum_{j=1}^m \tilde{V}_{Y_j}. \quad (2.9)$$

35 The two variance estimates have superscripts  $a$  and  $w$ , indicating that they  
36 are based on the variances *among* and *within* subintervals respectively. If  
37  $Y$  does not depend on  $X_1$ , these quantities are independent estimates of the  
38 variance of  $Y$ . If  $Y$  does depend on  $X_1$ , the ratio of one to the other is a  
39 measure of the degree of influence of  $X_1$ .

40 These equations apply when the points in an interval are randomly  
41 selected. Suppose instead that there is one deterministic value in the centre  
42 of the  $j$ th subinterval, at  $x_{j1} = (2j-1)/2N$ , for  $j$  from 1 to  $N$ , as in the

fourth line of Figure 2.2. Then estimates of the mean and variance must be based on some model of variation within the interval. The simplest assumption is that in the  $j$ th interval the function  $Y(X_1)$  is linear, with an unknown slope  $a_j$ :

$$y = y_j + a_j(x - x_{j1}). \quad (2.10)$$

Because the sample point is in the middle of the subinterval, contributions from the left and right sides of the subinterval cancel each other out, and the average value of  $y$  in the  $j$ th interval for a linear fit is

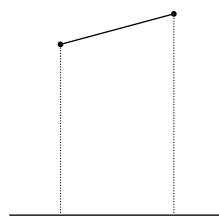
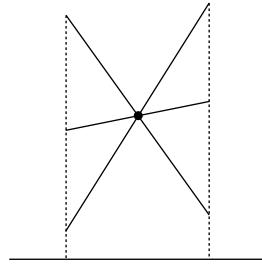
$$\begin{aligned} \bar{Y}_j &= \frac{1}{1/N} \int_{x_{j-1,1}}^{x_{j1}} (y_j + a_j(x - x_{j1})) dx \\ &= y_j \end{aligned} \quad (2.11)$$

irrespective of the value of  $a_j$ .

The diagram on the right shows several different trapezoids with different slopes, all passing through the same point in the middle of an interval. The area of each trapezoid (i.e. the width by the average height) is the same. The average value in Equation (2.11), which corresponds to the average height of each trapezoid, is the same. However, each of these trapezoids would have a different variance of heights in the interval, so it is not feasible to estimate  $\hat{V}_{Y_j}^w$ . Equations (2.7) and (2.8) still apply.

If we use endpoint values for each interval (as in the bottom line of Figure 2.2), the simplest model of the function  $Y = Y(X_1)$  is the line that interpolates the two endpoints, as shown on the right. One extra point  $(x_{01}, y_0)$  is required for  $X_1$  at the left end of the first subinterval.

This is not a bad approximation, as shown in Figure 2.3, where the nonpolynomial functions from Figure 2.1 have been interpolated at 11 evenly spaced points, and joined by straight lines. A sequence of connected straight lines like this is called a *piecewise linear* fit. In the last frame of Figure 2.3, it is clear that many more interpolation points would be required to fit this jagged function, but in the other two panels curves and discontinuities have been handled fairly well.



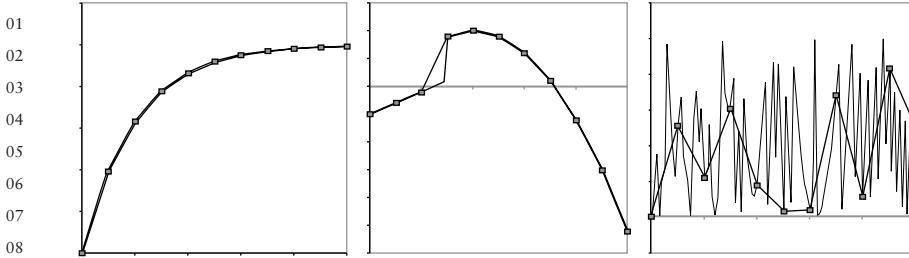


Figure 2.3 Piecewise linear fits to nonpolynomial functions

In this case the linear interpolating function in the  $j$ th subinterval for parameter  $X_1$  is

$$y = y_j + \frac{(x - x_{j1})}{(x_{j-1,1} - x_{j1})}(y_{j-1} - y_j) \quad (2.12)$$

for  $j$  from 1 to  $k$ . The average value is

$$\begin{aligned} \bar{Y}_j &= \frac{1}{1/N} \int_{x_{j-1,1}}^{x_{j1}} \left( y_j + \frac{(x - x_{j1})}{(x_{j-1,1} - x_{j1})}(y_{j-1} - y_j) \right) dx \\ &= \frac{1}{2}(y_{j-1} + y_j) \end{aligned} \quad (2.13)$$

and the estimated variance of  $Y$  in the  $j$ th interval is

$$\begin{aligned} \hat{V}_{Y_j} &= \frac{1}{1/N} \int_{x_{j-1,1}}^{x_{j1}} \left( y_j + \frac{(x - x_{j1})}{(x_{j-1,1} - x_{j1})}(y_{j-1} - y_j) - \bar{Y}_j \right)^2 dx \\ &= \frac{1}{12}(y_j - y_{j-1})^2 \end{aligned} \quad (2.14)$$

which is the variance of a uniform variate between  $y_{j-1}$  and  $y_j$ .

With these definitions the variance equations (2.8) and (2.9) apply. The overall estimate of the mean is slightly different in that the endpoints are given half as much weight as the other points.

$$\bar{Y} = \frac{1}{N} \sum_{j=1}^N \bar{Y}_j = \frac{1}{2N} (y_0 + 2y_1 + 2y_2 + \dots + 2y_{N-1} + y_N). \quad (2.15)$$

One disadvantage of using endpoints is that the extreme values  $X_1 = 0$  and  $X_1 = 1$  can cause problems. Suppose  $X_1$  is a transformed version of a normal (Gaussian) variate  $Z_1$ , as defined by Equation (2.1). Then points

01      $X_1 = 0$  and  $X_1 = 1$  correspond to  $-\infty$  and  $\infty$  for  $Z_1$  respectively. Even if  
 02     infinities are avoided by truncating the distribution,<sup>2</sup> the actual value of  $Y$   
 03     at such extreme values is likely to be determined by the truncation points,  
 04     and by our limited knowledge of the tail behaviour of the distribution.  
 05     There could be significant uncertainty attached to these values, and yet they  
 06     could affect both mean and variance estimates significantly. If endpoints are  
 07     used, distributions should be truncated judiciously and consistently before  
 08     performing sensitivity analysis.

09  
 10     **2.4 SENSITIVITY ANALYSIS OF MULTIPLE  
 11       PARAMETERS**

12  
 13     **HOW DO WE SAMPLE MANY PARAMETERS SO AS TO OBTAIN INFORMATION ABOUT  
 14       THE EFFECT OF EACH, OR AT LEAST OF THE MOST INFLUENTIAL? WHAT TYPES  
 15       OF ANALYSIS SHOULD A SAMPLING SCHEME SUPPORT? HOW MANY INFLUENTIAL  
 16       PARAMETERS DO WE EXPECT TO FIND? WHAT ARE ONE-AT-A-TIME DESIGNS AND  
 17       FRACTIONAL FACTORIAL DESIGNS? WHAT IS QUASI-RANDOM SAMPLING?**

18  
 19     Suppose the analyst has the capability to manipulate a set of  $k$  parameters,  
 20      $\{X_r\}_{r=1,k}$ . This is the situation discussed in general terms in Chapter 1. Each  
 21     parameter has properties like those described in the last section for  $X_1$ .  
 22     Specifically, the domain of  $X_r$  is the unitless interval from 0 to 1. Each  
 23      $X_r$  is uniformly distributed across this domain, possibly because it is the  
 24     transformed version of some variate  $Z_r$ .

25  
 26     For now, assume that the parameters are all statistically independent.  
 27     That is, knowing specific values for some subset of the parameters says  
 28     nothing about the distribution of the remaining parameters. That would *not*  
 29     typically be the case if there were a constraint linking the parameters. As  
 30     an example of a constraint, suppose that we know  $\sum_{r=1}^k X_r = k/2$  exactly.  
 31     The expected value of the sum of  $k$  independent parameters is  $k/2$ , so  
 32     this constraint is consistent with what we know about each parameter.  
 33     Should the situation arise where we have specified low values for half  
 34     the parameters, however, this constraint would limit our freedom to select  
 35     the rest. There are ways of dealing with such a situation, but sensitivity  
 36     analysis is much simpler if we avoid it in the first place. In this case, we

37  
 38  
 39     <sup>2</sup> Truncating the distribution means limiting the lower and upper values of  $Z_1$  to some finite  
 40     values, such as  $\pm 3$  standard deviations from the mean. There would be only about a quarter  
 41     of 1% chance of sampling values further out than that for a normal variate. The modified  
 42     cdf for  $Z_1$  after truncation would be  $F'_{Z_1}(z) = \int_{\mu-3\sigma}^z f_{Z_1}(z')dz' / \int_{\mu-3\sigma}^{\mu+3\sigma} f_{Z_1}(z')dz'$ , which means  
 43     that sampled points from the truncated distribution using Equation (2.3) would all be slightly  
 44     different from those sampled from the original distribution.

01 could change one of the parameters from a parameter to a derived quantity  
 02  $X_n = k/2 - \sum_{r \neq n} X_r$  to relieve pressure on the sampling.<sup>3</sup>

03 In the following discussion, we will assume that any combination of  
 04 parameter values  $\{x_r\}_{r=1,k}$  is equally likely. The  $k$  sampled parameter values  
 05 define a point in  $k$ -dimensional space, and sample points are uniformly  
 06 distributed throughout a  $k$ -dimensional hypercube of side 1.

#### 07 08 09 2.4.1 Linear Models

10 As in the analysis of a single parameter, the choice of experimental design  
 11 depends on how the experimenter expects the parameters to affect the model  
 12 output. As a first approximation, the dependency can be viewed as linear in  
 13 each parameter. That is, if  $Y$  is the output, and the inputs are the  $k$  variables  
 14  $X_1$  to  $X_k$ , the entire model being simulated would behave approximately  
 15 like so:

$$17 \quad Y = b_0 + \sum_{r=1}^k b_r X_r \\ 18 \quad = b_0 + b_1 X_1 + b_2 X_2 + \cdots + b_{k-1} X_{k-1} + b_k X_k \quad (2.16)$$

22 where the  $b_r$ 's are all constants that we assume are unknown at the start of  
 23 sensitivity analysis.

24 When the model is run with a set of parameter values, a data point  
 25 becomes available for sensitivity analysis. Any set of  $N$  simulations, where  
 26  $N \geq k+1$ , can be solved for the  $b_r$ 's, provided that the system of equations  
 27 that is produced is linearly independent (e.g. there can be no repeated simu-  
 28 lations). In general,  $N$  simulations will result in the following  $N \times (k+1)$   
 29 system of linear equations,

$$31 \quad \begin{bmatrix} 1 & x_{11} & \dots & x_{1k} \\ 1 & x_{21} & \dots & x_{2k} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_{N1} & \dots & x_{Nk} \end{bmatrix} \begin{pmatrix} b_0 \\ b_1 \\ \vdots \\ b_k \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{pmatrix} \quad (2.17)$$

36 which we can abbreviate as

$$38 \quad X_{Nk} B_k = Y_N \quad (2.18)$$

40 using matrix notation.

---

43 44 <sup>3</sup> Note that  $X_n$  would not necessarily lie in the interval  $[0, 1]$ .

01     The matrix  $X_{Nk}$  has 1's in the first column, and experimental values  
 02    for the  $k$  parameters in the  $N$  simulations in the remaining columns.  $B_k$   
 03    contains the  $k + 1$  unknown coefficients corresponding to the intercept  
 04     $b_0$  and the  $k$  parameters.  $Y_N$  contains the  $N$  output values from the  $N$   
 05    simulations.

06     If  $N \geq k + 1$ , it is generally possible to solve these equations. If  $N$  is  
 07    strictly greater than  $k + 1$ , it will not be possible to solve the equations  
 08    exactly, unless the model is in fact linear, as the system of equations is  
 09    overdetermined. However, a solution of the least-squares type will generally  
 10    be available. Solving an overdetermined system of equations for a least-  
 11    squares solution is computationally intensive. Numerical problems can also  
 12    arise if the equations are ill-conditioned (e.g. if several points are quite  
 13    close together). Random samples (i.e. a sample where every value in  $X_{Nk}$   
 14    outside the first column is sampled randomly) tend to be poorly conditioned  
 15    for large  $k$  because of clustering. Nevertheless, off-the-shelf software can  
 16    often solve such systems. Even general purpose spreadsheet packages like  
 17    Microsoft's Excel have regression equation solvers that can be used to  
 18    determine good estimates of the  $b_r$  coefficients, provided there are not too  
 19    many of them.

20     With only a small number of parameters, a reasonably good sensitivity  
 21    analysis can sometimes be carried out through a regression analysis alone.  
 22    After performing an initial regression using Equation (2.17) and random  
 23    or systematically sampled parameter values, the analyst can look at the  
 24    residuals (i.e. the discrepancies between the actual values for  $Y$ , and the  
 25    values estimated using the linear model). The residuals may exhibit a pattern  
 26    that suggests additional terms for the regression model, such as quadratic  
 27    terms in one or more of the parameters.<sup>4</sup>

28     If  $N < k + 1$ , or if the system has dependencies that reduce its effective  
 29    size (e.g. if a simulation is repeated two or more times), there will be an  
 30    infinite number of solutions to the equations. However, that does not mean  
 31    that the equations are devoid of useful information, as we shall see later  
 32    when discussing group sampling.

#### 35    2.4.2 One-at-a-time (OAT) Sampling

36  
 37     A sensitivity analyst can avoid or limit numerical problems in solving  
 38    Equation (2.17) by carefully selecting the data points that define  $X_{Nk}$ . One  
 39    way of simplifying  $X_{Nk}$  is to use a 'one-at-a-time' (OAT) design, where only

---

42     <sup>4</sup> In this exposition there is no need to resort to the standardized regression coefficients  
 43    mentioned in Chapter 1, since the assumption that every parameter has the same uniform  
 44    distribution eliminates differences among them that can be clarified by use of SRCs.

01 one parameter changes values between consecutive simulations. Suppose,  
 02 for example, that Equation (2.17) is rewritten as  
 03

$$04 \quad \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & \dots & 0 \\ 05 & 1 & 1 & 0 & 0 & 0 & \dots & 0 \\ 06 & 1 & 1 & 1 & 0 & 0 & \dots & 0 \\ 07 & 1 & 1 & 1 & 1 & 0 & \dots & 0 \\ 08 & 1 & 1 & 1 & 1 & 1 & \dots & 0 \\ 09 & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 10 & 1 & 1 & 1 & 1 & 1 & \dots & 1 \end{bmatrix} \begin{pmatrix} b_0 \\ b_1 \\ \vdots \\ b_k \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_{k+1} \end{pmatrix} \quad (2.19)$$

12 where every variable takes only two values, 0 and 1, and only one variable  
 13 changes its value between each pair of consecutive simulations. This system  
 14 of equations can be simplified by elementary row operations. In every row  
 15 but the first, subtract the entries from the previous row, yielding  
 16

$$17 \quad \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & \dots & 0 \\ 18 & 0 & 1 & 0 & 0 & 0 & \dots & 0 \\ 19 & 0 & 0 & 1 & 0 & 0 & \dots & 0 \\ 20 & 0 & 0 & 0 & 1 & 0 & \dots & 0 \\ 21 & 0 & 0 & 0 & 0 & 1 & \dots & 0 \\ 22 & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 23 & 0 & 0 & 0 & 0 & 0 & \dots & 1 \end{bmatrix} \begin{pmatrix} b_0 \\ b_1 \\ \vdots \\ b_k \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 - y_1 \\ y_3 - y_2 \\ y_4 - y_3 \\ \vdots \\ y_{k+1} - y_k \end{pmatrix}. \quad (2.20)$$

26 This equation demonstrates that if there is any change in value between  $y_i$   
 27 and  $y_{i+1}$ , it can only be attributed to a change in parameter  $X_i$  (complicated  
 28 by random effects if the model is stochastic). The quantity  $\Delta y_i = y_{i+1} - y_i$  is  
 29 an estimate of the effect on  $y$  of changing  $X_i$  from 0 to 1. It is applicable  
 30 everywhere if the linear model is appropriate, and for some region around  
 31 the current sample point otherwise.

32 As another form of analysis, consider that parameter  $X_i$  takes the value  
 33 0 in exactly  $i$  simulations and the value 1 in  $k+1-i$  simulations. Estimates  
 34 of the average values of  $Y$  when parameter  $X_i$  takes the values 0 and 1 are  
 35 given by  
 36

$$37 \quad \hat{y}_{X_i=0} = \frac{1}{i} \sum_{j=1}^i y_j \quad \hat{y}_{X_i=1} = \frac{1}{k+1-i} \sum_{j=i+1}^{k+1} y_j. \quad (2.21)$$

40 Equation (2.21) is clearly unbalanced. For instance, if  $k = 15$  and  $i = 1$ ,  
 41  $\hat{y}_{X_i=0}$  is based on one simulation result, whereas  $\hat{y}_{X_i=1}$  is calculated from 15  
 42 simulation results. A more balanced result can be obtained if the system of  
 43 equations in (2.19) is expanded to the  $2k+1$  equations below, representing  
 44

01 a round trip that returns to the starting point. Note that as the first and  
 02 last equation are the same, only  $2k$  of the equations are independent.  
 03

$$\begin{array}{ccccccccc}
 04 & \left[ \begin{array}{ccccccccc} 1 & 0 & 0 & 0 & 0 & \dots & 0 \\ 05 & 1 & 1 & 0 & 0 & 0 & \dots & 0 \\ 06 & 1 & 1 & 1 & 0 & 0 & \dots & 0 \\ 07 & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 08 & 1 & 1 & 1 & 1 & 1 & \dots & 1 \\ 09 & 1 & 0 & 1 & 1 & 1 & \dots & 1 \\ 10 & 1 & 0 & 0 & 1 & 1 & \dots & 1 \\ 11 & 1 & 0 & 0 & 0 & 1 & \dots & 1 \\ 12 & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 13 & 1 & 0 & 0 & 0 & 0 & \dots & 0 \end{array} \right] & \left( \begin{array}{c} b_0 \\ b_1 \\ \vdots \\ b_k \end{array} \right) & = & \left( \begin{array}{c} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_{k+1} \\ y_{k+2} \\ y_{k+3} \\ y_{k+4} \\ \vdots \\ y_1 \end{array} \right). & (2.22)
 \end{array}$$

16  
 17 Equation (2.23) is analogous to Equation (2.20) for this expanded set of  
 18 equations.  
 19

$$\begin{array}{ccccccccc}
 20 & \left[ \begin{array}{ccccccccc} 1 & 0 & 0 & 0 & 0 & \dots & 0 \\ 21 & 0 & 1 & 0 & 0 & 0 & \dots & 0 \\ 22 & 0 & 0 & 1 & 0 & 0 & \dots & 0 \\ 23 & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 24 & 0 & 0 & 0 & 0 & 0 & \dots & 1 \\ 25 & 0 & -1 & 0 & 0 & 0 & \dots & 0 \\ 26 & 0 & 0 & -1 & 0 & 0 & \dots & 0 \\ 27 & 0 & 0 & 0 & -1 & 0 & \dots & 0 \\ 28 & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 29 & 0 & 0 & 0 & 0 & 0 & \dots & -1 \end{array} \right] & \left( \begin{array}{c} b_0 \\ b_1 \\ \vdots \\ b_k \end{array} \right) & = & \left( \begin{array}{c} y_1 \\ y_2 - y_1 \\ y_3 - y_2 \\ \vdots \\ y_{k+1} - y_k \\ y_{k+2} - y_{k+1} \\ y_{k+3} - y_{k+2} \\ y_{k+4} - y_{k+3} \\ \vdots \\ y_1 - y_{2k} \end{array} \right). & (2.23)
 \end{array}$$

32  
 33 This system of equations can yield two estimates of the effect of changing  
 34 parameter  $X_i$ . First, the quantity  
 35

$$\Delta_i Y = \frac{1}{2}(y_{i+1} - y_i - y_{k+i+1} + y_{k+i}) \quad (2.24)$$

39  
 40 is a revised estimate of the effect on  $Y$  of changing  $X_i$  from 0 to 1. It  
 41 combines the two rows in Equation (2.23) where the only parameter change  
 42 is in  $X_i$ , and it would apply to the entire domain if  $Y$  varied linearly with  $X_i$ .

43 The other estimate,  $(\hat{y}_{X_i=1} - \hat{y}_{X_i=0})$ , is based on Equation (2.21). With  
 44 the  $k-1$  extra data points in Equation (2.22), the number of data points

01 contributing to each of these average quantities is now more balanced, as  
 02 each uses  $k$  data points:

$$04 \quad 05 \quad \hat{y}_{X_i=0} = \frac{1}{k} \left( \sum_{j=1}^i y_j + \sum_{j=k+i+1}^{2k} y_j \right) \quad \hat{y}_{X_i=1} = \frac{1}{k} \sum_{j=i+1}^{i+k} y_j. \quad (2.25)$$

06  
 07 In the OAT experimental design shown here, each parameter  $X_i$  takes  
 08 only two distinct values. These have been shown as the extreme values, 0 and  
 09 1, primarily to simplify the equations. More complicated paths through the  
 10 sample space would involve much smaller changes to the parameter values,  
 11 which would allow the estimation of elementary effects, as mentioned in  
 12 Chapter 1. This approach is described in more detail in Chapter 3.

13 Another simplification is that the parameters have been changed in the  
 14 order  $X_1, X_2, \dots, X_k$ . This choice simplifies Equations (2.17) through to  
 15 (2.25). However, the parameters could be changed in any order with similar  
 16 results, though the analyst would need to know the order to be able to  
 17 compute average values.

18 With the choices described here, each parameter change corresponds to a  
 19 move from one corner of the sample hypercube to an adjacent corner, along  
 20 an edge of the hypercube. If the order of the parameter changes is determined  
 21 randomly, the path defined by the successive parameter changes is a random  
 22 walk along the surface of the sample hypercube. In Equation (2.22), the  
 23 sample point for simulation  $l > k$  is diametrically opposite the point for  
 24 simulation  $l - k$ . (Such points, placed symmetrically with respect to the  
 25 centre of the hypercube, are called *mirror points*.) As a result, the design  
 26 described by Equation (2.22) is a walk along the surface of the sample  
 27 hypercube from a starting corner to the opposite corner, and then back  
 28 again following the mirror points of those used on the outward path. If  
 29 the order of the parameter changes is randomized, the path becomes a  
 30 random walk to the opposite point, followed by a return using mirror  
 31 points.

32 If a function  $Y$  follows a linear model as shown in Equation (2.16), the  
 33 average of two mirror point values is simply the constant  $b_0 + \frac{1}{2} \sum_{r=1}^k b_r$ ,  
 34 which is the value at the centre of the hypercube, where every parameter  
 35 takes the value 0.5. Averages of all the pairs of mirror points in an OAT  
 36 design give a set of values that all approximate to  $b_0 + \frac{1}{2} \sum_{r=1}^k b_r$ . The  
 37 variance of this set is one measure of the nonlinearity of the function.

38 Values other than 0 and 1 could be used in Equations (2.17) and (2.22).  
 39 Typically, an analyst would use values symmetrically placed around 0.5,  
 40 such as 0.2 and 0.8, so that points would be mirror points. The earlier  
 41 section on sampling values for a single parameter suggested an alternative,  
 42 but with only two values, the options are quite limited. A later chapter  
 43 discusses how the number of options can be expanded for this design.

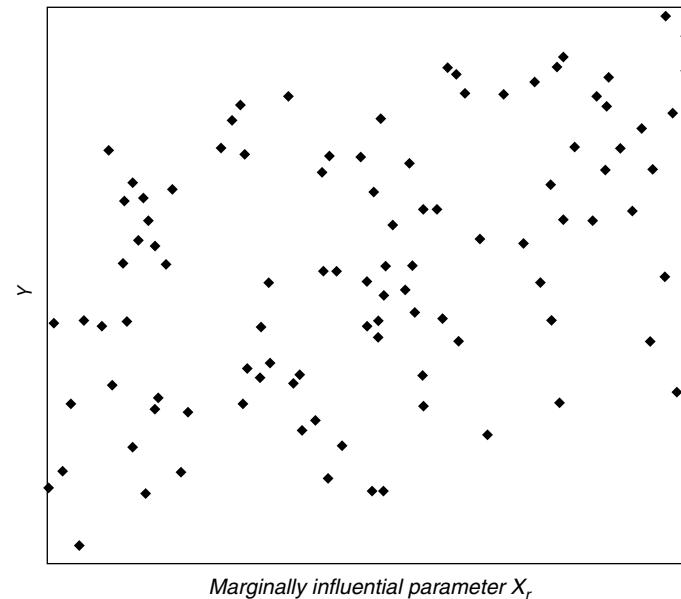
### 01            2.4.3 Limits on the Number of Influential Parameters

02  
 03        OAT sampling is inefficient when the number of parameters  $k$  is large and only  
 04        a few of them are influential. Each simulation changes the value of one param-  
 05        eter. If only a few parameters are influential, most of the simulations would  
 06        be devoted to determining the very small effects of noninfluential parame-  
 07        ters. These simulations would be duplicates as far as the values of influential  
 08        parameters are concerned. Very little new information would be generated.

09        It is not unusual to have only a few influential parameters. In fact,  
 10        even when the number of parameters is large, the number of *influential*  
 11        parameters is *always* small. Why is this the case?

12        The number of influential parameters in a model is akin to the number of  
 13        exceptional individuals in a group. For instance, it is common for a school to  
 14        have a small number of exceptional athletes who can outperform everyone  
 15        else at running events. Yet in some years there may be no exceptional  
 16        performances in a particular running event; all the times may be ordinary.  
 17        Do we then say that every participant is exceptional? No – we reserve that  
 18        term for situations in which one or a few athletes stand out from the rest.

19        Consider the scatterplot in Figure 2.4, showing values of  $Y$  resulting  
 20        from a random selection of sampled parameters. Assume  $Y$  is a linear  
 21        combination of several parameters (as in Equation 2.16), and the parameter



42            **Figure 2.4**  $X_r$  contributes 10% of the variance of  $Y$

01      $X_r$ , against which  $Y$  is plotted explains 10% of the variance of  $Y$ . The figure  
 02     shows some influence of  $X_r$  on  $Y$ , but this parameter would be considered  
 03     only marginally influential.

04     The linear function in Equation (2.16) has a variance that depends on  
 05     the sum of squares of the coefficients  $b_1, b_2, \dots, b_k$ . If the number of  
 06     influential parameters in a linear model comes to be as large as 10, the least  
 07     influential parameter cannot contribute more than 10% of the variance,  
 08     and it can contribute that much only if the influential parameters are all  
 09     equally influential.

10     With a nonlinear function, we can use the facts that first, the sensitivity  
 11     coefficients  $S_{ij\dots l}$  described in Chapter 1 are all nonnegative, and second,  
 12     they sum to 1. These sensitivity coefficients cannot all be influential, as they  
 13     are competing with each other to influence the output variable  $Y$ . Only  
 14     a small number can win that competition. Certainly one could not have  
 15     hundreds of influential parameters.

16     It is possible that there are *no* influential parameters for sensitivity anal-  
 17     ysis to reveal. For instance, consider the model

$$18 \quad 19 \quad 20 \quad 21 \quad Y = \sum_{r=1}^k X_r \quad (2.26)$$

22     in which all the parameters play exactly the same role. Sensitivity analysis  
 23     can reveal that many parameters have similar small effects, but cannot give  
 24     further insight into this model's behaviour. All of the parameters are equally  
 25     *noninfluential*.

26     Usually, however, there are a few parameters that stand out from the  
 27     rest. So with large numbers of parameters, it is desirable to find a more  
 28     efficient approach than changing one parameter at a time.

#### 31     2.4.4 Fractional Factorial Sampling

32     Table 2.1 shows a two-level factorial design for three parameters. These  
 33     34     35     36     37     38     39     40     41     42     43     44     eight simulations contain all possible combinations of low and high values  
 40     for  $X_1, X_2$  and  $X_3$ , where by convention ‘–1’ represents a low value, and  
 41     ‘1’ represents a high value.<sup>5</sup> These eight points occupy the eight corners  
 42     of the cube shown on the right, which represents the sample space for

---

<sup>5</sup> For practical reasons it is traditional to use the bounds –1 and 1 for each parameter  $X_i$  in a factorial design. The values in a column of the design form a *contrast*, a set of coefficients that tell you how to combine simulation results to estimate the influence of a particular parameter. Values from a factorial design can be scaled linearly to the interval [0, 1], used previously in this chapter for parameter values, by the transformation  $X'_i = (X_i + 1)/2$ .

three parameters. In general,  $k$  parameters would require  $2^k$  simulations to generate all combinations for a factorial design, and these combinations would represent the corners of the corresponding  $k$ -dimensional hypercube. One can generate full factorial designs with  $s > 2$  levels for each parameter, to determine behaviour at a grid of locations inside the hypercube. Then the number of simulations would be  $s^k$ , which is a much larger quantity than  $2^k$ . Because of the explosive growth of the quantity  $s^k$ , two levels are typically used for full factorial designs, except when  $k$  is very small.

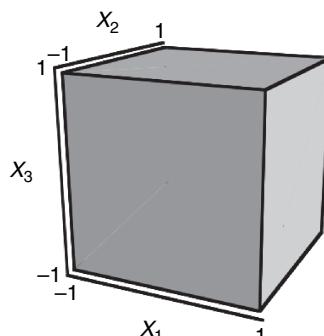
One benefit of using a full factorial design in designing simulations is that the analyst has the data to estimate the mean  $Y$  value for each level of every parameter  $X_r$ , by averaging over simulations where all other parameters take all possible combinations of high and low values. One disadvantage of using a factorial design is the enormous number of simulations required. Using two levels, 10 parameters would require  $2^{10} = 1024$  simulations, and 20 parameters would need more than a million. However, it is possible to select a fraction of these simulations to generate a smaller, feasible design that can still produce useful results.

Consider for example, the design for seven parameters in Table 2.2. The original three columns from Table 2.1 now appear in columns 1, 2 and 4, and the other four columns are obtained from the original three by multiplication as shown in the column headers. Note that exactly half the values in each column are 1, and that half are -1. Observe also that any *two* columns  $i$  and  $j$  of this design have the property that the four combinations  $(1, 1)$ ,  $(1, -1)$ ,  $(-1, 1)$  and  $(-1, -1)$  each occur twice. (For instance, in the first two columns of the table,  $(1, 1)$  occurs in rows 1 and 5, and  $(-1, -1)$  occurs in rows 4 and 8.)

In general, if one starts with a full factorial design on two levels for  $n$  parameters, requiring  $k = 2^n$  simulations, it can be converted into a fractional factorial (FF) design for  $k - 1$  parameters. Tables 2.1 and 2.2

**Table 2.1** A two-level full factorial design for three parameters

$X_1$	$X_2$	$X_3$
1	1	1
-1	1	1
1	-1	1
-1	-1	1
1	1	-1
-1	1	-1
1	-1	-1
-1	-1	-1



01                   **Table 2.2** A two-level fractional factorial design for seven  
 02                   parameters

$X_1$	$X_2$	$X_3 = X_1X_2$	$X_4$	$X_5 = X_1X_4$	$X_6 = X_2X_4$	$X_7 = X_1X_2X_4$
1	1	1	1	1	1	1
-1	1	-1	1	-1	1	-1
1	-1	-1	1	1	-1	-1
-1	-1	1	1	-1	-1	1
1	1	1	-1	-1	-1	-1
-1	1	-1	-1	1	-1	1
1	-1	-1	-1	-1	1	1
-1	-1	1	-1	1	1	-1

14                   started with  $n = 3$  and produced an FF design with  $k = 2^3 = 8$  simulations  
 15                   for  $k - 1 = 7$  parameters. Doing this by means of taking products of columns  
 16                   can be an involved and error-prone procedure. There is a much simpler way  
 17                   of generating a design like that of Table 2.2, namely by using Hadamard  
 18                   matrices.

19                   A Hadamard matrix is a matrix of 1's and -1's with the property that  
 20                   it is orthogonal (that is, the product of an  $n \times n$  Hadamard matrix and  
 21                   its transpose yields a multiple of the  $n \times n$  identity matrix). The smallest  
 22                   Hadamard matrix is  $H_2$ :

$$24                   H_2 = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}. \quad (2.27)$$

26                   When  $H_2$  is multiplied by its transpose (which is simply  $H_2$ , since it is  
 27                   symmetric), the result is twice the  $2 \times 2$  identity matrix,  $I_2$ .

$$29                   H_2 H_2^T = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} = \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix} = 2I_2. \quad (2.28)$$

32                   As a generalization of Equation (2.28),  $H_n H_n^T = nI_n$  for any  $n \times n$  Hadamard  
 33                   matrix  $H_n$ . A Hadamard matrix formed in this way makes a good FF design  
 34                   template. It is easy to generate a  $2^n \times 2^n$  Hadamard matrix recursively, using  
 35                   this identity:

$$37                   H_{2^n} = \left[ \begin{array}{c|cc} H_{2^{n-1}} & H_{2^{n-1}} \\ \hline H_{2^{n-1}} & -H_{2^{n-1}} \end{array} \right]. \quad (2.29)$$

39                   Specifically,

$$41                   H_4 = \left[ \begin{array}{c|cc} H_2 & H_2 \\ \hline H_2 & -H_2 \end{array} \right] = \left[ \begin{array}{cccc} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{array} \right] \quad (2.30)$$

01 and one more application of the recursion in Equation (2.29) gives  $H_8$ ,  
 02 which is the same as Table 2.2, except that  $H_8$  has a column of 1's on  
 03 the left.

04 A Hadamard matrix makes a design of *Resolution III*, which in practical  
 05 terms means that any two columns have an equal number of the combi-  
 06 nations  $(1, 1)$ ,  $(1, -1)$ ,  $(-1, 1)$  and  $(-1, -1)$ , as mentioned above. We can  
 07 construct an FF design matrix with even better properties in the following  
 08 way. Define  $M_k$  for  $k = 2^n$  as shown in Equation (2.31).

$$10 \quad M_k = \begin{bmatrix} H_k \\ -H_k \end{bmatrix}. \quad (2.31)$$

12 The matrix  $M_k$  has  $k$  columns and  $N = 2k$  rows. It can be used as a design  
 13 of *Resolution IV*. That means that this design has a much stronger version  
 14 of the rule given above for any two columns in Table 2.2. Any *three* columns  
 15  $p$ ,  $q$  and  $r$  of  $M_k$  have the property that the eight combinations  $(1, 1, 1)$ ,  
 16  $(1, 1, -1)$ ,  $(1, -1, 1)$ ,  $(1, -1, -1)$ ,  $(-1, 1, 1)$ ,  $(-1, 1, -1)$ ,  $(-1, -1, 1)$  and  
 17  $(-1, -1, -1)$  appear equally often in those columns. To put it another way,  
 18 the variables  $X_p$ ,  $X_q$  and  $X_r$  define a cube-shaped sample space like the one  
 19 shown beside Table 2.1. Each row in  $M_k$  then allocates values to  $X_p$ ,  $X_q$  and  
 20  $X_r$ , so that they occupy one of the corners of the cube. In a design constructed  
 21 from  $M_k$ , an equal number of simulations are allocated to each corner of the  
 22 design cube, *no matter which three parameters we consider*. This balance  
 23 in distribution is very helpful in determining which parameter and which  
 24 combinations of parameters working together influence the value of  $Y$ .

25 Utilizing  $M_k$  produces a design with  $k = 2^n$  columns and  $N = 2k = 2^{n+1}$   
 26 simulations. This is the same size as the OAT design in Equation (2.22) if  
 27  $k$  is a power of 2. If  $k$  is not a power of 2, we can treat it as one by adding  
 28 to the set of parameters enough ‘dummy’ or spare parameters<sup>6</sup> to make  
 29 the total equal the next higher power of 2.

30 In the case of FF analysis, a parameter’s contrast (the combination of  
 31  $-1$ ’s and 1’s that appear in the design) also represents the values of several  
 32 different interactions among two or more other parameters. For instance,  
 33 in Table 2.2  $X_3$  was explicitly defined to equal the interaction  $X_1 \times X_2$ . In a  
 34 design of Resolution IV, no parameter has the same contrast as any other,  
 35 nor as any two-factor interaction, but each parameter does have the same  
 36 contrast as some products of three or more other parameters. Therefore, if  
 37 a dummy parameter cannot be causing the estimated effect, it is likely that  
 38 an interaction among influential parameters is causing it.

40

---

41 <sup>6</sup> They are called dummy parameters because they do not appear in the model, and therefore  
 42 cannot influence the output of the model. Dummy parameters act as sentinels. If sensitivity  
 43 analysis purports to show that a dummy parameter is influential, the analyst knows that  
 44 something else is at work.

01 One advantage of using the OAT design in Equation (2.22) is that each  
 02 simulation changes only one parameter, and so, in a deterministic model,  
 03 the analyst can determine exactly what effect is caused by changing the  
 04 parameter.<sup>7</sup> One disadvantage is that parameter values for different param-  
 05 eters may be highly correlated. In Equation (2.22), consecutive parameters  
 06 like  $X_4$  and  $X_5$  differ in value in only two equations out of the total. The  
 07 average values estimated in Equation (2.25) will therefore be quite similar.

08 By contrast, designs based on the matrix in Equation (2.31) require  
 09 substantial computational effort to determine the influence of each param-  
 10 eter, but the parameters themselves have independent values that are not  
 11 correlated.

12 One traditional measure of the effect of a parameter in FF analysis is  
 13  $ME_r(Y)$ , the *main effect* of parameter  $X_r$  on  $Y$ . This quantity is obtained  
 14 by taking half the difference of average  $Y$  values for the two values of the  
 15 parameter. As the following equation shows, this definition is proportional  
 16 to the dot product between the contrast for the parameter and the vector  
 17 of simulation results.

$$\begin{aligned} 19 \quad ME_r(Y) &= \frac{1}{2} \left( \frac{1}{k} \sum_{x_{jr}=1} y_j - \frac{1}{k} \sum_{x_{jr}=-1} y_j \right) \\ 20 \\ 21 \quad &= \frac{1}{2} \left( \frac{1}{k} \sum_{x_{jr}=1} x_{jr} y_j + \frac{1}{k} \sum_{x_{jr}=-1} x_{jr} y_j \right) \\ 22 \\ 23 \quad &= \frac{1}{2k} \sum_{j=1}^{2k} x_{jr} y_j. \end{aligned} \tag{2.32}$$

28 It can be shown for a two-level FF design that the variance in the results  
 29 explained by parameter  $X_r$  alone is just

$$31 \quad \tilde{V}_{Yr} = [ME_r(Y)]^2. \tag{2.33}$$

33 A main effect could be estimated for OAT sampling using the estimated  
 34 means in Equation (2.25). However, the quantity  $\Delta_i Y$  from Equation (2.24)  
 35 typically gives a better estimate of the effect of changing  $X_i$  because  
 36 of the correlations among parameter values that affect the values in  
 37 Equation (2.25). In any case, the variance property in Equation (2.33)  
 38 would not apply to OAT sampling. It stems from the orthogonality of the  
 39 Hadamard matrix used in computing  $M_k$ .

41  
 42 <sup>7</sup> Of course, this information about changing one parameter applies only at the current point  
 43 in the sample space. Changing that parameter with some other combination of values for other  
 44 parameters might have quite a different effect in a nonlinear model.

01      Equation (2.33) creates a variance partitioning that is very useful in  
 02      making a quick search for influential parameters, when influence is defined  
 03      in terms of variance. Of course, the fact that the variance due to  $X_r$  is  
 04      based on the main effect, a linear estimator, emphasizes that variance due  
 05      to nonlinear effects is not accessible with this (or any other) two-level  
 06      design.

07

08

#### 09      2.4.5 Latin Hypercube Sampling

10

11      A two-level FF design gives no insight into the variation of an output  $Y$  as  
 12      a result of small changes in an influential parameter  $X_r$  inside its domain.  
 13      Section 2.3 discussed how to sample values of a single parameter considered  
 14      alone. Sometimes a single influential parameter is all we need to study in  
 15      sensitivity analysis, as all other parameters may have little influence. Just as  
 16      a two-level FF design is a small fraction of two-level full factorial design, so  
 17      we can define an  $s$ -level FF design that is a small fraction of an  $s$ -level full  
 18      factorial design. How do we select such a fraction with useful properties?  
 19      The following common method of selection is called Latin hypercube (LH)  
 20      sampling.

21

22      The key objective in LH sampling is to ensure that each parameter is  
 23      individually stratified over  $s > 2$  levels, and that each level contains the  
 24      same number of points. These conditions require that  $s$  divides into  $N$ ,  
 25      the sample size (some definitions require that  $s = N$ ). Table 2.3 shows 9  
 26      parameters and 6 levels, with each parameter having 2 simulations at each  
 27      level, for a total of 12 simulations.

28

29

30      **Table 2.3** An LH design with 12 simulations for  
 31      9 parameters on 6 levels

$X_1$	$X_2$	$X_3$	$X_4$	$X_5$	$X_6$	$X_7$	$X_8$	$X_9$
0	4	5	0	5	4	0	2	0
4	4	1	0	4	3	5	1	4
2	2	4	5	1	0	2	0	0
5	0	5	3	0	5	3	3	5
3	2	3	2	2	5	3	2	3
2	5	2	4	2	1	4	1	1
1	3	3	3	3	4	1	5	5
5	1	0	2	1	3	2	0	4
1	5	4	1	4	2	5	4	2
0	1	1	1	5	1	1	3	1
3	0	2	5	3	0	0	4	2
4	3	0	4	0	2	4	5	3

01 A randomized design like that of Table 2.3 is easy to generate. Simply  
 02 store the quantities 0, 0, 1, 1, 2, 2, 3, 3, 4, 4, 5, 5 in each column of an  
 03 array, and then randomize each column separately.<sup>8</sup> The result is a design  
 04 in coded form, using integer values 0 to  $s - 1$ , rather than parameter values  
 05 from the interval  $[0, 1]$ .

06 Table 2.4 is also a  $12 \times 9$  LH design on six levels, but it has a feature that  
 07 Table 2.3 does not. As indicated by the horizontal line separating top and  
 08 bottom, Table 2.4 consists of two LH designs, each with six simulations.  
 09 That means that in each column, the numbers 0 to 5 appear above and  
 10 below the line.

11 What is the practical difference between these designs? When Table 2.3 is  
 12 used to generate parameter values for simulations, an analyst can estimate  
 13 the mean value of output Y with the sample mean (Equation (2.5)), but it is  
 14 difficult to assess how good the estimate is. Because of the stratification, it  
 15 is likely that the estimate is better than what a random sample of the same  
 16 size would yield, but the traditional uncertainty estimate in Equation (2.5)  
 17 does not apply.

18 By contrast, the repeated design in Table 2.4 permits its own uncertainty  
 19 estimates. Any statistic that can be calculated separately for the top and the  
 20 bottom of the table, such as a sample mean for Y, now has two independent

21  
 22  
 23 **Table 2.4** A doubled LH design with 12  
 24 simulations, 9 parameters, 6 levels

$X_1$	$X_2$	$X_3$	$X_4$	$X_5$	$X_6$	$X_7$	$X_8$	$X_9$
0	4	5	0	5	4	0	2	0
4	3	1	1	4	3	5	1	4
2	2	4	5	1	0	2	0	2
5	0	0	3	0	5	3	3	5
3	1	3	2	2	2	1	4	3
1	5	2	4	3	1	4	5	1
<hr/>								
2	3	3	3	3	4	1	5	5
5	1	0	2	1	3	2	0	4
1	5	4	1	4	2	5	4	2
0	2	1	0	5	1	3	3	1
3	0	2	5	2	0	0	1	0
4	4	5	4	0	5	4	2	3

40     <sup>8</sup> An array  $a$  of length  $N$  can be randomized using a function  $random(N)$  that generates a  
 41 pseudo-random integer value from 0 to  $N - 1$ , and a method  $swap$  that interchanges two  
 42 entries of the array:

43     **for** ( int  $j = 0$  ;  $j < N$ ;  $j++$  )  
 44       **swap**( $a$ ,  $j$ ,  $random(N)$ ) ;

estimates. The uncertainty in these estimates can be obtained directly from the standard deviation of the two. That is,

$$\begin{aligned}\bar{Y}^{[1]} &= \frac{1}{6} \sum_{i=1}^6 y_i \\ \bar{Y}^{[2]} &= \frac{1}{6} \sum_{i=7}^{12} y_i \\ \bar{Y} &= \frac{1}{2} (\bar{Y}^{[1]} + \bar{Y}^{[2]})\end{aligned}\quad (2.34)$$

$$s_{\bar{Y}} = \sqrt{(\bar{Y}^{[1]} - \bar{Y})^2 + (\bar{Y}^{[2]} - \bar{Y})^2} = \frac{1}{\sqrt{2}} |\bar{Y}^{[1]} - \bar{Y}^{[2]}|. \quad (2.35)$$

Now examine Table 2.5. It is the same as Table 2.4, except that some randomly selected levels have been marked with a prime. Every column now has 12 levels: 0 and 0', 1 and 1', ...5 and 5'. If we replace these symbols by 0, 1, 2, ...11 respectively, we have an LH design with 12 levels. But because of the way it was constructed, the bottom and top halves are also LH designs on six levels. By constructing a two-level design this way, we can use the uncertainty estimate of Equation (2.35), while retaining the added benefit of using an LH sample on 12 levels. The uncertainty estimate will probably be an overestimate as a result.

The preceding discussion has addressed the issue of generating integer levels. To convert the integer levels to parameter values, the analyst can choose from several options. The design's integer value can be interpreted as identifying one subinterval out of  $s$  equal-length subintervals. The actual value to be used within that subinterval can be randomly generated from

**Table 2.5** An LH design with 12 simulations, 9 parameters, 12 levels

$X_1$	$X_2$	$X_3$	$X_4$	$X_5$	$X_6$	$X_7$	$X_8$	$X_9$
0'	4'	5	0	5'	4	0	2	0'
4'	3'	1	1'	4	3	5	1	4'
2'	2	4'	5	1	0	2'	0'	2
5	0'	0	3	0	5	3'	3'	5'
3	1	3'	2'	2	2'	1	4	3
1	5	2	4	3	1	4'	5'	1'
2	3	3	3'	3'	4'	1'	5	5
5'	1'	0'	2	1'	3'	2	0	4
1'	5'	4	1	4'	2	5'	4'	2'
0	2'	1'	0'	5	1'	3	3	1
3'	0	2'	5'	2'	0'	0'	1'	0
4	4	5'	4'	0'	5'	4	2'	3'

a uniform distribution, or it can be chosen at a fixed location within the interval (e.g. the midpoint). These are the same options illustrated in Figure 2.2 for a single parameter. One can even divide the interval  $[0, 1]$  into  $s - 1$  (rather than  $s$ ) subintervals, and interpret the numbers in the table as the  $s$  endpoints of these subintervals. This approach would lead to a piecewise linear fit of  $Y$  to each influential parameter, independently. Higher-order fits could be attempted to the mesh of points defined by interval endpoints for two or more influential parameters.

LH designs have attractive properties because values sampled for each parameter are stratified. In particular, one can use an LH sample mean as an estimate of a population mean. This estimate converges to the true mean more rapidly with increasing  $N$  than does a sample mean from a random sample. If  $Y$  is monotonic in each of the parameters  $X_i$ , a sample mean will have less uncertainty with LH sampling than a random sample mean at any sample size.

When the number of simulations  $N$  is much larger than the number of parameters  $k$ , a randomized LH design can be very effective in examining the influence of each parameter, through scatterplots and regression analysis. However, when  $N \leq k$ , the effects of different parameters cannot all be distinguished, because there are not enough data points to give independent estimates for each one. In this case the columns of the design matrix display excessive correlation. Excessive correlation between pairs of columns can persist even when  $N$  is somewhat greater than  $k$ . Then LH designs need extra structure, and that structure can be provided in various ways.

For example, orthogonal arrays are arrays of integers with properties similar in nature to those of a Hadamard matrix, but which can be much more complex. Orthogonal arrays can be used to generate LH samples where there is some degree of control over the similarities between columns for different parameters, to maximize the information available from a design of a particular size. Table 2.6 has nine simulations for four parameters operating at three levels. It has the additional balance property that each

**Table 2.6** A  $9 \times 4$  LH design on three levels based on an orthogonal array

	$X_1$	$X_2$	$X_3$	$X_4$
35	0	0	0	0
36	0	1	1	2
37	0	2	2	1
38	1	0	1	1
39	1	1	2	0
40	1	2	0	2
41	2	0	2	2
42	2	1	0	1
43	2	2	1	0

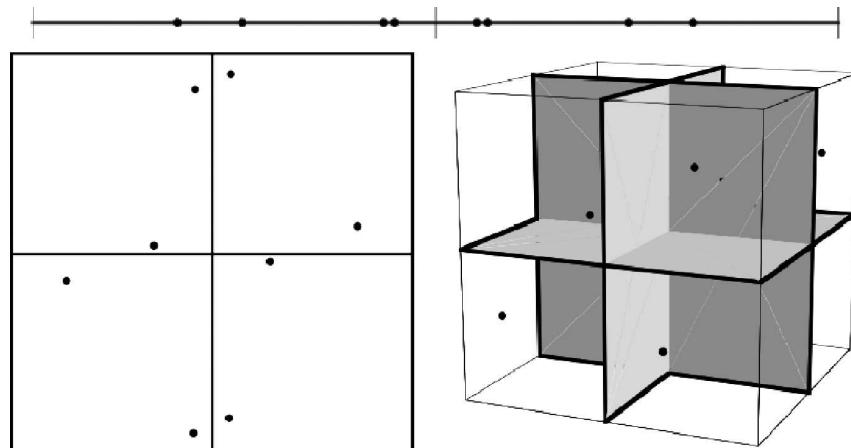
01 pair of columns contains all the nine combinations  $(0, 0), (0, 1), (0, 2), \dots$   
 02  $(2, 1), (2, 2)$ . It is not easy to create a new orthogonal array, but they have  
 03 been tabulated for many different sizes (Colbourn and Dinitz, 1996).

04 The next section describes a different way of adding structure to an LH  
 05 sample using a two-level FF design.

#### 07 2.4.6 Multivariate Stratified Sampling

08 The principle behind stratified sampling with a single variate was to  
 09 partition the sample space into nonoverlapping regions and to guarantee  
 10 sampling from each region. With a single parameter, the regions are  
 11 contiguous intervals. The purpose for stratified sampling is to ensure that all  
 12 parts of the sample space are represented, for improved (i.e. less uncertain)  
 13 mean and variance estimates. This goal is just as important in multivariate  
 14 sampling, but harder to achieve.

15 Suppose one pursues the goal by bisecting the domain for every parameter  
 16 and then taking at least one sample point from each ‘corner’ of the sample  
 17 space. One parameter has two ‘corners’, the regions  $[0, 0.5)$  and  $[0.5, 1]$ .  
 18 (The brackets indicate that the point 0.5 is in the second region only.) Two  
 19 parameters,  $X_p$  and  $X_q$ , have four ‘corners’, the quadrants of the  $X_p X_q$   
 20 plane. Three parameters  $X_p$ ,  $X_q$  and  $X_r$  have eight ‘corners’, the octants  
 21 of the  $X_p X_q X_r$  space. In general,  $k$  parameters have a sample space that  
 22 is a  $k$ -dimensional hypercube, with  $2^k$  ‘corners’. The first three cases are  
 23 illustrated in Figure 2.5.



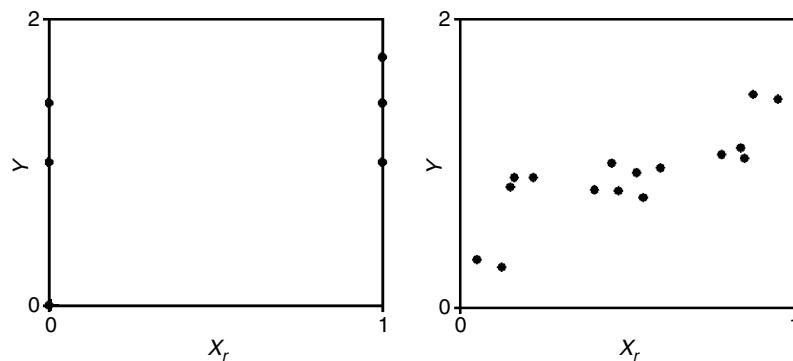
43 Figure 2.5 Bisecting the domain of each parameter for one [top], two [left] or three  
 44 [right] parameters

01 It would be desirable to have at least one point in each corner of the  
 02 sample space, but for large numbers of parameters, it is usually infeasible.  
 03 Attempting to do so would be equivalent to generating a two-level full facto-  
 04 rial design, requiring 1024 simulations for 10 parameters, over a million  
 05 for 20 parameters, and  $2^k$  simulations for  $k$  parameters.

06 However, the FF design approach partially solves this problem. Earlier we  
 07 used the interpretation that a value of ‘−1’ in the design matrix  $M_k$  should  
 08 correspond to the single parameter value 0 for  $X_r$ , and that ‘1’ in the design  
 09 matrix should correspond to a parameter value of 1. Suppose instead that  
 10 we use the interpretation that a ‘−1’ in an FF design means sampling from  
 11 the interval [0, 0.5) and a ‘1’ means to sample from the interval [0.5, 1].  
 12 Then the properties of a Resolution IV design will mean that there will  
 13 be an equal number of points in each of the octants of the sample space  
 14 for any three parameters viewed in isolation. Figure 2.5 would appear  
 15 approximately as shown for any selection of parameters. This balance helps  
 16 to expose dependencies of  $Y$  on interactions among parameters.

17 Figure 2.6 shows a plot of a function  $Y = (\sum_{i=1}^3 X_r^2)^{1/2}$  against  $X_r$  for  
 18 the two different interpretations. In the left panel, all parameter values are  
 19 either 0 or 1, and very little information about the dependence of  $Y$  on  $X_r$   
 20 is evident. Many of the points overlap since there are only four possible  
 21 values for  $Y$ , corresponding to zero, one, two or three parameters with a  
 22 value of 1. In the right panel parameter values span the domain of each  
 23 parameter and greater insight can be gained into the effect of an influential  
 24 parameter across its domain.

25 Unfortunately, there is a cost attached to this greater insight.  
 26 Equation (2.33) (using a main effect to estimate the variance explained  
 27 by parameter  $X_r$ ) no longer applies, except as a rough approximation.  
 28 That equation was based on the assumption that variation in  $Y$  due to



42 **Figure 2.6** Different interpretations of an FF design: [left] ‘−1’ maps to 0, ‘1’ maps  
 43 to 1; [right] ‘−1’ maps to the left half of the domain, and ‘1’ maps to the right half.  
 44 Both plots contain 16 points

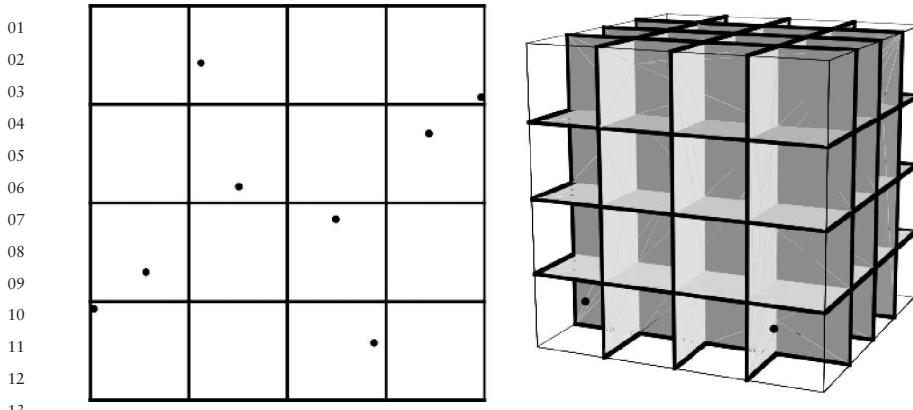


Figure 2.7 Combined fractional factorial – Latin hypercube design

changes in  $X_r$  could only occur as a result of the difference between low and high extreme values of  $X_r$ . If we let  $X_r$  vary within the upper or lower interval, those small changes could also affect the value of  $Y$ , and so should contribute to the variance of  $Y$  attributable to  $X_r$ .

It is possible to combine two-level FF and LH sampling, to secure the advantages of both. Figure 2.7 shows what happens in two and three dimensions when a two-level FF design is combined with stratified sampling inside each of the main two levels. In the pane on the left side, the two-level FF design ensures that each of the four quadrants contains the same number of points (two out of the eight). The LH sample ensures that each of the four columns contains two points, and similarly for the four rows. This behaviour would be observed for any pair of two parameters in the design. In the pane on the right side, the FF design ensures that each octant (corner) of the cube contains two points. The LH design ensures that each layer in each of the three directions contains two points. The two points in the closest vertical layer are visible. Once again, this distribution of points holds for any selection of three different parameters.

In Figure 2.7, points are randomly located within the subintervals designated by the design. It would also be possible to place them at specified locations, such as the centres of the regions.

#### 2.4.7 Quasi-random Sampling with Low-discrepancy Sequences

As experimental designs become more elaborate, more work must be devoted to the theory, implementation and selection of designs. How does one know that a combined FF–LH design with 128 parameters, 256

01 simulations and 64 LH strata was implemented correctly? How can it be  
 02 expanded to deal with more parameters? What if this design does not  
 03 yield adequate results – can one somehow make it part of a larger design  
 04 with more simulations? This section addresses the possibility of decreasing  
 05 sample complexity by using quasi-random sampling in much the same way  
 06 one would use pseudo-random sampling as discussed in Section 2.4.1.

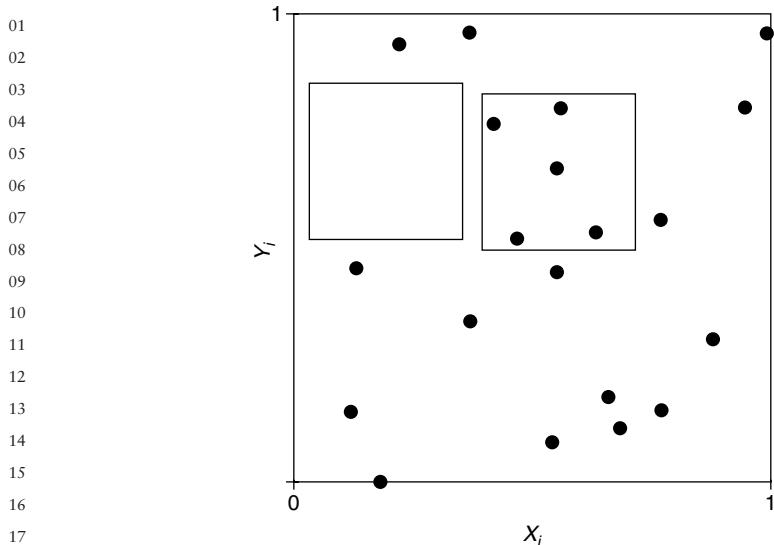
07 Using a pseudo-random generator for simple Monte Carlo sampling is  
 08 much simpler than using a complex design: as many values as necessary can  
 09 be generated, and if more parameters or more simulations are desired, it is  
 10 a simple matter to generate more.

11 Unfortunately, as shown earlier, samples generated randomly tend to have  
 12 clusters and gaps. Where a cluster occurs, function values in that vicinity are  
 13 overemphasized in statistical analysis. Where a gap arises, function values  
 14 within that gap are not sampled for statistical analysis. The net effect is that  
 15 mean values estimated with random samples have an uncertainty that dimin-  
 16 ishes slowly as  $1/\sqrt{N}$  (see Equation 2.5). To reduce an estimated uncertainty  
 17 by a factor of 10, the analyst must increase  $N$  by a factor of  $10^2 = 100$ .

18 A mathematical measure called *discrepancy* characterizes the lumpiness  
 19 of a sequence of points in a multidimensional space. Smaller discrepancy  
 20 values are better for sensitivity analysis (the distribution is less lumpy).  
 21 Figure 2.8 illustrates the concept in two dimensions. Each small square in  
 22 the figure occupies  $1/4 \times 1/4 = 1/16$  of the area of the unit square. Since  
 23 there are 20 randomly located points in the figure, each small square should  
 24 contain 1 or 2 of them, if the points are evenly distributed. However, one  
 25 of the small squares contains 5 points, and the other none. The discrepancy  
 26 of a sequence of points is the maximum absolute difference over a specified  
 27 set of regions between the area fraction and the point fraction. When the  
 28 regions are squares within the unit square, the discrepancy in Figure 2.8 is  
 29 at least  $5/20 - 1/16 = 3/16$ .

30 Random sequences of  $k$ -dimensional points have a relatively high discrep-  
 31 arity, as shown here. But there are infinite sequences of  $k$ -dimensional points  
 32 that behave much better with respect to this measure. They are called *low-*  
 33 *discrepancy sequences*. They have the property that as the sequence length  
 34  $N$  gets very large, the discrepancy shrinks at the theoretically optimal rate.  
 35 As a result, an estimated mean for a function  $Y(X_1, X_2, X_3, \dots, X_k)$  evaluated  
 36 on points  $\{X_{i1}, X_{i2}, \dots, X_{ik}\}_{i=1,N}$  from such a sequence will converge much  
 37 more quickly than would an estimated mean based on the same number of  
 38 random points.<sup>9</sup>

39  
 40  
 41     <sup>9</sup> How quickly? ‘For Monte Carlo integration of a smooth function in  $n$  dimensions, the  
 42 answer is that the fractional error will decrease with  $N$ , the number of samples, as  $(\ln N)^n/N$ ,  
 43 i.e. almost as fast as  $1/N$ ’ (Press *et al.*, 1997). This comment was made about the Sobol’  
 44 sequence, but all low-discrepancy sequences have the same asymptotic performance.



**Figure 2.8** Discrepancy is the maximum absolute difference between the fraction of the area a square occupies and the fraction of the points it contains. (Each small square is  $1/4$  of the width of the unit square.)

Samples made from a finite subset of such sequences are called *quasi-random* samples. These samples are not random, in the sense of being completely unpredictable. In fact, to maintain an even spread of points, an algorithm that generates low-discrepancy sequences must somehow bias the selection of new points to keep them away from the points already present. But they are like random points in the sense that they are uniformly distributed across the entire sample space.

In ‘small’ quasi-random samples, the effects of low-discrepancy may or may not be evident, as it is an asymptotic property that primarily comes into play as the sample size  $N$  gets very large. Whether a sample is large enough to display a low discrepancy depends in part on the number of parameters. When the number of parameters is large, a quasi-random sample will need to be large as well in order for the low discrepancy to become evident.

The Halton sequence is a well-known low-discrepancy sequence that is easy to generate. Table 2.7 shows how to generate values for  $X_1, X_2, X_3, \dots, X_{100}$  for the Halton sequence. On the left side of the table, successive position indices of the points are listed as ordinary numbers (base 10), and in bases 2, 3, 5, ..., 541.<sup>10</sup> These bases are the 1st, 2nd, 3rd and 100th

<sup>10</sup> The letters A, B, C, etc. are used as digits for base 541 because there are not enough digits in our number system to properly represent base-541 numbers.

**Table 2.7** Generating coordinates of points in a Halton sequence using the radical inverse transform

Index in base...					Parameter value			
10	2	3	5	... 541	$X_1$	$X_2$	$X_3$	... $X_{100}$
1	1	1	1	1	$0.1_2 = 0.5$	$0.1_3 = 0.333$	$0.1_5 = 0.2$	$0.1_{541} = 0.002$
2	10	2	2	2	$0.01_2 = 0.25$	$0.2_3 = 0.667$	$0.2_5 = 0.4$	$0.2_{541} = 0.004$
3	11	10	3	3	$0.11_2 = 0.75$	$0.01_3 = 0.111$	$0.3_5 = 0.6$	$0.3_{541} = 0.006$
4	100	11	4	4	$0.001_2 = 0.125$	$0.11_3 = 0.444$	$0.4_5 = 0.8$	$0.4_{541} = 0.007$
5	101	12	10	5	$0.101_2 = 0.625$	$0.21_3 = 0.778$	$0.01_5 = 0.04$	$0.5_{541} = 0.009$
6	110	20	11	6	$0.011_2 = 0.375$	$0.02_3 = 0.222$	$0.11_5 = 0.24$	$0.6_{541} = 0.011$
7	111	21	12	7	$0.111_2 = 0.875$	$0.12_3 = 0.556$	$0.21_5 = 0.44$	$0.7_{541} = 0.013$
8	1000	22	13	8	$0.0001_2 = 0.062$	$0.22_3 = 0.889$	$0.31_5 = 0.64$	$0.8_{541} = 0.015$
9	1001	100	14	9	$0.10001_2 = 0.562$	$0.001_3 = 0.037$	$0.41_5 = 0.84$	$0.9_{541} = 0.017$
10	1010	101	20	A	$0.0101_2 = 0.312$	$0.101_3 = 0.370$	$0.02_5 = 0.08$	$0.A_{541} = 0.018$
11	1011	102	21	B	$0.1101_2 = 0.812$	$0.201_3 = 0.704$	$0.12_5 = 0.28$	$0.B_{541} = 0.020$
12	1100	110	22	C	$0.0011_2 = 0.188$	$0.011_3 = 0.148$	$0.22_5 = 0.48$	$0.C_{541} = 0.022$

01 largest prime numbers, and in general,  $X_r$  is based on the  $r$ th largest prime  
02 number.

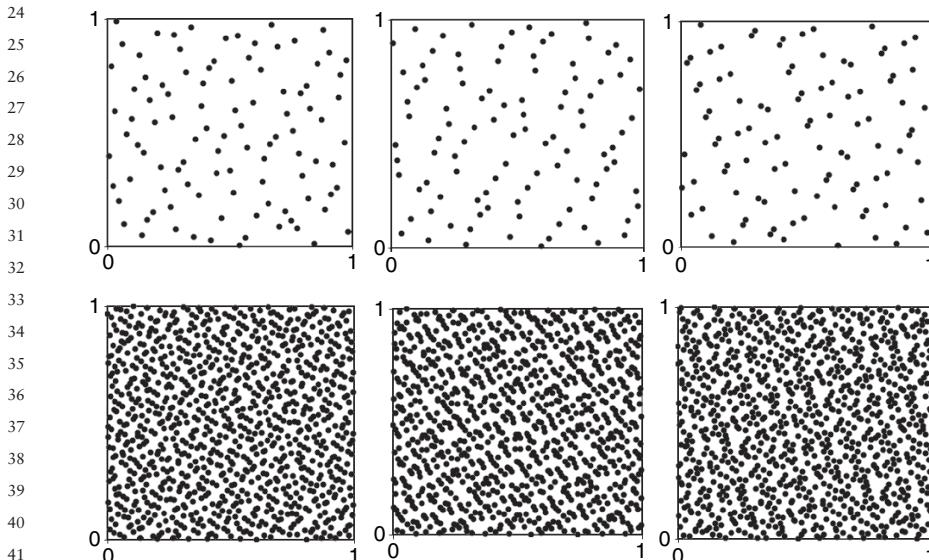
03 On the right side of the table, the digit sequences of the indices are  
04 reversed, and placed after a decimal point. This operation is called the  
05 radical inverse transform. The fractions so generated are then converted  
06 back to base 10 decimal fractions for comparison.

07 Figure 2.9 shows scatterplots of the first three parameters shown in  
08 Table 2.7 plotted against each other in pairs. The points look fairly evenly  
09 distributed, especially in the lower row where 1000 points are shown in  
10 each plot. However, there are also visible patterns in the dots (e.g. diagonal  
11 lines of dots). All low-discrepancy sequences have an even distribution, by  
12 definition, if the sample is large enough. Different sequences will display  
13 different patterns for small numbers of points.

14 Figure 2.10 shows scatterplots of  $X_1$  against  $X_{100}$  with 100 and 1000  
15 points. It is clear from this figure that more points are needed to hide  
16 artefacts of the way the points were generated.

17 One simple way to test a quasi-random sample with  $N$  points before  
18 using it in sensitivity analysis is to average each variable independently.  
19 That is,

$$20 \quad \int_0^1 X_j dX_j = 0.5 \cong (1/N) \sum_{i=1}^N x_{ij}. \quad (2.36)$$



42  
43 Figure 2.9 Parameters of Table 2.7 plotted against each other in pairs. Left to  
44 right:  $X_2$  vs  $X_1$ ,  $X_3$  vs  $X_1$ ,  $X_3$  vs  $X_2$ . Top row: 100 points; bottom row: 1000 points

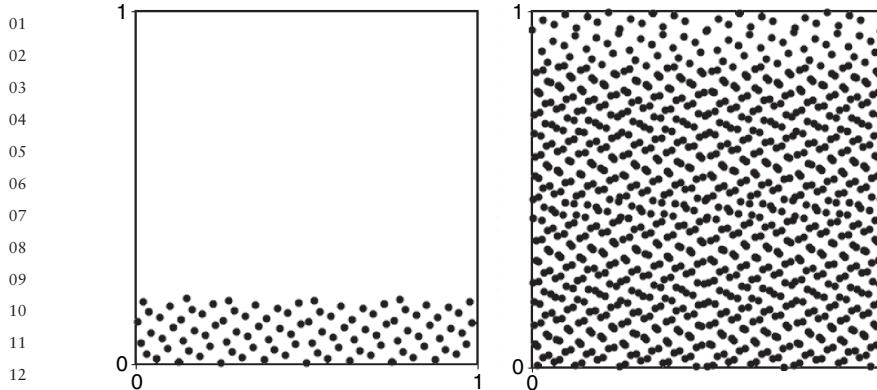


Figure 2.10  $X_{100}$  vs  $X_1$  from the Halton sequence (left: 100 points, right: 1000 points)

This fit should be very close, because of the quasi-random property. Similarly, it is a good idea to check at least some cross-products:

$$\int_0^1 (X_j X_k) dX_j dX_k = 0.25 \cong (1/N) \sum_{i=1}^N x_{ij} x_{ik}. \quad (2.37)$$

If the quasi-random sample cannot integrate these functions quite closely, it will probably not perform well in other sensitivity analysis tasks.

Table 2.8 shows how these quantities converge for the variables in Table 2.7, and for a couple of randomly generated variates,  $U$  and  $V$ . For  $N = 10\,000$ , parameters  $X_1$ ,  $X_2$  and  $X_3$  show tighter convergence than would be expected from random variables. However,  $X_{100}$  still shows worse convergence than the random variates. There is no apparent advantage at this sample size in using  $X_{100}$  in preference to a random variate.

Halton points are not the only quasi-random sequence described in the literature. One of the exercises at the end of this chapter challenges you to find other sequences, of which there are several. One that has been used in sensitivity analysis is the Sobol'  $LP_\tau$  sequence, for which Fortran code is given in Press *et al.* (1997). That code supports up to 51 dimensions (i.e.  $k = 51$ ), and up to about 1 billion values (i.e.  $N = 2^{30}$ ). Code that can handle larger problems is also available. Like the Halton sequence, more points are required for good behaviour in higher dimensions. An expedient to get the best possible results for a given  $N$  is to renumber the parameters so that those with lower numbers (e.g.  $X_1$ ,  $X_2$ ,  $X_3$ ) are the influential ones, if known. Another approach that has been explored is to randomize the entries for each parameter separately, to reduce correlations among parameters.

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**Table 2.8** Sample averages of single parameters and two-parameter products for different quasi-random sample sizes (sample averages should converge to 0.5, and product averages to 0.25)

N	Sample averages				Product averages				
	$X_1$	$X_2$	$X_3$	$X_{100}$	U	V	$X_1X_2$	$X_1X_{100}$	UV
1	0.500	0.333	0.200	0.002	0.738	0.135	0.167	0.001	0.099
3	0.500	0.370	0.400	0.004	0.831	0.644	0.139	0.002	0.562
10	0.444	0.441	0.428	0.010	0.660	0.521	0.172	0.004	0.354
30	0.484	0.472	0.470	0.029	0.563	0.522	0.223	0.014	0.304
100	0.490	0.489	0.492	0.093	0.542	0.518	0.237	0.046	0.291
300	0.496	0.495	0.495	0.278	0.524	0.501	0.245	0.138	0.260
1000	0.499	0.498	0.499	0.465	0.510	0.511	0.248	0.232	0.259
3000	0.4995	0.4994	0.4997	0.477	0.506	0.502	0.2494	0.238	0.252
10000	0.4998	0.4998	0.4999	0.492	0.5003	0.4976	0.2498	0.246	0.2487

01 Quasi-random samples can be analysed just as any empirical data set  
02 would be. One can calculate sample means and variances using the usual  
03 formulas. An output variable  $Y$  can be plotted against an input parameter  
04  $X_i$  to look for patterns. Two differences arise. First, traditional uncer-  
05 tainty estimates do *not* apply. For instance, an estimate  $\hat{Y}_N$  as calculated  
06 in Equation (2.4) would be expected to converge more rapidly than one  
07 based on random data as  $N$  increases, with the advantage growing for  
08 larger  $N$ . However, there is no obvious way of determining the uncertainty.  
09 The second difference is that small samples might not work well at all,  
10 depending on how the points are generated.

11

12

13 **2.5 GROUP SAMPLING**

14

15 **WHAT CAN BE DONE IF THE REQUIRED NUMBER OF SIMULATIONS IS NOT AFFORD-**  
16 **ABLE? IS THERE ANY WAY TO STUDY ONLY THE INFLUENTIAL PARAMETERS, IF**  
17 **THEY ARE NOT KNOWN IN ADVANCE?**

18 Designs considered so far require comparable numbers of simulations.  
19 For  $k$  parameters, an analyst should expect to use  $N = 2k$  simulations<sup>11</sup> or  
20 more. An OAT design needs that many to estimate the effect of changing  
21 each parameter, and an FF design of that size allows for estimation of main  
22 effects for each parameter. While LH samples can be of any size, strategies  
23 to reduce the correlations of different parameters in an LH design (such as  
24 combining FF with LH) tend to require  $N$  or more simulations.

25 This restriction on the minimum number of simulations could have an  
26 adverse effect on a modelling project. A model will generally become more  
27 complicated (i.e. acquire more parameters) over time as researchers add  
28 more features and elaborate on originally simple submodels. The natural  
29 evolution of a model could be curtailed if sensitivity analysis requirements  
30 make the simulation requirements with more parameters prohibitively  
31 expensive. Researchers need to find a way of reducing simulation require-  
32 ments for complex models.

33 One way to reduce the number of simulations required is to apply *group*  
34 *sampling*. It allows the analyst to generate smaller designs that can still  
35 isolate influential parameters and their effects. It is even possible to obtain  
36 sensitivity analysis information from *supersaturated designs*, where the  
37 number of simulations,  $N$ , is less than the number of parameters,  $k$ .

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40 <sup>11</sup> It should be noted that  $k$  does not affect the number of sample points required simply to  
41 estimate the mean of  $Y$  to a given level of uncertainty. The distribution of  $Y$  alone determines  
42 how many sample points are needed for an accurate estimate of the mean of  $Y$ . The number  
43 of parameters  $k$  does affect sensitivity analysis, however, because the analyst estimates not just  
44 one mean value, but also one or more coefficients for every parameter in the analysis.

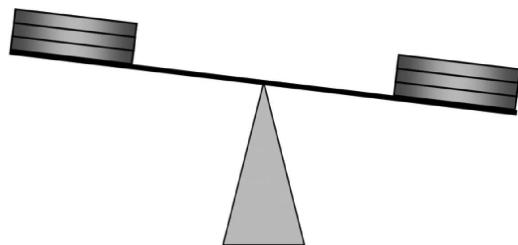
How can this be so? Look back at Equation (2.17) in Section 2.4.1. In matrix form, it specifies that  $X_{Nk}B_k = Y_k$ , which is a system of linear equations with  $N$  rows and  $k+1$  columns. From linear algebra, we know there is no unique solution to these equations when  $N < k+1$ . Furthermore, we will often be looking for functional forms more complex than a linear relationship, requiring the estimation of more coefficients. It seems unlikely that there is a mechanism for estimating these functions with too few simulations. It can be done only if we make some judicious assumptions.

The primary assumption (the null hypothesis) is that every parameter  $X_r$  has a negligible influence on the output variable  $Y$ . We will reject the null hypothesis for a particular parameter only if the data provide strong evidence of such an effect. This approach changes the statistical procedure from one of estimation (e.g. estimating the  $b_j$  coefficients in Equation 2.17) to one of statistical testing. We test each parameter for its effect, identify those for which we can reject the null hypothesis with high confidence, and then analyse the effects of only those parameters. Here we are aided by the conclusion in Section 2.4.3 that only about a dozen parameters can be influential compared to the rest. A supersaturated design can be effective if we focus on identifying and characterizing a small number of influential parameters.

Box 2.1 ‘A Counterfeit Coin Puzzle’ shows how clever design can extract the maximum amount of information from a small amount of data, given appropriate assumptions. In this puzzle, 12 coins need to be weighed on a balance scale only three times in order to find the one counterfeit coin and to tell whether it is lighter or heavier than the rest. A straightforward solution in which each coin is weighed against a standard reference coin would require as many as 11 comparisons, so reducing this number to three is a sound achievement. The solution works only if there is exactly one counterfeit coin. Moreover, the design is sequential: what is weighed in the second and third steps depends on the results of the first and second, respectively.

### Box 2.1 A Counterfeit Coin Puzzle (Fixx, 1972)

Suppose you are given 12 apparently identical coins, and you are told that one of them is counterfeit. It can only be told apart from the other coins by its weight – it is either lighter or heavier than a real coin. How many weighings with a balance scale would you need to find the fake coin, and determine if it is heavier or lighter than the rest?



Answer: only three.

1. Number the coins from 1 to 12. First weigh coins 1 to 4 together against coins 5 to 8.
  - (i) If the two sides balance, the fake coin is one of 9 to 12. Assume coins 1 to 8 are all good. Weigh 9 to 11 together against 1 to 3.
  - (ii) If the two sides still balance, the fake coin must be 12. Weigh it against any other coin to see if it is heavy or light.
  - (iii) If the second weighing does not balance, the fake coin is one of 9 to 11, and you know whether it is heavy or light by the way the scale tipped. Suppose it is heavy. Weigh 9 against 10 to see which one is the fake (i.e. the heavy one). If they balance, 11 is the counterfeit.
2. Suppose coins 1 to 4 were heavier than 5 to 8 in the first weighing. Then either the fake is heavy, and one of coins 1 to 4, or light, and one of 5 to 8. Coins 9 to 12 are assumed fair. Weigh coins 1 to 3 and 5 against coins 9 to 11 and 4.
  - (i) If the two sides balance, the fake coin is light, and one of 6 to 8. Weigh 6 against 7 to see which one is the fake (i.e. the light one). If they balance, 8 is the counterfeit.
  - (ii) If coins 1 to 3 and 5 are heavy in the second weighing, the fake coin is heavy, and must be one of 1 to 3. Weigh 1 against 2 to see which one is the fake (i.e. the heavy one). If they balance, 3 is the counterfeit.
  - (iii) If coins 1 to 3 and 5 are light in the second weighing, then either 5 is the fake and it is light, or 4 is the fake on the other side, and it is heavy. Weight 5 against 1 to see which case applies.

Suppose we analyse a model with 1000 parameters, and utilize a sample design with only 400 simulations. By statistical testing, we identify a dozen parameters for which we have strong evidence to reject insignificance. Then we reuse the 400 simulations to investigate the nature of the influence of those 12 parameters. The task seems feasible. The number of simulations actually required to perform sensitivity analysis is determined more by the number of parameters that are influential (which is always a small number) than by the total number of parameters.

What design might be suitable for testing the influences of a large number of parameters? The concept of *group sampling* provides one answer. In group sampling, all the parameters are assigned to a small number of groups. For example, with  $k = 1000$  parameters, we could designate 16 groups as follows:

$$\begin{aligned} G_1 &= \{X_1, X_2, X_3, \dots, X_{64}\} \\ G_2 &= \{X_{65}, X_{66}, \dots, X_{128}\} \\ &\vdots \\ G_{16} &= \{X_{961}, X_{962}, \dots, X_{1024}\} \end{aligned} \tag{2.38}$$

where the extra parameters from  $X_{1001}$  to  $X_{1024}$  would be dummy parameters.

This kind of grouping will be done several times, and each one will have a set of simulations. In each set of simulations, every parameter in a group takes the same sampled parameter values. That is,  $x_{i1} = x_{i2} = \dots = x_{i,64}$  for every simulation  $i$  in the set. The group itself acts like a parameter, just as in the coin-weighing example a group of coins would be weighed together. It is not possible to separate the effects of individual parameters, given the results of one set of simulations, just as one weighing tells us little about the weights of individual coins.

Why have 16 groups, rather than 3 or 300? As in the coin-weighing example, the size of the group can be optimized to yield the most information. If the number of groups is very small, influential parameters will be grouped together, and it will be more difficult to separate their effects and to examine their interactions (i.e. nonlinear effects when they are both varied). Accordingly, it is desirable to have more groups than influential parameters. However, if the number of groups is too large, then each set of simulations will be large, and it will not be possible to have more than a few sets of simulations. On the premise that only a dozen parameters can be influential, it makes sense to have 20 or 30 groups. A power of 2, such as 16 or 32, works well because it allows two-level FF designs to be used.

Given 16 groups, an analyst could conduct 32 simulations in an OAT or Resolution IV FF sample, treating the groups as parameters. From the

01 results the analyst could determine which groups were influential. Suppose  
 02 two parameters are individually influential. If they are in separate groups,  
 03 then their effects would appear independently as group effects. If they are  
 04 in the same group, their effects either sum together, or partially cancel each  
 05 other. Since the number of influential parameters cannot be large, there will  
 06 typically be some groups that have no influential parameters, and most of  
 07 the rest will appear in separate groups.

08 Then the analyst would redo the group analysis using a different allocation  
 09 of groups, such as

$$\begin{aligned} G_{12} &= \{X_1, X_{17}, X_{33}, \dots, X_{993}, X_{1009}\} \\ G_{22} &= \{X_2, X_{18}, \dots, X_{994}, X_{1010}\} \\ &\vdots \\ G_{16,2} &= \{X_{16}, X_{32}, \dots, X_{1008}, X_{1024}\}. \end{aligned} \tag{2.39}$$

17 Parameters that were grouped together in Equation (2.38) are mostly  
 18 separated in Equation (2.39). When the analyst carries out another 32-  
 19 simulation study, each influential parameter will influence a different group  
 20 from before, in combination with a different collection of other parameters.  
 21

22 The rearrangement from Equation (2.38) to (2.39) is obviously system-  
 23 atic, designed to suggest how different the groupings are. In practice, an  
 24 analyst can randomly assign parameters to groups. If two influential param-  
 25 eters appear in the same group in the first grouping, there is only a 1/16  
 26 chance they will appear together in the second grouping, and in each subse-  
 27 quent grouping. Given enough groupings, the analyst can separate the effects  
 28 of different influential parameters.

29 To make this argument quantitative, we denote with  $M$  the number of  
 30 different groupings, each with its set of simulations. If the grouping is  
 31 done randomly, two influential parameters will be grouped together on  
 32 average  $M/16$  times. For example, if  $M = 8$ , two influential parameters  
 33 will share a group, on average,  $8/16$  times. We would expect to find them  
 34 together perhaps once, and not likely more than two or three times. With  
 35 10 influential parameters, each one will have a probability of more than  
 36 50% of not having any other influential parameters in its group each time.

37 A more difficult problem arises in weeding out noninfluential parame-  
 38 ters that masquerade as influential parameters because they share a group  
 39 several times with influential parameters. For example, suppose that  $X_1$  is  
 40 influential. The probability that  $X_1$  shares a group  $t$  times out of  $M$  with a  
 41 noninfluential parameter  $X_j$  is

$$P_{1j}(t, M) = \binom{M}{t} \left(\frac{1}{16}\right)^t \left(\frac{15}{16}\right)^{M-t}. \tag{2.40}$$

If  $M = 8$  and  $t = 4$ , the probability is  $P_{1j}(4, 8) = 0.0008$ . While this value is small, it may not be small enough. If there are 1000 parameters, there is a significant probability of  $1 - (1 - P_{1j}(4, 8))^{999} = 0.56$  that one of the other parameters, probably a noninfluential one, shares a group four times with  $X_1$ . And that coincidence could be enough to make that parameter look influential.

If two or more influential parameters have similar effects, the situation becomes even worse. Suppose the three parameters  $X_1$ ,  $X_2$  and  $X_3$  have significant effects of similar magnitude. Then a noninfluential parameter that shares a group with any one of them several times can appear influential. By analogy with Equation (2.40), the probability of parameter  $X_j$  sharing a group with one of these parameters is roughly<sup>12</sup>

$$P_{123j}(t, M) = \binom{M}{t} \left(\frac{3}{16}\right)^t \left(\frac{13}{16}\right)^{M-t} \quad (2.41)$$

which evaluates to  $P_{123j}(4, 8) = 0.038$  for four repetitions in eight groupings. With 1000 parameters, many noninfluential parameters would create a halo around the influential ones, concealing the parameters that are actually influential.

Three simple steps can help to clarify which parameters are influential. Examine Table 2.9, in which the first two steps will be demonstrated. The left

**Table 2.9** Analysis of results for three parameters, showing effects of steps to eliminate noninfluential parameters

<i>Grouping</i>	<i>Before analysis</i>			<i>Using signs</i>		<i>After <math>X_1</math> correction</i>	
	$X_1$	$X_2$	$X_j$	$X_j$	$X_1$	$X_2$	$X_j$
1	9.5	-5.2	9.5	-9.5	2.0	-5.2	-2.0
2	2.3	2.3	0.2	0.2	-5.2	-5.2	0.2
3	4.7	-4.6	-0.2	0.2	-2.8	-4.6	-0.2
4	9.9	-4.8	2.6	2.6	2.4	-4.8	2.6
5	7.2	-3.9	7.2	-7.2	-0.3	-3.9	-0.3
6	7.7	-0.6	-3.3	-3.3	0.2	-0.6	-3.3
7	9.6	-7.3	9.6	9.6	2.1	-7.3	2.1
8	8.9	-1.3	0.6	-0.6	1.4	-1.3	0.6
Average	7.5	-3.2	3.3	-1.0	0.0	-4.1	0.5

<sup>12</sup> This is not an exact formulation because it does not allow for cases where influential parameters are themselves in the same group.

01 side of the table shows the main effects of parameters  $X_1$ ,  $X_2$  and  $X_j$ . Parameters  $X_1$  and  $X_2$  are both influential parameters, with main effects of similar magnitude, but opposite sign. Parameter  $X_j$  is noninfluential, but by chance it shares a grouping with  $X_1$  three times out of the eight groupings. As a result, its average effect is larger than that of  $X_2$ . The rectangles around some of the numbers represent values that are repeated in the table because two of the tabulated parameters were in the same group. For instance,  $X_1$  and  $X_j$  shared a group in Grouping 7, and so both received the same main effect, 9.6.

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The first improvement in group sampling is a simple trick that greatly reduces the probability that impostors like  $X_j$  will appear. Sample a random sign variable  $s_{rm}$  for each parameter  $X_r$  in each grouping  $m$  from 1 to  $M$ . Each sign variable is either 1 or  $-1$ , with equal probability. If  $s_{rm} = 1$ , then parameter  $X_r$  follows the group sampling in grouping  $m$ . That is, if  $X_r$  belongs to group  $G_1$  in the  $m$ th grouping, and if the parameter value for group  $G_1$  is 0.69237 in simulation 5, then  $x_{5r} = 0.69237$ . If  $s_{rm} = -1$ , on the other hand, parameter  $X_r$  takes values complementary to the group value in the  $m$ th grouping. In the case above, the value for  $x_{5r}$  would not be 0.69237, but rather  $1 - 0.69237 = 0.30763$ .

The sign variables for each grouping must be stored and used when calculating a sensitivity statistic, such as a main effect. Toggling the sign variable between 1 and  $-1$  toggles the sign of many sensitivity statistics. Since  $X_1$  causes the large main effects in groups where it occurs, these groups always have a positive main effect after corrections are made for the sign variable associated with  $X_1$ . The same cannot be said for a noninfluential variable like  $X_j$ . It is just as likely to have a negative main effect as a positive one.

The centre section of Table 2.9 shows what happens to  $X_j$  if some of the signs are flipped because the sign variable of  $X_j$  is different from the sign variable of the controlling parameter in a group. Instead of having three large main effects that add up to make  $X_j$  look like an influential parameter, there is some cancellation, and the resulting average effect for  $X_j$  is quite small ( $-1.0$ ). This first step reduces the number of impostors substantially, but alone it is not enough.

The second step occurs at the analysis stage. When the amount of data available is limited, it is important that an analyst perform sensitivity analysis in a stepwise manner. That is, the analyst should identify the most influential parameter, characterize its effect, and try to remove that effect, leaving a set of residuals to analyse, instead of the original  $Y$  values. The analyst should then proceed to analyse the residuals in a stepwise manner.

For example, the right side of Table 2.9 shows what happens when the effect of the most influential parameter,  $X_1$ , is removed from the analysis. (To make this effect clear, sign variables have not been used on the right-hand side of the table.) The main effect of  $X_1$  is best estimated as 7.5, its average value from all groupings. Assume that the presence of  $X_1$  adds 7.5

01 to the main effect of any group to which  $X_1$  belongs. Subtract 7.5 from the  
02 main effect of all those groups to which  $X_1$  belonged.

03 The right side of the table shows what happens after the reduction. The  
04 remaining average effect of  $X_1$  after this correction is 0.0. The remaining  
05 average effect of the other influential parameter,  $X_2$ , has strengthened  
06 from -3.2 to -4.1. It looks more influential because the cancellation  
07 that occurred with  $X_1$  in Grouping 2 has been eliminated. In contrast,  
08 the remaining average effect of the noninfluential parameter,  $X_3$ , has been  
09 reduced from 3.3 to 0.5. The removal of the effect of  $X_1$  eliminates impos-  
10 tors that gained their apparent influence simply by sharing a group with  $X_1$   
11 several times.

12 These two approaches, sign variables and stepwise analysis, can be used  
13 together to increase the capability of the analyst to identify truly influential  
14 parameters. There is one more step that can be taken, if the analyst is  
15 observant while carrying out the experimental design.

16 Suppose the analyst carries out one grouping, and looks at the results.  
17 They may show one influential group, several influential groups, or the  
18 effects of all the groups may be of a similar magnitude. As in the coin  
19 puzzle, the analyst has the option of controlling the group assignments in  
20 later groupings based on earlier results. Suppose group  $G_5$  out of 16 groups  
21 has an effect that is much larger than the effect of any other group. In the  
22 next grouping, the analyst could choose to divide the parameters from  $G_5$   
23 into groups  $G_1$  to  $G_8$ , while combining all the other parameters into a pool  
24 from which to construct  $G_9$  to  $G_{16}$ . This would be an effective technique to  
25 isolate a single dominant parameter, by allocating it to ever smaller groups.

26 Alternatively, it may happen that 12 out of 16 groups show effects of  
27 similar magnitude. The implication is that there may be a large number  
28 of semi-influential parameters, without any really dominant ones. At that  
29 point the analyst could choose to allocate 32 groups instead of 16 at the  
30 next grouping, to try to separate these semi-influential parameters.

31 Sequential analysis of this type is very powerful, but not well understood.  
32 It illustrates one of many possible lines of inquiry to be followed by future  
33 research in sensitivity analysis. The choice of appropriate experimental  
34 designs remains an open and fascinating field.

## 37 2.6 EXERCISES

- 39 1. Suppose a parameter  $Z$  is uniformly distributed between 5 and 9 metres.  
40  
 41 (a) What are its pdf  $f_Z(z)$  and cdf  $F_Z(z)$ ?  
 42 (b) What transform would convert  $Z$  to a parameter  $X$  uniformly  
43 distributed between 0 and 1? What transform would convert values  
44 of  $X$  back to  $Z$  values?

- 01 (c) What if  $Z$  had a triangular distribution instead? That is, suppose the  
02 pdf is a straight line between the points  $(5m, 0)$  and  $(9m, 0.5)$ , and 0  
03 elsewhere. Find its pdf, cdf and transforms.

04 2. Identify a pseudo-random generator in a computer language or  
05 software package that you frequently use. For example, Java has  
06 `Math.random()` and Excel has `rand()`.

07 (a) What is the algorithm by which this generator computes numbers?  
08 How long a period does the generator have before it starts to repeat  
09 itself?

10 (b) How would you regenerate a sequence of numbers so that you could  
11 repeat an earlier set of simulations? [Hint: how do you use a random  
12 seed with your generator?] How would you generate a new sample  
13 that did *not* overlap with the previous one?

14 (c) Suppose you want to change both the number of parameters in  
15 your model and the number of simulations carried out. How could  
16 you arrange to regenerate the same values for parameters that  
17 were used before and new values for new parameters and new  
18 simulations?

19 3. Generate a long sequence of random values for the triangular variate  
20  $Z$  described in Question 1. Estimate the sample mean and variance  
21 using Equation (2.4). How many simulations are needed to estimate  
22 these quantities reliably to one decimal place? [Hint: generate multiple  
23 sequences of the same length and ensure they have the same mean and  
24 variance to one decimal place.]

25 4. Generate a stratified random sample for the triangular variate  $Z$   
26 described in Question 1. Use  $N$  points, with two random points sampled  
27 from each of  $N/2$  equal-length intervals for  $X$ . For instance, if  $N =$   
28 8, divide the interval from 0 to 1 into four subintervals:  $[0, 0.25]$ ,  
29  $[0.25, 0.5]$ ,  $[0.5, 0.75]$  and  $[0.75, 1]$  and sample two points in each subin-  
30 terval.  
31 (a) How many simulations are needed to estimate the mean value of  $Z$   
32 reliably to one decimal place (see previous question)?  
33 (b) How do the variance estimates  $\tilde{V}_Y^a$  and  $\tilde{V}_Y^w$  differ, if  $Y = Z$ ?

34 5. Suppose  $v = 3a - 2bc + 4d^2$ , where  $a$ ,  $b$ ,  $c$  and  $d$  are parameters,  
35 each with values in the domain  $[0, 1]$ . Write out a list of eight linear  
36 equations generated by a randomized return-trip OAT design starting  
37 from  $\{1, 1, 1, 1\}$ .

38 (a) Determine the two effects of changes to the values of each param-  
39 eter, as in Equation (2.24). Which parameter change causes the  
40 largest single change in  $v$ ? Which parameter has the largest difference  
41 between its two effects?

- 01                   (b) What is the average value of  $\nu$  for  $a$  at 0 and  $a$  at 1, as in  
02                   Equation (2.25)? What are the average values for the other parame-  
03                   ters? Which one has the largest difference between averages?  
04                   (c) Which method of assessing the impact of the parameters is most  
05                   representative in this example?  
06                   (d) Calculate the average value for each pair of mirror points in your  
07                   sample. Can you determine that the model is nonlinear from these  
08                   averages?
- 09                 6. Construct a two-level full factorial design for five parameters. How many  
10                  simulations are there?  
11  
12                   (a) Consider just the fraction of the design consisting of simulations  
13                  where an odd number of parameters have value  $-1$ . How many  
14                  simulations are there in this fraction?  
15                   (b) How many simulations would be needed for the same five parameters  
16                  for a full factorial design on five levels?  
17                   (c) In the factorial design on five levels, every parameter has a value  
18                  that is 0, 1, 2, 3 or 4. How many simulations would there be in  
19                  the fraction of the design consisting of simulations where the sum of  
20                  values for all the parameters is a multiple of 5?  
21                 7. Use Equation (2.31) to produce a Resolution IV FF design for 12 param-  
22                  eters. [Hint: how many parameters would the design have to handle?] Evaluate  $Y$  values for this design, given that  $Y = X_1 + 2X_2 + 3X_3 + 4X_7X_{12}$ . Assume each  $X_i$  takes values 1 or  $-1$  only.  
23  
24                   (a) Work out the main effects for all the parameters  $X_1$  to  $X_{12}$ . How do  
25                  they relate to the coefficients of the formula for  $Y$ ?  
26                   (b) Use your design to work out the contrast (i.e. the pattern of 1's and  
27                   $-1$ 's) for  $X_7X_{12}$  and for two other two-factor interactions. Evaluate  
28                  interaction effects for these interactions by applying these contrasts  
29                  using Equation (2.32).  
30                   (c) Can you find a three-factor interaction that has the same contrast as  
31                   $X_1$ ?  
32  
33                 8. Generate:  
34  
35                   (a) one LH sample with 5 parameters, 12 levels and 12 simulations;  
36                   (b) three LH samples with 5 parameters, 4 levels and 4 simulations each;  
37                   (c) one LH sample with 5 parameters, 12 levels and 12 simulations by  
38                  combining the three samples in part (b), and splitting levels 0 to 3  
39                  into three sub-levels each (e.g. 0, 0' and 0'' become new levels 0, 1  
40                  and 2);  
41                   (d) an orthogonal array as shown in Table 2.6 that has 16 simulations on  
42                  5 parameters at 4 levels, with the property that all the combinations  
43  
44

- 01                   (0, 0), (0, 1), (0, 2), (0, 3), (1, 0), . . . (3, 2), (3, 3) occur for any pair of  
 02                   parameters. [Difficult]
- 03     9. Generate a combined FF and LH design with eight simulations and four  
 04                   parameters using the following steps:  
 05  
 06       (a) Generate a  $4 \times 4$  Hadamard matrix, and then replace every  $-1$  by  $0$   
 07                   and every  $1$  by  $4$ . (In general you use  $0$  and  $2^n$  for a  $2^n \times 2^n$  Hadamard  
 08                   matrix.)  
 09       (b) Generate an LH design with four simulations for four variables on  
 10                   four levels. Each column will have a permutation of the numbers  $0$ ,  
 11                    $1$ ,  $2$  and  $3$ . Add this design to the one from step (a) in the following  
 12                   way. If the entry in the modified Hadamard matrix is  $4$ , add the  
 13                   entry in the same location of the LH design to it. If the entry in the  
 14                   modified Hadamard matrix is  $0$ , add to it  $3 - w$ , where  $w$  is the entry  
 15                   in the same location of the LH design. Entries in the new design will  
 16                   now range from  $0$  to  $7$ , but in each column there will only be four  
 17                   different values.  
 18       (c) Double the number of rows to make a Resolution IV design by adding  
 19                   to the design the complement of every simulation currently there.  
 20                   The complement is found by subtracting each entry in the original  
 21                   row from  $7$  to get the entry in the new row.
- 22     10. Several low-discrepancy sequences are described in the literature. Find  
 23                   papers or books containing algorithms for generating at least three other  
 24                   low-discrepancy sequences beside the Halton points. In each case cite  
 25                   the source, name the sequence (usually named after the person who  
 26                   discovered it), and describe briefly how the numbers are generated.
- 27     11. Suppose you have access to a model with the functional form  $Y =$   
 28                    $aX_m - bX_n$  for some unknown  $a$ ,  $b$ ,  $m$  and  $n$ . How many groupings and  
 29                   runs would you need to find the unknowns with high confidence using  
 30                   FF designs, given that the number of parameters is  $k = 1000$ ? What if  
 31                    $k = 10^6$ ?

## 2.7 EXERCISE SOLUTIONS

- 35     1. Suppose a parameter  $Z$  is uniformly distributed between  $5$  and  $9$   
 36                   metres . . .

37       (a)

$$f_Z(z) = \begin{cases} 0 \text{ m}^{-1} & z < 5 \text{ m} \\ 1/(9 \text{ m} - 5 \text{ m}) & 5 \text{ m} \leq z < 9 \text{ m} \\ 0 \text{ m}^{-1} & 9 \text{ m} \leq z \end{cases} \quad (2.42)$$

$$F_Z(z) = \begin{cases} 0 & z < 5 \text{ m} \\ (z - 5 \text{ m})/(9 \text{ m} - 5 \text{ m}) & 5 \text{ m} \leq z < 9 \text{ m} \\ 1 & 9 \text{ m} \leq z \end{cases} \quad (2.43)$$

01                   (b)  $X = F_Z(Z)$   
 02                    $Z = 5 \text{ m} + X(9 \text{ m} - 5 \text{ m})$   
 03  
 04  
 05                   (c)  $f_Z(z) = \begin{cases} 0 \text{ m}^{-1} & z < 5 \text{ m} \\ 2(z - 5 \text{ m})/(9 \text{ m} - 5 \text{ m})^2 & 5 \text{ m} \leq z < 9 \text{ m} \\ 0 \text{ m}^{-1} & 9 \text{ m} \leq z \end{cases}$                    (2.44)  
 06  
 07  
 08                    $F_Z(z) = \begin{cases} 0 & z < 5 \text{ m} \\ ((z - 5 \text{ m})/(9 \text{ m} - 5 \text{ m}))^2 & 5 \text{ m} \leq z < 9 \text{ m} \\ 1 & 9 \text{ m} \leq z \end{cases}$                    (2.45)  
 09  
 10  
 11  
 12                    $X = F_Z(Z)$   
 13                    $Z = 5 \text{ m} + \sqrt{X}(9 \text{ m} - 5 \text{ m}).$

14                   2. Identify a pseudo-random generator in a computer language or software  
 15                   package that you frequently use. ...Take Excel's `rand()`.

16  
 17                   (a) Prior to 2003, Excel used a poor pseudo-random generator that  
 18                   started to repeat (approximately) after a cycle of about 1 million  
 19                   values. Excel 2003 upgraded `rand` to use a 48-bit pseudo-random  
 20                   generator published by Wichman and Hill (1982). It has a cycle of  
 21                   more than  $10^{13}$  before repetition occurs. The Fortran algorithm is  
 22                   as follows:<sup>13</sup>

23                   C IX, IY, IZ SHOULD BE SET TO INTEGER VALUES BETWEEN  
 24                   C 1 AND 30000 BEFORE FIRST ENTRY  
 25  
 26                   IX = MOD(171 \* IX, 30269)  
 27                   IY = MOD(172 \* IY, 30307)  
 28                   IZ = MOD(170 \* IZ, 30323)  
 29                   RANDOM = AMOD(FLOAT(IX) / 30269.0 + FLOAT(IY) /  
 30                   30307.0 + FLOAT(IZ) / 30323.0, 1.0)

31                   (b) According to one website,<sup>14</sup> it is not possible to set the starting seed in  
 32                   Excel 2003's (and Excel 2007's) version of `rand()`. The Visual Basic  
 33                   method `RANDOMIZE()` is supposed to perform this function, but does  
 34                   not. It is possible, however, to generate a fixed sequence in Excel by  
 35                   filling a large number of cells with the formula `=rand()`, and then  
 36                   copying and pasting the values (not the formulas) of these cells into  
 37                   another range of cells of the same size. Thereafter these values will  
 38                   stay fixed. Similarly, it is not possible to guarantee that two different  
 39                   samples will not overlap. However, because of the long cycle, overlap  
 40                   is unlikely unless you use many random numbers. For example, if you  
 41                   use two separate sample of 10 000 numbers, the odds are less than

42  
 43  
 44                   <sup>13</sup> <http://support.microsoft.com/kb/828795>

<sup>14</sup> <http://www.daheiser.info/excel/main/section15.pdf>

$10\ 000/10^{13} = 10^{-9}$  that the second sequence starts within the range of the first sequence. In a programming language where you can set the random seed, you would regenerate the first sequence and then take the following numbers to form a new sequence, thereby guaranteeing they do not overlap. Some pseudo-random generators (e.g. l'Ecuyer and Andres, 1997) offer the facility of generating independent and nonoverlapping subsequences.

- (c) If your simulation generates pseudo-random numbers as it goes along, start from the same seed and you will get the same sequence. If the number of parameters can change between runs, it helps to have a distinct subsequence for each parameter so that the number of parameters will not affect the numbers produced. It is important that if you have a distinct subsequence for each parameter, the subsequence is made much longer than you expect to use, so that you can expand the number of runs later. In Excel, generate a large table of pseudo-random numbers that is made constant by copying and pasting values from a table where the formula =rand() is used. Assign one parameter to each column, and make sure the number of rows is much larger than what you expect to use. If necessary, you can copy more numbers into the bottom of the table to support more simulations.
- 3. Generate a long sequence of random values for the triangular variate  $Z$  described in Question 1. . . . no answer provided.
- 4. Generate a stratified random sample for the triangular variate  $Z$  described in Question 1. . . . no answer provided.
- 5. Suppose  $v = 3a - 2bc + 4d^2$ , where  $a, b, c$  and  $d$  are parameters, each with values in the domain  $[0, 1]$ . Write out a list of eight linear equations generated by a randomized round-trip OAT design starting from  $\{1, 1, 1, 1\}$ . The coefficients  $b_j$  in the following equation are based on Equation (2.16), and are not related to the variable  $b$ .

$$\begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 & 1 \end{bmatrix} \begin{pmatrix} b_0 \\ b_1 \\ b_2 \\ b_3 \\ b_4 \end{pmatrix} = \begin{pmatrix} 5 \\ 7 \\ 4 \\ 0 \\ 0 \\ 0 \\ 3 \\ 7 \end{pmatrix} \quad (2.46)$$

(a)	<i>a</i>	<i>b</i>	<i>c</i>	<i>d</i>	
1st effect	3	0	-2	4	
2nd effect	3	-2	0	4	
largest				✓	
largest difference		✓	✓		
avg $\nu$ at 0	1	2.5	2.75	0.75	(2.47)
avg $\nu$ at 1	5.5	4.0	3.75	5.75	
difference	4.5	1.5	1.0	5.0	
largest difference				✓	
mirror point avg	2.5	3.5	3.5	3.5	

(b) See table above.

(c) In this case, the single simulation change best measures the coefficient of each parameter. It gets the correct coefficient for  $a$ , gets the right coefficient for  $b$  and  $c$  part of the time, and gets the right coefficient for  $d$ , although with two levels it cannot distinguish between a linear effect and a squared effect.

(d) See the table above for averages of each pair of mirror points. Three are the same, but one is different, indicating some nonlinearity. If you plug  $a = b = c = d = 0.5$  into the actual formula, you get  $\nu = 2$ , which is quite different from these values, indicating a higher degree of nonlinearity.

6. Construct a two-level full factorial design for five parameters. There are 32 simulations, as shown in the following table:

Run	$X_1$	$X_2$	$X_3$	$X_4$	$X_5$	Run	$X_1$	$X_2$	$X_3$	$X_4$	$X_5$
1	1	1	1	1	1	17	-1	1	1	1	1
2	1	1	1	1	-1	18	-1	1	1	1	-1
3	1	1	1	-1	1	19	-1	1	1	-1	1
4	1	1	1	-1	-1	20	-1	1	1	-1	-1
5	1	1	-1	1	1	21	-1	1	-1	1	1
6	1	1	-1	1	-1	22	-1	1	-1	1	-1
7	1	1	-1	-1	1	23	-1	1	-1	-1	1
8	1	1	-1	-1	-1	24	-1	1	-1	-1	-1
9	1	-1	1	1	1	25	-1	-1	1	1	1
10	1	-1	1	1	-1	26	-1	-1	1	1	-1
11	1	-1	1	-1	1	27	-1	-1	1	-1	1
12	1	-1	1	-1	-1	28	-1	-1	1	-1	-1
13	1	-1	-1	1	1	29	-1	-1	-1	1	1
14	1	-1	-1	1	-1	30	-1	-1	-1	1	-1
15	1	-1	-1	-1	1	31	-1	-1	-1	-1	1
16	1	-1	-1	-1	-1	32	-1	-1	-1	-1	-1

- 01           (a) Consider just the fraction of the design consisting of simulations in  
 02           which an odd number of parameters have value  $-1$ . There is one  
 03           simulation in each row of the table above, for 16 in total.

04

05

06

<i>Run</i>	$X_1$	$X_2$	$X_3$	$X_4$	$X_5$
17	-1	1	1	1	1
2	1	1	1	1	-1
3	1	1	1	-1	1
20	-1	1	1	-1	-1
5	1	1	-1	1	1
22	-1	1	-1	1	-1
23	-1	1	-1	-1	1
8	1	1	-1	-1	-1
9	1	-1	1	1	1
26	-1	-1	1	1	-1
27	-1	-1	1	-1	1
12	1	-1	1	-1	-1
29	-1	-1	-1	1	1
14	1	-1	-1	1	-1
15	1	-1	-1	-1	1
32	-1	-1	-1	-1	-1

23

24

25

- (b) On five levels,  $5^5 = 3125$  simulations would be required.  
 (c) There would be  $5^4 = 625$  simulations in the fraction. Whatever the sum of the first four parameters is, one and only one value for  $X_5$  would make the total sum a multiple of 5.

26

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7. Use Equation (2.31) to produce a Resolution IV FF design for 12 parameters (see next page).

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- (a) Main effects: see the last line of the table on the next page. All coefficients of terms linear in the variables are estimated correctly. The effects of the two-way interaction do not affect the main effects.  
 (b) Two-way interaction: see table above for the column  $X_7X_{12}$ . Other two-way interactions are not shown. The interaction effect of 4 is correct and it is shown in the ME row of the table.  
 (c) The product  $X_2X_3X_4$  has the same contrast (sign structure) as  $X_1$ .

41

42

43

44

8. Generate:

- (a) one LH sample with 5 parameters, 12 levels and 12 simulations (not shown)

Run	$X_1$	$X_2$	$X_3$	$X_4$	$X_5$	$X_6$	$X_7$	$X_8$	$X_9$	$X_{10}$	$X_{11}$	$X_{12}$	$X_7X_{12}$	Y
1	1	1	1	1	1	1	1	1	1	1	1	1	1	10
2	1	-1	1	-1	1	-1	1	-1	1	-1	1	-1	-1	-2
3	1	1	-1	-1	1	1	-1	-1	1	1	-1	-1	1	-4
4	1	-1	-1	1	1	-1	-1	1	1	-1	-1	1	-1	-8
5	1	1	1	1	-1	-1	-1	-1	1	1	-1	-1	1	2
6	1	-1	1	-1	-1	1	-1	1	1	1	-1	-1	-1	6
7	1	1	-1	-1	-1	-1	1	1	1	-1	-1	1	-1	0
8	1	-1	-1	1	1	-1	1	-1	1	-1	-1	-1	-1	2
9	1	1	1	1	1	1	1	1	-1	-1	-1	1	-1	6
10	1	-1	1	-1	1	-1	1	-1	-1	-1	-1	1	-1	-4
11	1	1	-1	-1	1	1	-1	-1	-1	-1	1	1	-1	0
12	1	-1	-1	1	1	-1	-1	-1	-1	-1	-1	-1	1	10
13	1	1	1	1	-1	-1	-1	-1	-1	-1	-1	-1	1	-2
14	1	-1	1	-1	-1	-1	1	-1	-1	-1	-1	1	-1	-4
15	1	1	-1	-1	-1	-1	1	1	-1	-1	-1	1	-1	-8
16	1	-1	-1	1	-1	-1	1	1	-1	-1	-1	-1	1	-2
17	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	1	-6
18	-1	1	-1	1	-1	-1	1	-1	1	-1	1	-1	1	4
19	-1	-1	1	1	-1	-1	-1	1	1	-1	-1	1	-1	0
20	-1	1	1	-1	-1	1	1	1	-1	-1	1	-1	-1	-10
21	-1	-1	-1	-1	1	1	1	1	1	-1	-1	-1	1	2
22	-1	1	-1	1	1	-1	1	-1	-1	-1	1	-1	1	-4
23	-1	-1	1	1	1	1	-1	-1	-1	-1	1	1	-1	8
24	-1	1	1	-1	1	-1	-1	1	1	-1	1	-1	1	-10
25	-1	-1	-1	-1	-1	-1	-1	-1	1	1	1	-1	1	2
26	-1	1	-1	1	-1	1	-1	-1	1	1	-1	-1	-1	-4
27	-1	-1	1	1	-1	-1	1	1	1	1	-1	1	1	8
28	-1	1	1	-1	-1	1	1	-1	1	1	-1	1	1	-2
29	-1	-1	-1	-1	1	1	1	1	-1	1	-1	1	-1	-6
30	-1	1	-1	1	1	1	-1	-1	-1	1	1	-1	-1	4
31	-1	-1	1	1	1	1	-1	-1	-1	1	-1	-1	1	0
32	-1	1	1	-1	-1	1	-1	-1	1	1	-1	-1	-1	4
ME	1	2	3	0	0	0	0	0	0	0	0	0	0	0

01           (b) three LH samples with 5 parameters, 4 levels and 4 simulations  
 02           each:

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<i>Run</i>	$X_1$	$X_2$	$X_3$	$X_4$	$X_5$
1	1	3	0	3	2
2	3	0	1	2	1
3	2	1	3	1	0
4	0	2	2	0	3
<hr/>					
5	1	2	1	2	3
6	3	1	3	1	0
7	2	3	2	3	2
8	0	0	0	0	1
<hr/>					
9	2	3	0	2	2
10	1	1	1	3	1
11	0	2	3	1	0
12	3	0	2	0	3

23           (c) a derived LH sample with 5 parameters, 12 levels and 12 simula-  
 24           tions:

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<i>Run</i>	$X_1$	$X_2$	$X_3$	$X_4$	$X_5$
1	4	10	0	9	6
2	9	1	3	8	5
3	8	5	11	4	1
4	2	6	7	2	10
<hr/>					
5	5	7	4	6	11
6	10	3	9	5	0
7	6	11	8	10	7
8	1	0	2	1	3
<hr/>					
9	7	9	1	7	8
10	3	4	5	11	4
11	0	8	10	3	2
12	11	2	6	0	9

01 (d) An orthogonal array:

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<i>Run</i>	$X_1$	$X_2$	$X_3$	$X_4$	$X_5$
1	0	0	0	0	0
2	0	1	1	1	1
3	0	2	2	2	2
4	0	3	3	3	3
<hr/>					
5	1	0	1	2	3
6	1	1	0	3	2
7	1	2	3	0	1
8	1	3	2	1	0
<hr/>					
9	2	0	2	3	1
10	2	1	3	2	0
11	2	2	0	1	3
12	2	3	1	0	2
<hr/>					
13	3	0	3	1	2
14	3	1	2	0	3
15	3	2	1	3	0
16	3	3	0	2	1

9. Generate a combined FF and LH design with 8 simulations and 4 parameters:

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<i>Run</i>	$X_1$	$X_2$	$X_3$	$X_4$
1	4	7	6	5
2	5	1	5	3
3	7	5	0	0
4	6	3	3	6
<hr/>				
5	3	0	1	2
6	2	6	2	4
7	0	2	7	7
8	1	4	4	1

10. No answer provided. Hint: look in the ACM journal *Transactions on Mathematical Software*.

- 01    11. Use Resolution IV designs with 8 parameters and 16 runs for each  
02    grouping. There are only two influential parameters, so the probability  
03    is only 1/8 that they will share the same grouping if grouping is done  
04    randomly. Suppose in the first set of 16 simulations two groups appear  
05    to be influential. In the next grouping, divide the parameters in those  
06    groups into four groups, and divide the rest among the other four  
07    groups. Again only two groups (at worst) appear to be influential. At  
08    the next grouping, divide the parameters in those two into four groups,  
09    and all the rest into four groups. And so on. If we start with 1000  
10    parameters, the number of parameters in each influential group will be:  
11     $125 \rightarrow 63 \rightarrow 32 \rightarrow 16 \rightarrow 8 \rightarrow 4 \rightarrow 2 \rightarrow 1$ . A total of eight groupings  
12    with 128 simulations would be required. In general, the number of  
13    groupings is  $1 + \log_2(k/8)$ . With  $k = 1\,000\,000$ , the number of groupings  
14    would be about 18, and the number of simulations would be only 288.
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# 3

## Elementary Effects Method

### 3.1 INTRODUCTION

IS THERE A METHOD WHICH CAN COPE WITH COMPUTATIONALLY EXPENSIVE MODELS AND GIVE SENSITIVITY RESULTS WITH A SMALL NUMBER OF MODEL EVALUATIONS?

In the previous chapter we noted that the amount of information revealed via a sensitivity analysis depends heavily on the number of sample points that are simulated and where they are located.

In this chapter we will describe a sensitivity analysis method which is effective in identifying the few important factors in a model that contains many factors, with a relatively small number of sample points properly distributed.

The method is conceptually simple and easy to implement. It belongs to the class of OAT designs described in Chapter 2 but partially overcomes their main limitations. While adhering to the concept of local variation around a base point, this method makes an effort to overcome the limitations of the derivative-based approach by introducing wider ranges of variations for the inputs and averaging a number of local measures so as to remove the dependence on a single sample point.

This method is ideal when the number of input factors is too large to allow the application of computationally expensive variance-based techniques, but at the same time not large enough to demand the use of group techniques such as those described at the end of Chapter 2. With respect to group techniques it has the advantage of examining each factor individually so as

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

01 to avoid the problem of cancellation effects (i.e. two factors, individually  
 02 influential, may belong to the same group and have effects that partially  
 03 cancel each other out).

04

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### 06 3.2 THE ELEMENTARY EFFECTS METHOD

07

08 **WHAT IS AN ELEMENTARY EFFECT? HOW CAN I DEFINE A SENSITIVITY MEASURE**  
 09 **USING THE ELEMENTARY EFFECTS? HOW CAN I INTERPRET THE SENSITIVITY**  
 10 **RESULTS? WHEN CAN I USE THIS METHOD?**

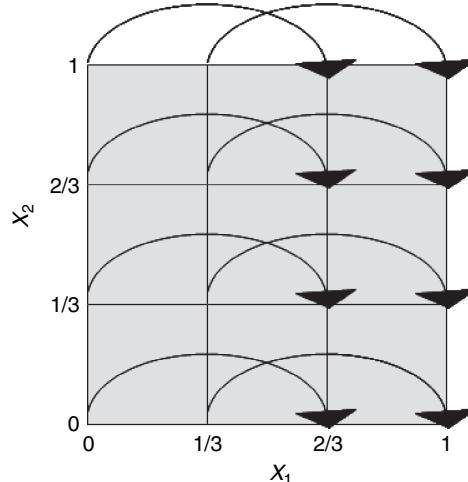
11 The elementary effects (EE) method is a simple but effective way of  
 12 screening a few important input factors among the many that can be  
 13 contained in a model. The fundamental idea behind the method is owed  
 14 to Morris, who introduced the concept of elementary effects in 1991,  
 15 proposing the construction of two sensitivity measures with the aim of  
 16 determining which input factors could be considered to have effects which  
 17 were (a) negligible, (b) linear and additive, or (c) nonlinear or involved  
 18 in interactions with other factors. An elementary effect is defined as  
 19 follows. Consider a model with  $k$  independent inputs  $X_i, i = 1, \dots, k$ ,  
 20 which varies in the  $k$ -dimensional unit cube across  $p$  selected levels. In  
 21 other words, the input space is discretized into a  $p$ -level grid  $\Omega$ . For  
 22 a given value of  $\mathbf{X}$ , the elementary effect of the  $i$ th input factor is  
 23 defined as

$$24 \\ 25 EE_i = \frac{[Y(X_1, X_2, \dots, X_{i-1}, X_i + \Delta, \dots, X_k) - Y(X_1, X_2, \dots, X_k)]}{\Delta}, \quad (3.1) \\ 26$$

27 where  $p$  is the number of levels,  $\Delta$  is a value in  $\{1/(p-1), \dots, 1-1/(p-1)\}$ ,  
 28  $\mathbf{X} = (X_1, X_2, \dots, X_k)$  is any selected value in  $\Omega$  such that the transformed  
 29 point  $(\mathbf{X} + e_i \Delta)$  is still in  $\Omega$  for each index  $i = 1, \dots, k$ , and  $e_i$  is a vector of  
 30 zeros but with a unit as its  $i$ th component.

32 The distribution of elementary effects associated with the  $i$ th input factor  
 33 is obtained by randomly sampling different  $\mathbf{X}$  from  $\Omega$ , and is denoted  
 34 by  $F_i$ , i.e.  $EE_i \sim F_i$ . The  $F_i$  distribution is finite and, if  $p$  is even and  $\Delta$   
 35 is chosen to be equal to  $p/(2(p-1))$ , the number of elements of  $F_i$  is  
 36  $p^{k-1} [p - \Delta(p-1)]$ . Assume, for instance, that  $k = 2$ ,  $p = 4$  and  $\Delta = 2/3$ ,  
 37 for a total number of eight elements for each  $F_i$ . The four-level grid in the  
 38 input space is represented in Figure 3.1. The total number of elementary  
 39 effects can be counted from the grid by simply keeping in mind that each  
 40 elementary effect relative to a factor  $i$  is computed by using two points  
 41 whose relative distance in the coordinate  $X_i$  is  $\Delta$ , and zero in any other  
 42 coordinate.

43 The sensitivity measures,  $\mu$  and  $\sigma$ , proposed by Morris, are respectively  
 44 the estimates of the mean and the standard deviation of the distribution  $F_i$ .



**Figure 3.1** Representation of the four-level grid ( $p = 4$ ) in the two-dimensional input space ( $k = 2$ ). The value of  $\Delta$  is  $2/3$ . The arrows identify the eight points needed to estimate the elementary effects relative to factor  $X_1$

The mean  $\mu$  assesses the overall influence of the factor on the output. The standard deviation  $\sigma$  estimates the ensemble of the factor's effects, whether nonlinear and/or due to interactions with other factors. An intuitive explanation of the meaning of  $\sigma$  is the following. Assume that for factor  $X_i$  we obtain a high value of  $\sigma$ . The elementary effects relative to this factor thus differ notably from one another, implying that the value of an elementary effect is strongly affected by the choice of the sample point at which it is computed, i.e. by the choice of the other factors' values. By contrast, a low value of  $\sigma$  indicates very similar values among the elementary effects, implying that the effect of  $X_i$  is almost independent of the values taken by the other factors. Campolongo *et al.* (2007) proposed replacing the use of the mean  $\mu$  with  $\mu^*$ , which is defined as the estimate of the mean of the distribution of the absolute values of the elementary effects that we denote with  $G_i$ , i.e.  $|EE_i| \sim G_i$ .

The use of  $\mu^*$  is convenient as it solves the problem of type II errors (failing to identify a factor with considerable influence on the model), to which the original measure  $\mu$  is vulnerable. Type II errors might occur when the distribution  $F_i$  contains both positive and negative elements, i.e. when the model is nonmonotonic or has interaction effects. In these cases, some effects may cancel each other out when computing  $\mu$ , thus producing a low mean value even for an important factor. To avoid such type II errors, Morris (1991) recommended considering the values of  $\mu$  and  $\sigma$  simultaneously, since a factor with elementary effects of different signs (i.e. that cancel each other out) would have a low value of  $\mu$  but a considerable

value of  $\sigma$ . A graphical representation in the  $(\mu, \sigma)$  plane allows for a better interpretation of results by taking into account at the same time the two sensitivity measures. Morris's approach is in general valuable, but it may become problematic in the case of large models with multiple outputs (see Campolongo *et al.*, 2007). On the other hand,  $\mu^*$  is a practical and concise measure to use, especially when there are several output variables. Moreover, in contrast to  $\mu$ ,  $\mu^*$  has the advantage that it can be adjusted to work with a group of factors, i.e. to produce an overall sensitivity measure relative to a group (see Section 3.5). Campolongo *et al.* (2007) have also shown that  $\mu^*$  is a good proxy of the total sensitivity index  $S_T$  discussed in Chapter 4. The total sensitivity index is a measure of the overall effect of a factor on the output (inclusive of interactions) and corresponds to the expected variance that is left when all factors but  $X_i$  are fixed, i.e.  $E_{X_{\sim i}}(V_{X_i}(Y|X_{\sim i}))$ , and

$$S_{T_i} = \frac{E_{X_{\sim i}}(V_{X_i}(Y|X_{\sim i}))}{V(Y)}.$$

$S_{T_i}$  is to be used when the goal is that of identifying noninfluential factors in a model (rather than prioritizing the most influential ones).  $\mu^*$  is an effective substitute for the total index when the computational cost of  $S_T$  is unaffordable.

In general, as the estimate of  $\mu$  comes at no extra computational cost (the same number of model executions is required), we recommend computing all three statistics,  $\mu$ ,  $\sigma$  and  $\mu^*$ , so as to extract the maximum amount of sensitivity information. For instance, the comparison between  $\mu$  and  $\mu^*$  provides information on the signs of the effects that the factor has on the output. If  $\mu$  and  $\mu^*$  are both high, it implies not only that the factor has a large effect on the output, but also that the sign of this effect is always the same. If, by contrast,  $\mu$  is low while  $\mu^*$  is high, it means that the factor examined has effects of different signs depending on the point of the space at which the effect is computed. The sampling strategy to estimate the three statistics is described in detail in the next section.

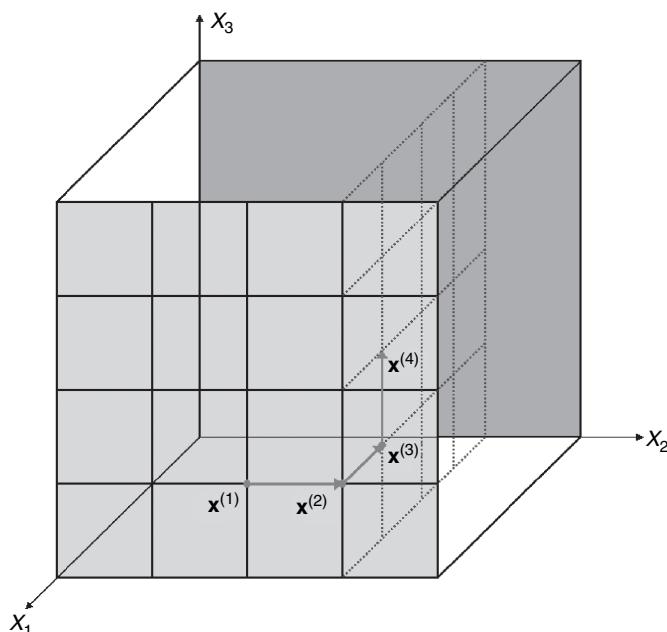
### 3.3 THE SAMPLING STRATEGY AND ITS OPTIMIZATION

#### HOW CAN I BUILD AN EFFICIENT SAMPLE TO ESTIMATE THE ELEMENTARY EFFECTS?

In order to estimate the sensitivity measures (i.e. the statistics of the distributions  $F_i$  and  $G_i$ ), the design focuses on the problem of sampling a number  $r$  of elementary effects from each  $F_i$ . As the computation of each elementary effect requires two sample points, the simplest design would

01 require  $2r$  sample points for each input, for a total of  $2rk$ , where  $k$  is the  
 02 number of input factors. Morris (1991) suggested a more efficient design  
 03 that builds  $r$  trajectories of  $(k+1)$  points in the input space, each providing  $k$   
 04 elementary effects, one per input factor, for a total of  $r(k+1)$  sample points.

05 The trajectories are generated in the following manner. A *base* value  $\mathbf{x}^*$   
 06 for the vector  $\mathbf{X}$  is randomly selected in the  $p$ -level grid  $\Omega$ .  $\mathbf{x}^*$  is not part  
 07 of the trajectory but is used to generate all the trajectory points, which are  
 08 obtained from  $\mathbf{x}^*$  by increasing one or more of its  $k$  components by  $\Delta$ . The  
 09 first trajectory point,  $\mathbf{x}^{(1)}$ , is obtained by increasing one or more components  
 10 of  $\mathbf{x}^*$  by  $\Delta$ , in such a way that  $\mathbf{x}^{(1)}$  is still in  $\Omega$ . The second trajectory  
 11 point,  $\mathbf{x}^{(2)}$ , is generated from  $\mathbf{x}^*$  with the requirement that it differs from  
 12  $\mathbf{x}^{(1)}$  in its  $i$ th component, which has been either increased or decreased by  
 13  $\Delta$ , i.e.  $\mathbf{x}^{(2)} = \mathbf{x}^{(1)} + \mathbf{e}_i\Delta$  or  $\mathbf{x}^{(2)} = \mathbf{x}^{(1)} - \mathbf{e}_i\Delta$ . The index  $i$  is randomly selected  
 14 in the set  $\{1, 2, \dots, k\}$ . The third sampling point,  $\mathbf{x}^{(3)}$ , is generated from  
 15  $\mathbf{x}^*$  with the property that  $\mathbf{x}^{(3)}$  differs from  $\mathbf{x}^{(2)}$  for only one component  $j$ ,  
 16 for any  $j \neq i$ . It can be either  $\mathbf{x}^{(3)} = \mathbf{x}^{(2)} + \mathbf{e}_j\Delta$  or  $\mathbf{x}^{(3)} = \mathbf{x}^{(2)} - \mathbf{e}_j\Delta$ . And so on  
 17 until  $\mathbf{x}^{(k+1)}$ , which closes the trajectory. The design produces a trajectory  
 18 of  $(k+1)$  sampling points  $\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \dots, \mathbf{x}^{(k+1)}$  with the key properties that  
 19 two consecutive points differ in only one component and that any value  
 20 of the *base vector*  $\mathbf{x}^*$  has been selected at least once to be increased by  $\Delta$ .  
 21 An example of a trajectory for  $k = 3$  is illustrated in Figure 3.2.



43                   **Figure 3.2** An example of a trajectory in the input space when  $k = 3$

01 A technical scheme to generate trajectories with the required properties  
 02 is as follows. A trajectory can be seen in the form of a matrix,  $\mathbf{B}^*$ , with  
 03 dimension  $(k+1) \times k$ , whose rows are the vectors  $\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \dots, \mathbf{x}^{(k+1)}$ . To  
 04 build  $\mathbf{B}^*$ , the first step is the selection of a matrix  $\mathbf{B}$ , whose dimensions are  
 05  $(k+1) \times k$ , with elements that are 0's and 1's and the key property that  
 06 for every column index  $j, j = 1, \dots, k$ , there are two rows of  $\mathbf{B}$  that differ  
 07 only in the  $j$ th entry. A convenient choice for  $\mathbf{B}$  is a strictly lower triangular  
 08 matrix of 1's:

$$\mathbf{B} = \begin{bmatrix} 0 & 0 & 0 & \dots & 0 \\ 1 & 0 & 0 & \dots & 0 \\ 1 & 1 & 0 & \dots & 0 \\ 1 & 1 & 1 & 0 & \dots \\ \dots & \dots & \dots & \dots & \dots \end{bmatrix}.$$

15 The matrix  $\mathbf{B}'$ , given by

$$17 \quad \mathbf{B}' = \mathbf{J}_{k+1,k} \mathbf{x}^* + \Delta \mathbf{B},$$

19 where  $\mathbf{J}_{k+1,k}$  is a  $(k+1) \times k$  matrix of 1's and  $\mathbf{x}^*$  is a randomly chosen *base*  
 20 *value* of  $\mathbf{X}$ , is a potential candidate for the desired design matrix, but it  
 21 has the limitation that the  $k$ th elementary effect it produces would not be  
 22 randomly selected.

23 A randomized version of the sampling matrix is given by

$$25 \quad \mathbf{B}^* = (\mathbf{J}_{k+1,1} \mathbf{x}^* + (\Delta/2) [(2\mathbf{B} - \mathbf{J}_{k+1,k}) \mathbf{D}^* + \mathbf{J}_{k+1,k}]) \mathbf{P}^*, \quad (3.2)$$

27 where  $\mathbf{D}^*$  is a  $k$ -dimensional diagonal matrix in which each element is either  
 28 +1 or -1 with equal probability, and  $\mathbf{P}^*$  is a  $k$ -by- $k$  random permutation  
 29 matrix in which each row contains one element equal to 1, all others are  
 30 0, and no two columns have 1's in the same position. Read row by row,  $\mathbf{P}^*$   
 31 gives the order in which factors are moved;  $\mathbf{D}^*$  states whether the factors  
 32 will increase or decrease their value along the trajectory.  $\mathbf{B}^*$  provides one  
 33 elementary effect per input, which is randomly selected.

### 37 Example 3.1

39 Consider a model with two input factors uniformly distributed in  $[0, 1]$ .  
 40 Consider the following set of levels  $\{0, 1/3, 2/3, 1\}$ . In this case  $k = 2, p = 4$ ,  
 41 and we choose  $\Delta = 2/3$ . Suppose the randomly generated  $\mathbf{x}^*$ ,  $\mathbf{D}^*$  and  $\mathbf{P}^*$  are

$$43 \quad \mathbf{x}^* = \{1/3, 1/3\} \quad \mathbf{D}^* = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \quad \mathbf{P}^* = \mathbf{I}.$$

01 The matrix  $\mathbf{B}$  is given by

$$02 \\ 03 \\ 04 \\ 05 \quad \mathbf{B} = \begin{bmatrix} 0 & 0 \\ 1 & 0 \\ 1 & 1 \end{bmatrix}$$

06 and for these values we get

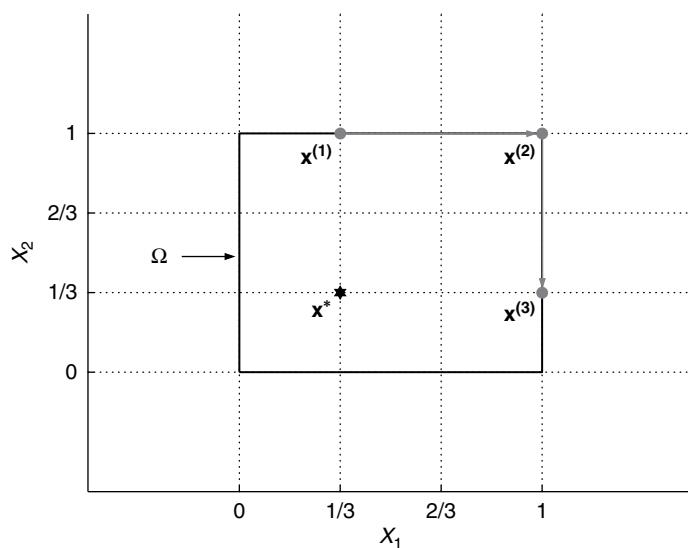
$$07 \\ 08 \quad (\Delta/2) [(2\mathbf{B} - \mathbf{J}_{k+1,k}) \mathbf{D}^* + \mathbf{J}_{k+1,k}] = \begin{bmatrix} 0 & \Delta \\ \Delta & \Delta \\ \Delta & 0 \end{bmatrix} = \begin{bmatrix} 0 & 2/3 \\ 2/3 & 2/3 \\ 2/3 & 0 \end{bmatrix}$$

11 and

$$12 \\ 13 \quad \mathbf{B}^* = \begin{bmatrix} 1/3 & 1 \\ 1 & 1 \\ 1 & 1/3 \end{bmatrix}$$

14 so that  $\mathbf{x}^{(1)} = (1/3, 1)$ ;  $\mathbf{x}^{(2)} = (1, 1)$ ;  $\mathbf{x}^{(1)} = (1, 1/3)$  (see Figure 3.3). This  
15 procedure is repeated a number of times in order to build the distributions  
16  $F_i$  and  $G_i$  for each factor.

17 Campolongo *et al.* (2007) proposed an improvement of the sampling  
18 strategy just described that facilitates a better scanning of the input domain  
19 without increasing the number of model executions needed. The idea is to  
20 select the  $r$  trajectories in such a way as to maximize their spread in the  
21



43 Figure 3.3 The trajectory obtained in Example 3.1  
44

01 input space. The design starts by generating a high number of different  
 02 trajectories, e.g.  $M \sim 500\text{--}1000$ , and then selects the subset of  $r$  (e.g.  $r =$   
 03 10, 20) with the highest spread, where the concept of *spread* is based on  
 04 the following definition of distance,  $d_{ml}$ , between a pair of trajectories  
 05  $m$  and  $l$ :

$$06 \quad d_{ml} = \begin{cases} \sum_{i=1}^{k+1} \sum_{j=1}^{k+1} \sqrt{\sum_{z=1}^k [X_z^{(i)}(m) - X_z^{(j)}(l)]^2} & m \neq l \\ 0 & \text{otherwise} \end{cases} \quad (3.3)$$

11 where  $k$  is the number of input factors and  $X_z^{(i)}(m)$  indicates the  $z$ th  
 12 coordinate of the  $i$ th point of the  $m$ th trajectory. In other words,  
 13  $d_{ml}$  is the sum of the geometric distances between all the pairs of  
 14 points of the two trajectories under analysis. The best  $r$  trajectories  
 15 from  $M$  are selected by maximizing the distance  $d_{ml}$  among them. First  
 16 we consider for each possible combination of  $r$  trajectories from  $M$   
 17 the quantity  $D^2$ , which is the sum of the squared distances between  
 18 all possible pairs of trajectories belonging to the combination. For  
 19 instance, for the combination 4, 6, 7, and 9 (i.e.  $r = 4$ ) from the possible  
 20  $M = \{1, 2, 3, 4, 5, 6, 7, 8, 9, 10\}$ , we define  $D_{4,6,7,9}$  as  
 21

$$22 \quad D_{4,6,7,9} = \sqrt{d_{4,6}^2 + d_{4,7}^2 + d_{4,9}^2 + d_{6,7}^2 + d_{6,9}^2 + d_{7,9}^2}.$$

23 Then, we consider the combination with the highest value of  $D$ , of the  
 24

$$\binom{10}{4}$$

25 possible choices of  $r = 4$  from  $M = 10$ . This sampling strategy optimizes  
 26 the scanning of the input space and is simple to implement.  
 27

### 34    3.4 THE COMPUTATION OF THE SENSITIVITY 35    MEASURES

36    HOW CAN I DEFINE A SENSITIVITY MEASURE USING THE ELEMENTARY EFFECTS?  
 37    HOW MANY LEVELS SHOULD I CHOOSE? HOW CAN I DEAL WITH NON-UNIFORM  
 38    DISTRIBUTIONS? WHAT IS THE ROLE OF  $\Delta$ ?

39    The sampling strategy described above results in the construction of  $r$   
 40    trajectories in  $\Omega$ . Each trajectory corresponds to  $(k+1)$  model executions  
 41    and allows the computation of an elementary effect for each factor  $i$ , for  
 42     $i = 1, \dots, k$ . If  $\mathbf{x}^{(l)}$  and  $\mathbf{x}^{(l+1)}$ , with  $l$  in the set  $\{1, \dots, k\}$ , are two sampling

01 points of the  $j$ th trajectory differing in their  $i$ th component, the elementary  
02 effect associated with factor  $i$  is

$$03 \\ 04 EE_i^j(\mathbf{x}^{(l)}) = \frac{[y(\mathbf{x}^{(l+1)}) - y(\mathbf{x}^{(l)})]}{\Delta} \\ 05 \\ 06$$

07 if the  $i$ th component of  $\mathbf{x}^{(l)}$  is increased by  $\Delta$ , and  
08

$$09 \\ 10 EE_i^j(\mathbf{x}^{(l+1)}) = \frac{[y(\mathbf{x}^{(l)}) - y(\mathbf{x}^{(l+1)})]}{\Delta} \\ 11 \\ 12$$

13 if the  $i$ th component of  $\mathbf{x}^{(l)}$  is decreased by  $\Delta$ . Once  $r$  elementary effects per  
14 input are available ( $EE_i^j, i = 1, 2, \dots, k, j = 1, 2, \dots, r$ ), the statistics  $\mu_i$ ,  
15  $\mu_i^*$  and  $\sigma_i^2$  relative to the distributions  $F_i$  and  $G_i$  can be computed for each  
16 factor by using the same estimators that would be used with independent  
17 random samples, as the  $r$  elementary effects belong to different trajectories  
18 and are therefore independent:  
19

$$20 \\ 21 \mu_i = \frac{1}{r} \sum_{j=1}^r EE_i^j \quad (3.4) \\ 22 \\ 23$$

$$24 \\ 25 \mu_i^* = \frac{1}{r} \sum_{j=1}^r |EE_i^j| \quad (3.5) \\ 26$$

$$27 \\ 28 \sigma_i^2 = \frac{1}{r-1} \sum_{j=1}^r (EE_i^j - \mu)^2 \quad (3.6) \\ 29$$

30 where  $EE_i^j$  indicates the elementary effects relative to factor  $i$  computed  
31 along trajectory  $j$ .  
32

33 A critical choice related to the implementation of the method is the  
34 choice of the parameters  $p$  and  $\Delta$ . The choice of  $p$  is strictly linked to  
35 the choice of  $r$ . If one considers a high value of  $p$ , thus producing a high  
36 number of possible levels to be explored, one is only seemingly enhancing  
37 the accuracy of the sampling. If this is not coupled with the choice of a  
38 high value of  $r$ , the effort will be wasted, since many possible levels will  
39 remain unexplored. In general, when the sampling size  $r$  is small, it is likely  
40 that not all possible factor levels will be explored within the experiment.  
41 For instance, in the above example, if  $r = 1$  the two factors never take the  
42 values 0 and  $2/3$ . If possible, it is convenient to choose an even value for  $p$   
43 as this affects the choice of  $\Delta$ . In fact, assuming  $p$  to be even, a convenient  
44 choice for  $\Delta$  is  $\Delta = p/[2(p-1)]$ . This choice has the advantage that the

design's sampling strategy guarantees equal-probability sampling from each  $F_i$  (for details see Morris, 1991).

The top part of Figure 3.4 (grey arrows) shows that when  $p = 4$ , the choice of  $\Delta = p/[2(p - 1)] = 2/3$  (left plot) guarantees that the four levels have equal probability of being selected. On the other hand, a choice of  $\Delta = 1/3$  (right plot) would imply that the levels  $1/3$  and  $2/3$  are sampled more often, since there are two arrays pointing there. The two histograms

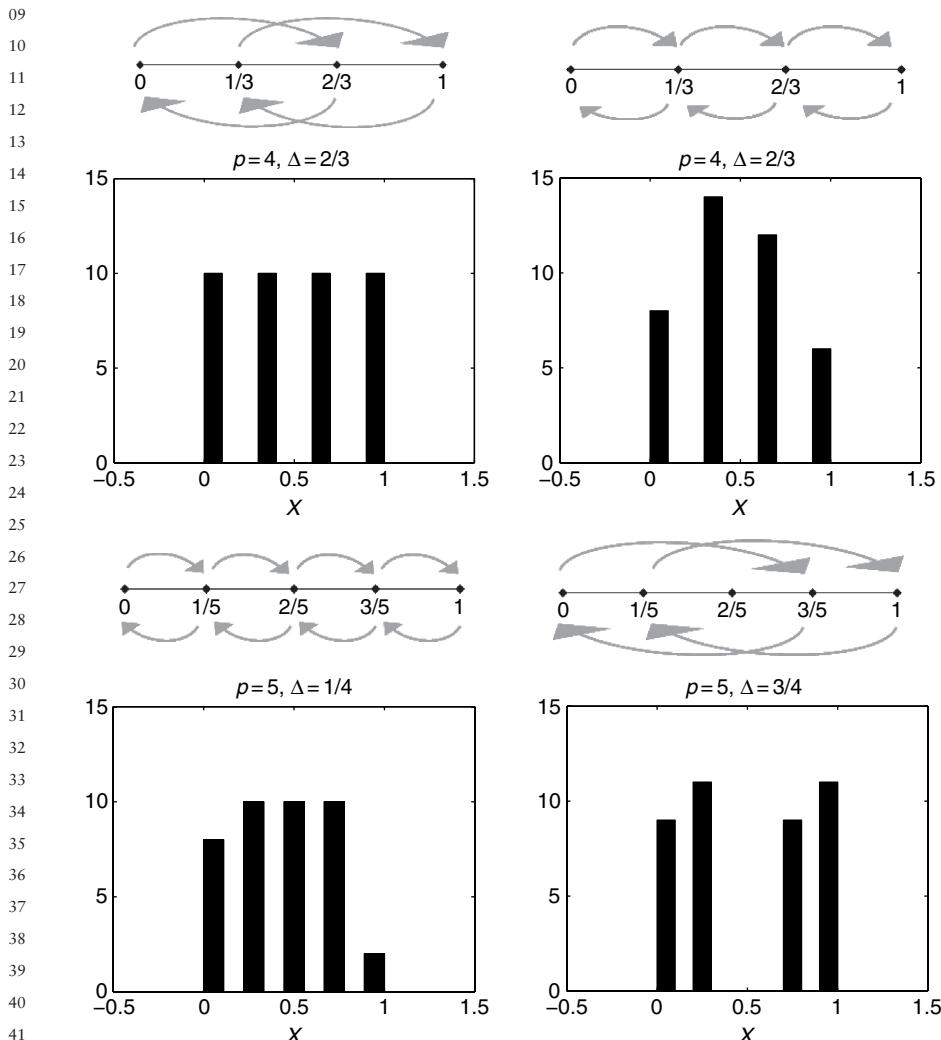


Figure 3.4 Empirical distributions obtained by choosing different values of  $p$  and  $\Delta$  and sampling  $r = 20$  trajectories

below the arrows plot the empirical distributions obtained when generating  $r = 20$  trajectories for  $p = 4$  levels, in the case of  $\Delta = 2/3$  (left plot) and  $\Delta = 1/3$  (right plot). The bottom part of the figure illustrates the case in which an odd number of levels is considered ( $p = 5$ ). Under this condition, no matter what value of  $\Delta$  is chosen, it is impossible to achieve equal probability for the elementary effects. In some cases, e.g. for  $p = 5$  and  $\Delta = 3/4$ , there are elementary effects which can never be sampled. Previous experiments (Campolongo and Saltelli, 1997; Campolongo *et al.*, 1999b; Saltelli *et al.*, 2000) have demonstrated that the choice of  $p = 4$  and  $r = 10$  has produced valuable results.

If a factor follows a uniform distribution, the levels are obtained simply by dividing into equal parts the interval in which each factor varies. If a factor follows nonuniform distributions, then input values are not sampled directly; rather, the sampling is carried out in the space of the quantiles of the distributions, which is a  $k$ -dimensional hypercube (each quantile varies in  $[0, 1]$ ). The actual factor values are then derived from its known statistical distribution (Campolongo *et al.*, 1999b). Figure 3.5 shows the case where a factor  $X$  follows a normal standard distribution and the space of quantiles is investigated via six quantiles ( $q_1, q_2, \dots, q_6$ ). Using the inverse of the normal cumulative distribution function (grey curve), corresponding levels for  $X$  are obtained ( $L_1, L_2, \dots, L_6$ ). If the distribution to be sampled has an infinite support, the quantiles to be used can be chosen for instance cutting the tails of the distribution. A good alternative is to divide the entire

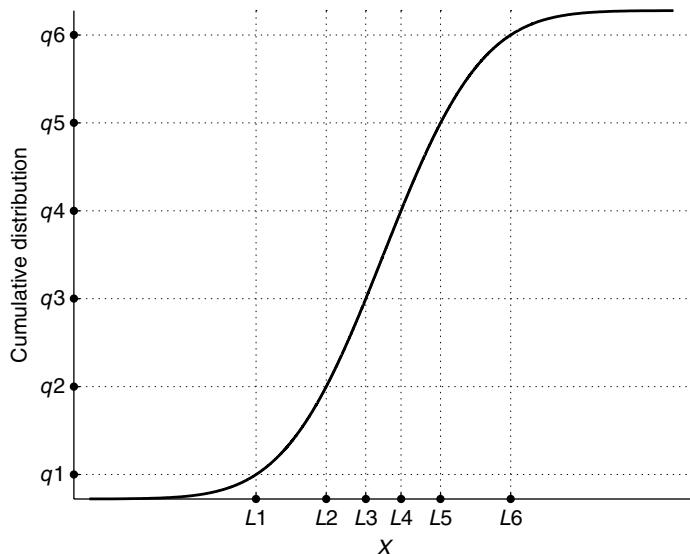


Figure 3.5 Sampling procedure for factors with standard normal distribution

support into a number of intervals equal to  $(r + 1)$  and then to use the centres of the bins (see also Section 2.3.2).

At this point, it is worth considering briefly the role of  $\Delta$ . If  $\Delta$  is chosen to be equal for all input factors, its role in the definition of the elementary effect for sensitivity purposes becomes irrelevant.  $\Delta^{-1}$  is simply a constant multiplying each elementary effect, which does not affect the sensitivity analysis results. A question may arise in the case that an input factor needs to be rescaled because its original distribution is not uniform between 0 and 1: *Should  $\Delta$  be rescaled so as to represent the actual sampling step in the factor range of variation, or should it remain the same so as to represent the sampling step between [0, 1] equal for each factor?* The following example addresses this question.

Assume the output  $Y$  is the simple function  $Y = X_1 + X_2$ , with  $X_1$  and  $X_2$  uniformly distributed in  $[0, 1]$  and  $[0, 10]$  respectively. In our sensitivity results one expects that input factor  $X_2$  is much more important than input factor  $X_1$ , since a variation in its value affects  $Y$  much more than a variation in  $X_1$ , i.e.  $X_2$  is much more uncertain than  $X_1$ . Here we consider  $p = 4$  levels,  $\Delta = 1/3$ , and  $r = 1$  trajectory, i.e. we compute just one elementary effect for each input and consider these as the final sensitivity measures. Assume that we randomly generate the following trajectory of quantiles for  $X_1$  and  $X_2$ :  $(0, 1/3); (0, 2/3); (1/3, 2/3)$ . The reader familiar with the method can easily verify that this is a typical sample. Applying the inverse cumulative function we obtain this sample for the two factors:  $(0, 10/3); (0, 20/3); (1/3, 20/3)$ . Finally, the elementary effects relative to each input are estimated as

$$EE_1(\mathbf{X}) = \frac{y(1/3, 20/3) - y(0, 20/3)}{\Delta} = \frac{1/3}{\Delta}$$

$$EE_2(\mathbf{X}) = \frac{y(0, 20/3) - y(0, 10/3)}{\Delta} = \frac{10/3}{\Delta}.$$

If in the computation of  $EE_2(\mathbf{X})$  the sampling step  $\Delta$  was rescaled and set to be equal to  $10/3$ , then both elementary effects would prove to be equal to 1, implying that both factors are to be considered equally influential in determining the value of  $Y$ . If instead  $\Delta$  is left equal to  $1/3$  for both factors, independently of the actual range of variation of factor  $X_2$ , we would obtain a sensitivity measure for  $X_2$  10 times higher than that of  $X_1$ . This second result is the correct one. In this way we are considering a sensitivity measure capable of taking into account not only the specifications of the model function, but also the effect of the statistical distributions assumed for the inputs. In general, whatever type of distribution is considered,  $\Delta$  must always represent the sampling step in the scale  $[0, 1]$ , i.e. in the case of non-uniform

distributions it should represent the variation in the quantiles of the factors.

## 05 3.5 WORKING WITH GROUPS

07 HOW CAN I EXTEND THE EE METHOD TO DEAL WITH GROUPS OF FACTORS?  
08 DOES THE SAMPLING STRATEGY CHANGE?

The EE method presented above can also be extended to work with groups using the  $\mu^*$  measure alone. When working with groups, the idea is to move all factors of the same group simultaneously. In the original definition given by Morris, the elementary effect is obtained by subtracting the function evaluated at  $\mathbf{X}$  from that evaluated after incrementing one factor see Equation (3.1). This definition cannot be extended straightforwardly to cases in which more than one factor is moved at the same time, as two factors may have been changed in opposite directions, i.e. one increased and one decreased by  $\Delta$ . By contrast, using  $\mu^*$  overcomes this problem, as the focus is not on the elementary effect itself but on its absolute value, i.e. the elementary effect is always positive, regardless of the displacement of the factors. For a two-factor group  $\mathbf{u} = (X_{i_1}, X_{i_2})$ , the absolute elementary effect in point  $\mathbf{X}$  is

$$|EE_u(\mathbf{X})| = \left| \frac{y(\tilde{\mathbf{X}}) - y(\mathbf{X})}{\Delta} \right| \quad (3.7)$$

where  $\mathbf{X}$  is any selected value in  $\Omega$  such that the transformed point  $\tilde{\mathbf{X}}$  is still in  $\Omega$ , and each of the components  $(\tilde{X}_{i_1}, \tilde{X}_{i_2})$  has been either increased or decreased by  $\Delta$  with respect to  $(X_{i_1}, X_{i_2})$ .

In order to treat groups of factors, the sampling strategy described in Section 3.3 needs to be modified slightly. It is first necessary to consider a matrix  $G$  describing how factors are allocated into groups. This matrix is defined as follows: its element  $G(i, j)$  equals 1 if factor  $i$  belongs to group  $j$ ; otherwise  $G(i, j) = 0$ . If  $g$  is the number of groups in the experiment,  $G$  has sizes  $k \times g$ . In this case the matrix of trajectories  $B^*$  has dimensions  $(g+1) \times k$ , since all the factors in a group move together.  $B^*$  can be built considering a lower triangular matrix  $B$  whose dimensions are  $(g+1) \times g$  and setting

$$\mathbf{B}^* = \mathbf{J}_{g+1,1}\mathbf{x}^* + (\Delta/2) \left[ \left( 2\mathbf{B}(\mathbf{G}\mathbf{P}^*)^T - \mathbf{J}_{g+1,k} \right) \mathbf{D}^* + \mathbf{J}_{g+1,k} \right],$$

where, similarly to the single-factor experiment,  $J_{i,j}$  is a matrix of 1's with dimensions  $(i \times j)$ ;  $D^*$  is a diagonal matrix  $(k \times k)$  describing whether the factors increase or decrease value; and  $P^*$  is a  $(g \times g)$  matrix, describing the

01 order in which the groups move. The following example illustrates how to  
 02 handle groups of factors.

05 **Example 3.2**

07 Consider three factors  $X_1, X_2$  and  $X_3$ , uniformly distributed on  $[0, 1]$ , and  
 08 assigned to a number of groups  $g = 2$ . The first group ( $G_1$ ) contains only  
 09 factor  $X_1$ ; the second ( $G_2$ ) contains the other two factors. The matrix  $\mathbf{G}$  is  
 10 therefore defined as

$$11 \quad 12 \quad 13 \quad 14 \quad \mathbf{G} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 1 \end{bmatrix}.$$

15 Consider an experiment with  $p = 4$  levels and the choice  $\Delta = 2/3$ . Suppose  
 16 we obtain the following matrices for  $\mathbf{x}^*$ ,  $\mathbf{D}^*$  and  $\mathbf{P}^*$ :

$$18 \quad 19 \quad 20 \quad 21 \quad \mathbf{x}^* = (1/3, 1/3, 0) \quad \mathbf{D}^* = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \mathbf{P}^* = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}.$$

22 In this case we get

$$24 \quad 25 \quad (\Delta/2) \left[ \left( 2\mathbf{B}(\mathbf{GP}^*)^T - \mathbf{J}_{g+1,k} \right) \mathbf{D}^* + \mathbf{J}_{g+1,k} \right] \\ 26 \quad 27 \quad = \Delta/2 \left[ \left( 2 \begin{bmatrix} 0 & 0 \\ 1 & 0 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 1 \end{bmatrix} - \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix} \right) \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} + \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix} \right] \\ 28 \quad 29 \quad 30 \quad 31 \quad 32 \quad = \begin{bmatrix} 0 & \Delta & 0 \\ \Delta & \Delta & 0 \\ \Delta & 0 & \Delta \end{bmatrix}$$

33 which makes clear that  $X_1$  (i.e.  $G_1$ ) moves first and increases in value, and  
 34 then that the factors in  $G_2$  change their values in opposite directions ( $X_2$   
 35 decreases and  $X_3$  increases). The final matrix is then:

$$37 \quad 38 \quad 39 \quad 40 \quad \mathbf{B}^* = \begin{bmatrix} 1/3 & 1 & 0 \\ 1 & 1 & 0 \\ 1 & 1/3 & 2/3 \end{bmatrix}.$$

41 Note that the two factors in the same group also take values on different  
 42 levels.

### 01           3.6 THE EE METHOD STEP BY STEP

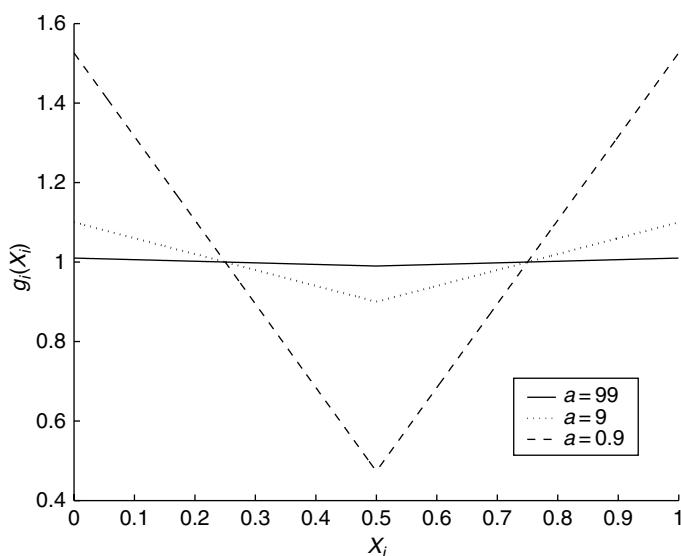
02  
 03       In this section we show how to put the EE method illustrated above into  
 04       practice. The method is tested on the analytical  $g$ -function attributed to  
 05       Sobol' (1990):

$$06 \quad Y = \prod_{i=1}^k g_i(X_i) \quad \text{where} \quad g_i(X_i) = \frac{|4X_i - 2| + a_i}{1 + a_i}$$

10       and  $a_i$  are parameters, such that  $a_i \geq 0$ . This function is widely used as  
 11       a test function in sensitivity analysis because it is a very difficult one: it  
 12       is strongly nonlinear and nonmonotonic, and all its interaction terms are  
 13       nonzero by definition. Moreover it is possible to compute analytically the  
 14       output variance decomposition and therefore the variance-based sensitivity  
 15       indices  $S_i$  and  $S_{T_i}$ . The values of the  $a_i$  determine the relative importance of  
 16       the  $X_i$  as they determine the range of variation of each  $g_i(X_i)$ :

$$17 \quad 1 - \frac{1}{1 + a_i} \leq g_i(X_i) \leq 1 + \frac{1}{1 + a_i}.$$

21       Thus, the higher the  $a_i$  value, the lower the importance of the  $X_i$  variable.  
 22       This is also shown by Figure 3.6, which illustrates the behaviour of  $g_i(X_i)$   
 23       as a function of  $X_i$  for the values of  $a_i = 0.9$ ,  $a_i = 9$  and  $a_i = 99$ .



44       Figure 3.6  $g_i(X_i)$  as a function of  $X_i$  for  $a_i = 0.9$ ,  $a_i = 9$  and  $a_i = 99$

01      The partial variances of the first order are given by  
 02  
 03       $V_i = V(E(Y|X_i)) = \frac{1}{3(1+a_i)^2}$ ,  
 04  
 05  
 06      while the higher-order partial variances are simply the product of the lower  
 07      ones, i.e.  $V_{12} = V_1 V_2$ . Finally, the total variance can be written as a function  
 08      of the first-order terms only:  
 09  
 10       $V(Y) = -1 + \prod_{i=1}^k (1 + V_i)$ .

13      This allows us to calculate analytically the first- and total-order sensitivity  
 14      indices for the  $g$ -function. In our example we assume  $k = 6$  and we set the  
 15       $a_i$  parameter values as shown in Table 3.1.

16      We now perform the sensitivity analysis by making use of the EE  
 17      method introduced in this chapter. The uncertainty in the input variables  
 18      is modelled by assuming that all the  $X_i$  are uniformly distributed in the  
 19      six-dimensional unit cube (i.e.  $X_i \sim U[0, 1], \forall i$ ). The optimized strategy  
 20      described in Section 3.3 is used to estimate the sensitivity measures  $\mu$ ,  $\mu^*$   
 21      and  $\sigma$ .  $p = 4$  levels and  $\Delta = 2/3$  are chosen;  $r = 4$  trajectories are employed,  
 22      selected out of a group of 100. The sampled input matrix is presented in  
 23      Table 3.2, columns 2–7. The last column reports the corresponding values  
 24      for the  $g$ -function. The graphs in Figure 3.7 present the scatterplots of the  
 25  
 26

27      **Table 3.1** Values of the parameters of the  $g$ -function  
 28      for each input

$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$
78	12	0.5	2	97	33

34      **Table 3.2** Sampled trajectories and corresponding  $g$ -function values

	$X_1$	$X_2$	$X_3$	$X_4$	$X_5$	$X_6$	$g$
$t_1$	0	2/3	1	0	0	1/3	2.193
	0	2/3	1	0	0	1	2.280
	0	0	1	0	0	1	2.520
	2/3	0	1	0	0	1	2.478
	2/3	0	1	2/3	0	1	1.652
	2/3	0	1/3	2/3	0	1	0.771
	2/3	0	1/3	2/3	2/3	1	0.761

01								
02		0	1/3	1/3	1	1	2/3	1.024
03		0	1	1/3	1	1	2/3	1.131
04		0	1	1	1	1	2/3	2.424
05	$t_2$	2/3	1	1	1	1	2/3	2.384
06		2/3	1	1	1	1	0	2.478
07		2/3	1	1	1	1/3	0	2.445
08		2/3	1	1	1/3	1/3	0	1.630
09		1	2/3	0	2/3	1	0	1.520
10		1	2/3	0	0	1	0	2.280
11	$t_3$	1/3	2/3	0	0	1	0	2.242
12		1/3	2/3	0	0	1/3	0	2.212
13		1/3	0	0	0	1/3	0	2.445
14		1/3	0	2/3	0	1/3	0	1.141
15		1/3	0	2/3	0	1/3	2/3	1.097
16		1	1/3	2/3	1	0	1/3	1.024
17	$t_4$	1	1/3	2/3	1	0	1	1.064
18		1	1/3	0	1	0	1	2.280
19		1	1/3	0	1/3	0	1	1.520
20		1	1/3	0	1/3	2/3	1	1.500
21		1	1	0	1/3	2/3	1	1.657
22		1/3	1	0	1/3	2/3	1	1.630

output as a function of each input. In this example, in which the number of inputs is not too large, the use of scatterplots already reveals that one factor ( $X_3$ ) plays a key role in the function. For more complex examples, in which the number of factors is larger, the use of scatterplots is cumbersome.

As an example, Table 3.3 shows how to estimate the sensitivity measures for factor  $X_4$ . The values of  $\mu$ ,  $\mu^*$  and  $\sigma$  are reported in Table 3.4. Results indicate that  $X_3$  and  $X_4$  are important factors, while factors  $X_1$ ,  $X_5$  and  $X_6$  can be regarded as noninfluential (see the  $\mu^*$  values in the first column). The high values of  $\sigma$  for some factors also demonstrate that interactions play an important role in the model. Moreover, the low values of  $\mu$  associated with high values of  $\mu^*$  indicate that factors have effects of oscillating signs. Figure 3.8 shows in a barplot the values of  $\mu^*$  in increasing order. It is clear that in this example,  $\mu^*$  alone can be used to assess the importance of each factor of the model. These results can be used to fix unimportant factors in the model (the *Factor Fixing* setting, see also Chapters 1 and 4). The extremely low values of  $\mu^*$  for  $X_1$  and  $X_5$  show that these factors can be fixed without affecting the variance of  $g$  to a great extent. On the other hand, it is clear that factors  $X_3$  and  $X_4$  cannot be fixed. The remaining factors ( $X_2$  and  $X_6$ ) stay in-between. The decision to fix them or not depends on how much importance is assigned to type II errors.

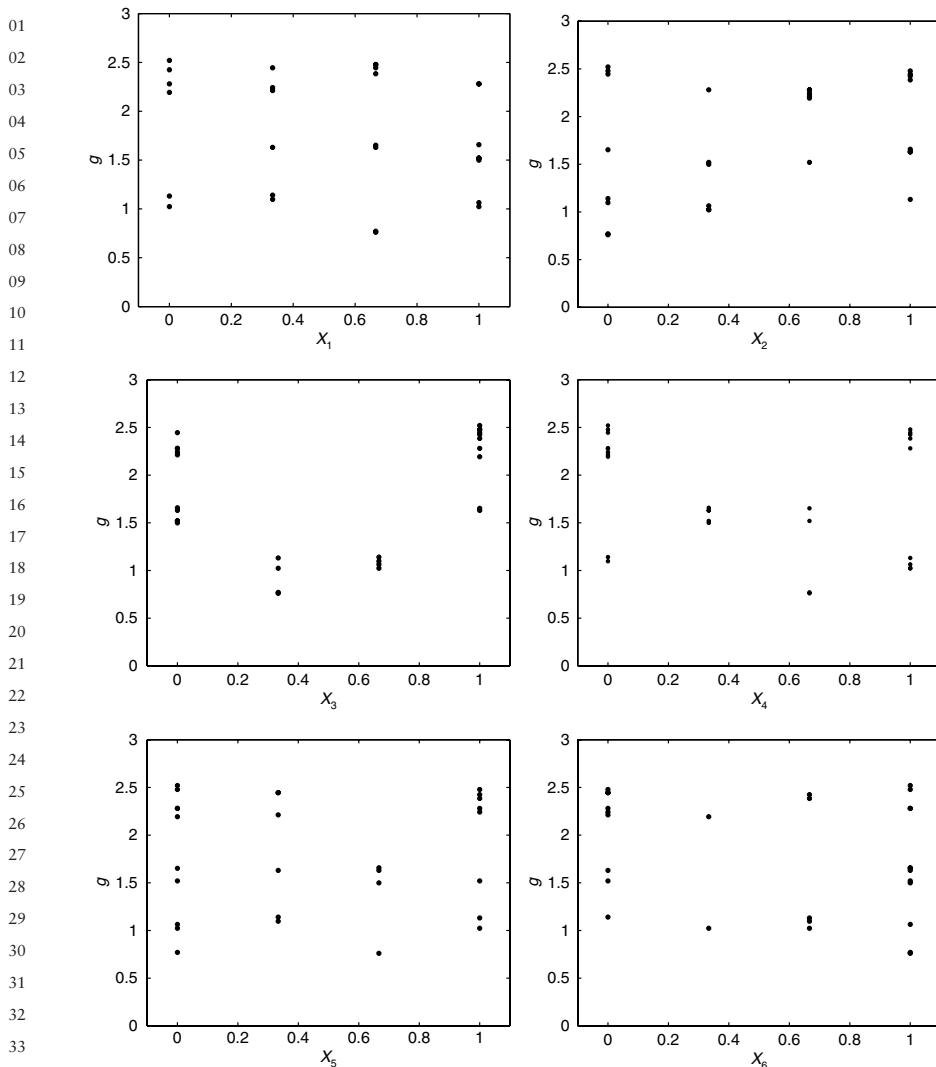


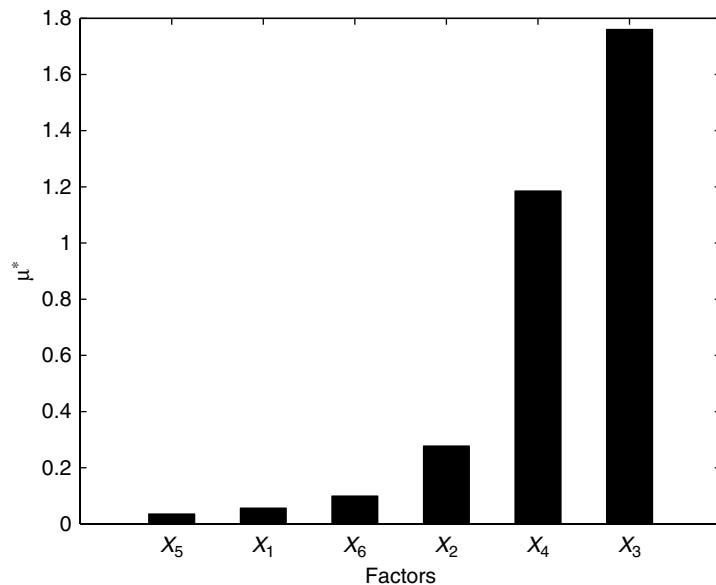
Figure 3.7 Scatterplot of the  $g = \prod_{i=1}^k g_i(X_i)$  as a function of each input

Table 3.3 Estimation of the distribution of the elementary effects (and their absolute values) for factor  $X_4$

	$g(X_1, \dots, X_4 + \Delta, \dots, X_6)$	$g(X_1, \dots, X_4, \dots, X_6)$	$EE_4(\mathbf{X})$	$ EE_4(\mathbf{X}) $
$t_1$	1.652	2.478	-1.239	1.239
$t_2$	2.445	1.630	1.222	1.222
$t_3$	1.520	2.280	-1.140	1.140
$t_4$	2.280	1.520	1.140	1.140

Table 3.4 Estimated sensitivity measures. The measures are estimated using  $r = 4$  trajectories

	$\mu^*$	$\mu$	$\sigma$
$X_1$	0.056	-0.006	0.064
$X_2$	0.277	-0.078	0.321
$X_3$	1.760	-0.130	2.049
$X_4$	1.185	-0.004	1.370
$X_5$	0.035	0.012	0.041
$X_6$	0.099	-0.004	0.122



**Figure 3.8** Barplot of  $\mu^*$  for the  $g$ -function

### 3.7 CONCLUSIONS

The EE method illustrated in this chapter is effective in identifying the few important factors in a model that contains many factors, with a relatively small number of model evaluations. The method is convenient when the number of factors is large and/or the model execution time is such that the computational cost of more sophisticated techniques is excessive, but not large enough to oblige the modeller to make use of grouping techniques.

With respect to a group technique, the EE method has the advantage of examining each factor individually so as to prevent cancellation effects and to offer a well-defined strategy to assess the importance of each individual factor. The method is conceptually simple. It can be thought of as an expansion of a derivative-based approach: when a single trajectory is considered, and the variations of input factors are small, it reduces to a incremental ratio estimation. Nevertheless, it overcomes the limitations of a local derivative-based approach in that it attempts to explore the whole input space. The method is computationally easy and has the flexibility typical of OAT approaches in handling unstable models. When a model is unstable it threatens to crash if executed on a set of input values rather different from the nominal values on which it was calibrated. Similarly to OAT designs, which allow for the substitution of a sample point when the model fails, without changing the full design, the EE method, being based on trajectories independent of one another, allows for the substitution of a trajectory on which the model execution fails with another one better handled by the model. Last but not least, when necessary, the method can be applied to groups, thus increasing the efficiency of the design.

### 3.8 EXERCISES

1. Given three input factors,  $X_1$ ,  $X_2$  and  $X_3$ , all uniformly distributed in  $[0, 1]$ , build some examples of trajectories for  $p = 4$ ,  $p = 6$ , and  $p = 8$ .
2. Given three input factors,  $X_1$ ,  $X_2$  and  $X_3$ , all normally distributed with mean 0 and variance 1, build an example of trajectories for  $p = 6$  levels (consider cutting the tails at quantiles 0.5 and 99.5%, or using the centres of the bins as described in Section 2.4.3).
3. Consider two input factors,  $X_1$  and  $X_2$ , uniformly distributed in  $[0, 1]$  and a number of levels  $p = 4$ .
  - (a) Following the revised sampling strategy, generate randomly a number  $M = 6$  of trajectories and then select, according to the approach described in Section 3.3, the best four out of six.
  - (b) Show by means of graphical representation that the new strategy outperforms the old one in terms of input-space scanning
4. As a follow-up to Exercise 3, given the model

$$y = \sin(\pi X_1) + \cos(\pi X_2/4) + \sqrt{X_1 X_2},$$

make use of the full set of  $M = 6$  trajectories and compute the sensitivity measures  $\mu$ ,  $\mu^*$  and  $\sigma$  for the two input factors  $X_1$  and  $X_2$ .

- 01       5. Consider a model with 15 input factors with standard normal distribution, i.e.  $X_i \sim N(0, 1)$ . Consider the function (Oakley and O'Hagan, 2004)

04                   $y = \mathbf{a}_1^T + \mathbf{a}_2^T \cos(\mathbf{X}) + \mathbf{a}_3^T \sin(\mathbf{X}) + \mathbf{X}^T \mathbf{M} \mathbf{X}$

06                  where  $\mathbf{a}_j$ , ( $j = 1, 2, 3$ ) and  $\mathbf{M}$  are respectively three vectors and a matrix of parameters, whose values are reported in Tables 3.5 and 3.6. Consider cutting the tails of the normal distributions at quantiles 5 and 95%. For this model estimate the sensitivity measures  $\mu^*$ ,  $\mu$ .

- 10       6. As a follow-up to Exercise 5, group the 15 factors into the two groups described by the matrix  $\mathbf{G}$  below and compute the sensitivity measures for the groups using  $r = 10$  trajectories.

14                  
$$\mathbf{G}^T = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

- 17       7. Consider the function introduced by Morris (1991):

19                  
$$y = \beta_0 + \sum_{i=1}^{20} \beta_i \omega_i + \sum_{i < j}^{20} \beta_{i,j} \omega_i \omega_j + \sum_{i < j < l}^{20} \beta_{i,j,l} \omega_i \omega_j \omega_l + \sum_{i < j < l < s}^{20} \beta_{i,j,l,s} \omega_i \omega_j \omega_l \omega_s$$

22                  where  $\omega_i = 2(X_i - 1/2)$  except for  $i = 3, 5$ , and  $7$ , where

24                  
$$\omega_i = 2(1.1X_i / (X_i + 0.1) - 1/2).$$

27                  **Table 3.5** Vectors of parameters for the Oakley–O'Hagan  
28                  function

<i>Factor</i>	$a_1$	$a_2$	$a_3$
$X_1$	0.01	0.43	0.10
$X_2$	0.05	0.09	0.21
$X_3$	0.23	0.05	0.08
$X_4$	0.04	0.32	0.27
$X_5$	0.12	0.15	0.13
$X_6$	0.39	1.04	0.75
$X_7$	0.39	0.99	0.86
$X_8$	0.61	0.97	1.03
$X_9$	0.62	0.90	0.84
$X_{10}$	0.40	0.81	0.80
$X_{11}$	1.07	1.84	2.21
$X_{12}$	1.15	2.47	2.04
$X_{13}$	0.79	2.39	2.40
$X_{14}$	1.12	2.00	2.05
$X_{15}$	1.20	2.26	1.98

44 01  
43 02  
42 03  
41 04  
40 05  
39 06  
38 07  
37 08  
36 09  
35 10  
34 11  
33 12  
32 13  
31 14  
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**Table 3.6** Matrix of parameters for the Oakley–O'Hagan function

	$X_1$	$X_2$	$X_3$	$X_4$	$X_5$	$X_6$	$X_7$	$X_8$	$X_9$	$X_{10}$	$X_{11}$	$X_{12}$	$X_{13}$	$X_{14}$	$X_{15}$
$X_1$	-0.02	-0.19	0.13	0.37	0.17	0.14	-0.44	-0.08	0.71	-0.44	0.5	-0.02	-0.05	0.22	0.06
$X_2$	0.26	0.05	0.26	0.24	-0.59	-0.08	-0.29	0.42	0.5	0.08	-0.11	0.03	-0.14	-0.03	-0.22
$X_3$	-0.06	0.2	0.1	-0.29	-0.14	0.22	0.15	0.29	0.23	-0.32	-0.29	-0.21	0.43	0.02	0.04
$X_4$	0.66	0.43	0.3	-0.16	-0.31	-0.39	0.18	0.06	0.17	0.13	-0.35	0.25	-0.02	0.36	-0.33
$X_5$	-0.12	0.12	0.11	0.05	-0.22	0.19	-0.07	0.02	-0.1	0.19	0.33	0.31	-0.08	-0.25	0.37
$X_6$	-0.28	-0.33	-0.1	-0.22	-0.14	-0.14	-0.12	0.22	-0.03	-0.52	0.02	0.04	0.36	0.31	0.05
$X_7$	-0.08	0.004	0.89	-0.27	-0.08	-0.04	-0.19	-0.36	-0.17	0.09	0.4	-0.06	0.14	0.21	-0.01
$X_8$	-0.09	0.59	0.03	-0.03	-0.24	-0.1	0.03	0.1	-0.34	0.01	-0.61	0.08	0.89	0.14	0.15
$X_9$	-0.13	0.53	0.13	0.05	0.58	0.37	0.11	-0.29	-0.57	0.46	-0.09	0.14	-0.39	-0.45	-0.15
$X_{10}$	0.06	-0.32	0.09	0.07	-0.57	0.53	0.24	-0.01	0.07	0.08	-0.13	0.23	0.14	-0.45	-0.56
$X_{11}$	0.66	0.35	0.14	0.52	-0.28	-0.16	-0.07	-0.2	0.07	0.23	-0.04	-0.16	0.22	0	-0.09
$X_{12}$	0.32	-0.03	0.13	0.13	0.05	-0.17	0.18	0.06	-0.18	-0.31	-0.25	0.03	-0.43	-0.62	-0.03
$X_{13}$	-0.29	0.03	0.03	-0.12	0.03	-0.34	-0.41	0.05	-0.27	-0.03	0.41	0.27	0.16	-0.19	0.02
$X_{14}$	-0.24	-0.44	0.01	0.25	0.07	0.25	0.17	0.01	0.25	-0.15	-0.08	0.37	-0.3	0.11	-0.76
$X_{15}$	0.04	-0.26	0.46	-0.36	-0.95	-0.17	0.003	0.05	0.23	0.38	0.46	-0.19	0.01	0.17	0.16

01      Each input factor  $X_i$  is uniformly distributed in  $[0, 1]$ . Coefficients with  
 02      relatively large values are:  $\beta_i = 20$ ,  $i = 1, \dots, 10$ ;  $\beta_{i,j} = -15$ ,  $i, j =$   
 03       $1, \dots, 6$ ;  $\beta_{i,j,l} = -10$ ,  $i, j, l = 1, \dots, 5$ ;  $\beta_{i,j,l,s} = 5$ ,  $i, j, l, s = 1, \dots, 4$ . The  
 04      remaining first- and second-order coefficients are independently gener-  
 05      ated from a normal distribution with zero mean and unit standard  
 06      deviation. The remaining third- and fourth-order coefficients are set  
 07      to zero. For this test case, estimate the sensitivity analysis measures  
 08       $\mu^*$ ,  $\mu$  and  $\sigma$  using the optimized sampling strategy with  $r = 10$   
 09      trajectories and discuss the results, considering also the structure of  
 10      the function  $y$ .

11      8. As a follow-up to Exercise 7, group the 20 factors into  $g = 4$  groups  
 12      described by the matrix  $\mathbf{G}$  below and compute the sensitivity measures  
 13      for the groups using  $r = 10$  trajectories. Discuss the results, using the  
 14      sensitivity information from Exercise 7.

$$\mathbf{G}^T = \begin{bmatrix} 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \end{bmatrix}.$$

### 3.9 SOLUTIONS

1. We treat separately the three cases  $p = 4, 6, 8$ .

- **Number of levels  $p = 4$**

The levels are  $\{0, 1/3, 2/3, 1\}$ . Consider the optimal value for  $\Delta$ , which is  $\Delta = 2/3$ , and suppose that the randomly generated  $\mathbf{x}^*$ ,  $\mathbf{D}^*$  and  $\mathbf{P}^*$  are

$$\mathbf{x}^* = [0, 1/3, 1/3] \quad \mathbf{D}^* = \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \mathbf{P}^* = \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}.$$

For these values,

$$(\Delta/2) [(2\mathbf{B} - \mathbf{J}_{k+1,k}) \mathbf{D}^* + \mathbf{J}_{k+1,k}] = \begin{bmatrix} \Delta & 0 & 0 \\ 0 & 0 & 0 \\ 0 & \Delta & 0 \\ 0 & \Delta & \Delta \end{bmatrix}$$

and then

$$\mathbf{B}^* = \begin{bmatrix} 1/3 & 1/3 & 2/3 \\ 1/3 & 1/3 & 0 \\ 1 & 1/3 & 0 \\ 1 & 1 & 0 \end{bmatrix}.$$

The trajectory obtained is  $\mathbf{x}^{(1)} = (1/3, 1/3, 2/3); \mathbf{x}^{(2)} = (1/3, 1/3, 0); \mathbf{x}^{(3)} = (1, 1/3, 0); \mathbf{x}^{(4)} = (1, 1, 0)$ .

- **Number of levels  $p = 6$**

The levels are  $\{0, 1/5, 2/5, 3/5, 4/5, 1\}$ . Suppose that  $\Delta = 3/5$ , and suppose that the randomly generated  $\mathbf{x}^*$ ,  $\mathbf{D}^*$  and  $\mathbf{P}^*$  are  $\mathbf{x}^* = [0, 1/5, 2/5];$

$$\mathbf{D}^* = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \quad \mathbf{P}^* = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}.$$

For these values,

$$(\Delta/2) [(2\mathbf{B} - \mathbf{J}_{k+1,k}) \mathbf{D}^* + \mathbf{J}_{k+1,k}] = \begin{bmatrix} \Delta & \Delta & \Delta \\ 0 & \Delta & \Delta \\ 0 & 0 & \Delta \\ 0 & 0 & 0 \end{bmatrix}$$

and then

$$\mathbf{B}^* = \begin{bmatrix} 1 & 3/5 & 4/5 \\ 1 & 0 & 4/5 \\ 1 & 0 & 1/5 \\ 2/5 & 0 & 1/5 \end{bmatrix}.$$

The trajectory obtained is  $\mathbf{x}^{(1)} = (1, 3/5, 4/5); \mathbf{x}^{(2)} = (1, 0, 4/5); \mathbf{x}^{(3)} = (1, 0, 1/5); \mathbf{x}^{(4)} = (2/5, 0, 1/5)$ .

- **Number of levels  $p = 8$**

The levels are  $\{0, 1/7, 2/7, 3/7, 4/7, 5/7, 6/7, 1\}$ . Suppose that  $\Delta = 3/7$ , and suppose that the randomly generated  $\mathbf{x}^*$ ,  $\mathbf{D}^*$  and  $\mathbf{P}^*$  are  $\mathbf{x}^* = [1/7, 3/7, 2/7];$

$$\mathbf{D}^* = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \quad \mathbf{P}^* = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}.$$

For these values,

$$(\Delta/2) [(2\mathbf{B} - \mathbf{J}_{k+1,k}) \mathbf{D}^* + \mathbf{J}_{k+1,k}] = \begin{bmatrix} 0 & 0 & \Delta \\ \Delta & 0 & \Delta \\ \Delta & \Delta & \Delta \\ \Delta & \Delta & 0 \end{bmatrix}$$

01           and then

$$02 \quad 03 \quad 04 \quad 05 \quad \mathbf{B}^* = \begin{bmatrix} 1/7 & 5/7 & 3/7 \\ 4/7 & 5/7 & 3/7 \\ 4/7 & 5/7 & 6/7 \\ 4/7 & 2/7 & 6/7 \end{bmatrix}.$$

06           The trajectory obtained is  $\mathbf{x}^{(1)} = (1/7, 5/7, 3/7); \mathbf{x}^{(2)} =$   
 07            $(4/7, 5/7, 3/7); \mathbf{x}^{(3)} = (4/7, 5/7, 6/7); \mathbf{x}^{(4)} = (4/7, 2/7, 6/7)$ .

09           **2. • Cut off the tails**

11           Since the factors are not uniformly distributed, the quantiles are first  
 12           sampled and the corresponding values for the factors are obtained  
 13           subsequently. In this exercise we cut 0.5% of the distribution in each  
 14           tail. We first sample the quantiles:

$$15 \quad \{0.0, 0.2, 0.4, 0.6, 0.8, 1.0\}.$$

17           Suppose that  $\Delta = 0.6$  and that the randomly generated  $\mathbf{x}^*$ ,  $\mathbf{D}^*$  and  
 18            $\mathbf{P}^*$  are

$$20 \quad 21 \quad 22 \quad 23 \quad \mathbf{x}^* = [0.2, 0.4, 0.4] \quad \mathbf{D}^* = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \quad \mathbf{P}^* = \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}.$$

24           For these values,

$$26 \quad 27 \quad 28 \quad 29 \quad \mathbf{B}^* = \begin{bmatrix} 1.0 & 1.0 & 0.2 \\ 1.0 & 1.0 & 0.8 \\ 0.4 & 1.0 & 0.8 \\ 0.4 & 0.4 & 0.8 \end{bmatrix}.$$

30           To cut the tails, we rescale these values in the range [0.005, 0.995],  
 31           thus obtaining

$$33 \quad 34 \quad 35 \quad 36 \quad \mathbf{B}^* = \begin{bmatrix} 0.995 & 0.995 & 0.203 \\ 0.995 & 0.995 & 0.797 \\ 0.401 & 0.995 & 0.797 \\ 0.401 & 0.401 & 0.797 \end{bmatrix}.$$

37           Finally, by applying the inverse normal cumulative function  $\Phi^{-1}$ , the  
 38           final values for the factors are obtained:

$$40 \quad 41 \quad 42 \quad 43 \quad \Phi^{-1}\mathbf{B}^* = \begin{bmatrix} 2.576 & 2.576 & -0.831 \\ 2.576 & 2.576 & 0.831 \\ -0.251 & 2.576 & 0.831 \\ -0.251 & -0.251 & 0.831 \end{bmatrix}.$$

01     • Centres of bins

02     In this case we divide the interval  $[0, 1]$  into six subintervals and we  
03     consider the centres of the bins as levels:

04

$$05 \quad \{0.083, 0.250, 0.417, 0.583, 0.750, 0.917\}.$$

06

07     Suppose that  $\Delta = 0.5$ ,  $x^* = [0.083, 0.417, 0.250]$ , and that the  
08     randomly generated  $D^*$  and  $P^*$  are as above. Then we obtain

09

$$10 \quad B^* = \begin{bmatrix} 0.917 & 0.750 & 0.083 \\ 0.917 & 0.750 & 0.583 \\ 0.417 & 0.750 & 0.583 \\ 0.417 & 0.250 & 0.583 \end{bmatrix}.$$

11

12     By applying the inverse normal cumulative function  $\Phi^{-1}$ , the corre-  
13     sponding values for the factors are obtained:

14

$$15 \quad \Phi^{-1}B^* = \begin{bmatrix} 1.383 & 0.675 & -1.383 \\ 1.383 & 0.675 & 0.210 \\ -0.210 & 0.675 & 0.210 \\ -0.210 & -0.675 & 0.210 \end{bmatrix}.$$

16

17     3. (a) Consider generating the following six trajectories:

18

$$19 \quad B_1^* = \begin{bmatrix} 0 & 1/3 \\ 0 & 1 \\ 2/3 & 1 \end{bmatrix} \quad B_2^* = \begin{bmatrix} 0 & 1/3 \\ 2/3 & 1/3 \\ 2/3 & 1 \end{bmatrix} \quad B_3^* = \begin{bmatrix} 2/3 & 0 \\ 2/3 & 2/3 \\ 0 & 2/3 \end{bmatrix}$$

20

$$21 \quad B_4^* = \begin{bmatrix} 1/3 & 1 \\ 1 & 1 \\ 1 & 1/3 \end{bmatrix} \quad B_5^* = \begin{bmatrix} 1/3 & 1 \\ 1/3 & 1/3 \\ 1 & 1/3 \end{bmatrix} \quad B_6^* = \begin{bmatrix} 1/3 & 2/3 \\ 1/3 & 0 \\ 1 & 0 \end{bmatrix}.$$

22

23     Following the notation introduced in Section 3.3, we denote with  
24      $X_z^{(i)}(m)$  the  $z$ -component ( $z = 1, 2$ ) of the  $i$ th point ( $i = 1, 2, 3$ ) of  
25     the  $m$ th trajectory ( $m = 1, 2, \dots, 6$ ). We show, for instance, how to  
26     calculate the distance between trajectories  $B_1^*$  and  $B_3^*$ :

27

$$28 \quad EE_{13} = \sqrt{\left[ X_1^{(1)}(1) - X_1^{(1)}(3) \right]^2 + \left[ X_2^{(1)}(1) - X_2^{(1)}(3) \right]^2}$$

29

$$30 \quad + \sqrt{\left[ X_1^{(1)}(1) - X_1^{(2)}(3) \right]^2 + \left[ X_2^{(1)}(1) - X_2^{(2)}(3) \right]^2}$$

31

$$32 \quad + \sqrt{\left[ X_1^{(1)}(1) - X_1^{(3)}(3) \right]^2 + \left[ X_2^{(1)}(1) - X_2^{(3)}(3) \right]^2}$$

33

$$\begin{aligned}
& + \sqrt{\left[ X_1^{(2)}(1) - X_1^{(1)}(3) \right]^2 + \left[ X_2^{(2)}(1) - X_2^{(1)}(3) \right]^2} \\
& + \sqrt{\left[ X_1^{(2)}(1) - X_1^{(2)}(3) \right]^2 + \left[ X_2^{(2)}(1) - X_2^{(2)}(3) \right]^2} \\
& + \sqrt{\left[ X_1^{(2)}(1) - X_1^{(3)}(3) \right]^2 + \left[ X_2^{(2)}(1) - X_2^{(3)}(3) \right]^2} \\
& + \sqrt{\left[ X_1^{(3)}(1) - X_1^{(1)}(3) \right]^2 + \left[ X_2^{(3)}(1) - X_2^{(1)}(3) \right]^2} \\
& + \sqrt{\left[ X_1^{(3)}(1) - X_1^{(2)}(3) \right]^2 + \left[ X_2^{(3)}(1) - X_2^{(2)}(3) \right]^2} \\
& + \sqrt{\left[ X_1^{(3)}(1) - X_1^{(3)}(3) \right]^2 + \left[ X_2^{(3)}(1) - X_2^{(3)}(3) \right]^2} \\
& = \sqrt{(2/3)^2 + (1/3)^2} + \sqrt{(2/3)^2 + (1/3)^2} + \sqrt{(1/3)^2} \\
& + \sqrt{(2/3)^2} + \sqrt{(2/3)^2 + (1)^2} + \sqrt{(2/3)^2 + (1/3)^2} \\
& + \sqrt{(1/3)^2} + \sqrt{(1)^2} + \sqrt{(1/3)^2} + \sqrt{(2/3)^2 + (1/3)^2} \\
& = 6.18.
\end{aligned}$$

The complete matrix of distances obtained by applying the definition of distance between each pair of the sampled trajectories (see Equation (3.3)) is

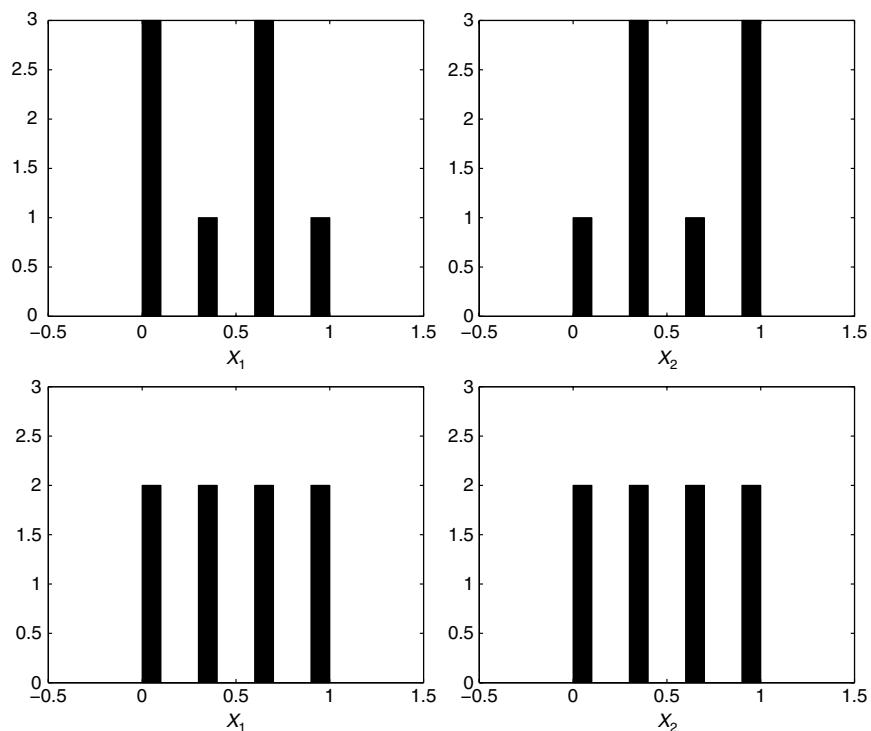
$$d_{ml} = \begin{bmatrix} 0.00 & & & & & \\ 5.50 & 0.00 & & & & \\ 6.18 & 5.31 & 0.00 & & & \\ 6.89 & 6.18 & 6.57 & 0.00 & & \\ 6.18 & 5.31 & 5.41 & 5.50 & 0.00 & \\ 7.52 & 5.99 & 5.52 & 7.31 & 5.77 & 0.00 \end{bmatrix}.$$

To select the optimal set of trajectories it is necessary to consider all the possible combinations of four trajectories out of six and to evaluate the squared root of the sum of their squared distances,  $D$ . Table 3.7 shows the possible combinations for the present exercises. The optimal set of trajectories is  $\mathbf{B}_1^*, \mathbf{B}_3^*, \mathbf{B}_4^*, \mathbf{B}_6^*$ .

- (b) Figure 3.9 shows the histograms of the values sampled for  $X_1$  and  $X_2$  when using the optimal trajectories scheme (bottom plot) and the original trajectories scheme (top plot), assuming that the original scheme would have taken the first four generated (i.e.  $\mathbf{B}_1^*, \mathbf{B}_2^*$ ,

01           **Table 3.7** Possible combinations of four trajectories out of six and corresponding  
 02           values of the measure used to identify the optimal set

<i>Trajectories {i, j, l, m}</i>	<i>D</i>	<i>Trajectories {i, j, l, m}</i>	<i>D</i>
1-2-3-4	15.022	1-3-5-6	15.685
1-2-3-5	13.871	1-4-5-6	16.098
1-2-3-6	14.815	2-3-4-5	14.049
1-2-4-5	14.582	2-3-4-6	15.146
1-2-4-6	16.178	2-3-5-6	14.333
1-2-5-6	14.912	2-4-5-6	14.807
1-3-4-5	15.055	3-4-5-6	14.825
1-3-4-6	16.410		



37           **Figure 3.9** Original (top plots) versus optimized (bottom plots) sampled distribu-  
 38           tions obtained in Exercise 3

40  
 41           **B\***<sub>3</sub> and **B\***<sub>4</sub>). Figure 3.10 plots the paths of the original (top plot)  
 42           and optimized (bottom plot) trajectories. The optimized strategy has  
 43           produced a better sample, in terms of both the level explored (the  
 44

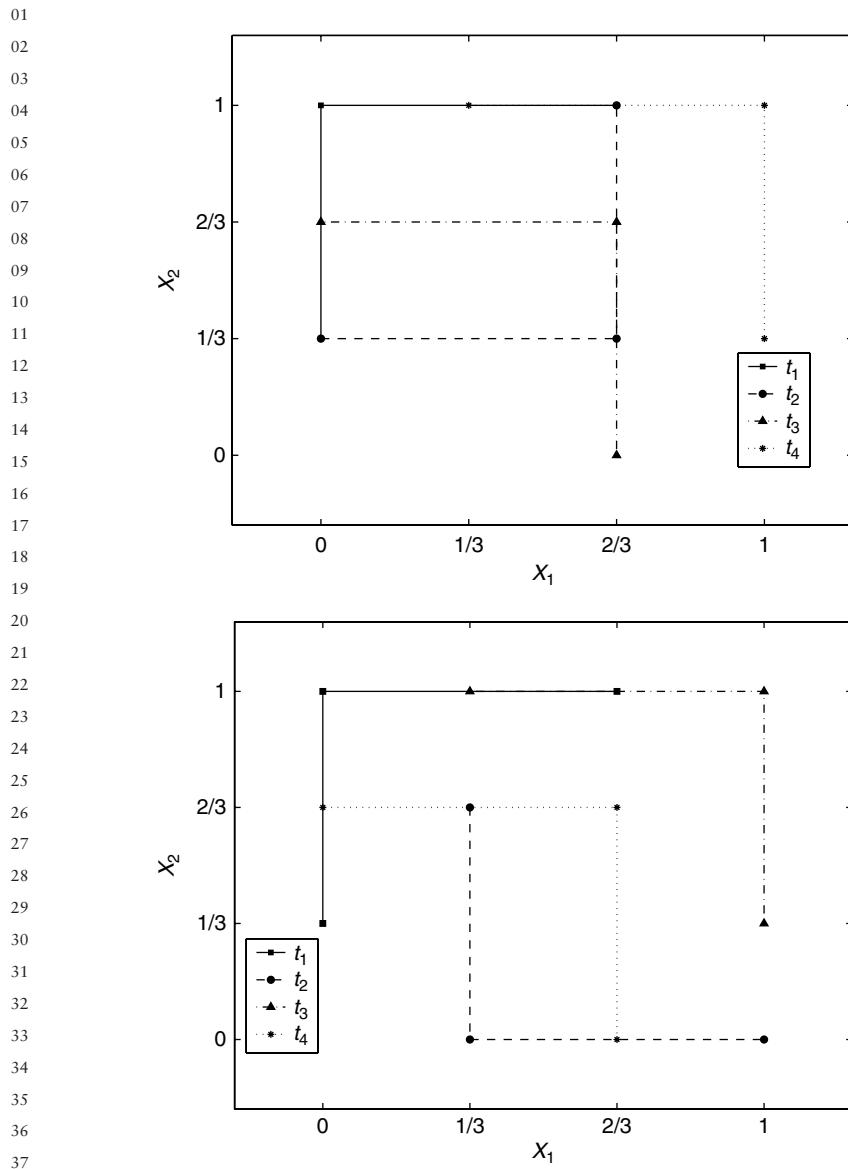


Figure 3.10 Original (top plot) versus optimized (bottom plot) paths of sampled trajectories for Exercise 3

sampled distributions match the theoretical ones) and the spread of the trajectories.

4. Given the values of the sampled inputs, the corresponding values for the output are reported in Table 3.8. The plots in Figure 3.11 show the output as a function of  $X_1$  (top plot) and  $X_2$  (bottom plot).

To compute the sensitivity measures  $\mu$ ,  $\mu^*$  and  $\sigma$  we estimate the elementary effects of  $X_1$  and  $X_2$  and their absolute values on each trajectory, which are shown in Table 3.9. The measures  $\mu$  and  $\sigma$  are the mean and the standard deviation of these elementary effects:

$$\mu(X_1) = \frac{2.52 + 2.01 + 2.30 - 0.66 - 0.93 - 1.30}{6} = 0.66$$

$$\sigma(X_1) = \sqrt{\frac{(2.52 - 0.66)^2 + 1.35^2 + 1.64^2 + (-1.32)^2 + (-1.59)^2 + (-1.96)^2}{5}} = 1.79$$

$$\mu(X_2) = \frac{-0.39 + 0.13 + 0.80 + 0.25 - 0.02 + 0.51}{6} = 0.21$$

$$\sigma(X_2) = \sqrt{\frac{(-0.6)^2 + (-0.08)^2 + 0.59^2 + 0.03^2 + (-0.23)^2 + 0.30^2}{5}} = 0.41$$

**Table 3.8** Sample and output values for Exercise 4 in the case of  $r = 6$  trajectories

	$X_1$	$X_2$	Y
$t_1$	0	1/3	0.97
	0	1	0.71
	2/3	1	2.39
$t_2$	0	1/3	0.97
	2/3	1/3	2.30
	2/3	1	2.39
$t_3$	2/3	0	1.87
	2/3	2/3	2.40
	0	2/3	0.87
$t_4$	1/3	1	2.15
	1	1	1.71
	1	1/3	1.54
$t_5$	1/3	1	2.15
	1/3	1/3	2.17
	1	1/3	1.54
$t_6$	1/3	2/3	2.20
	1/3	0	1.87
	1	0	1.00

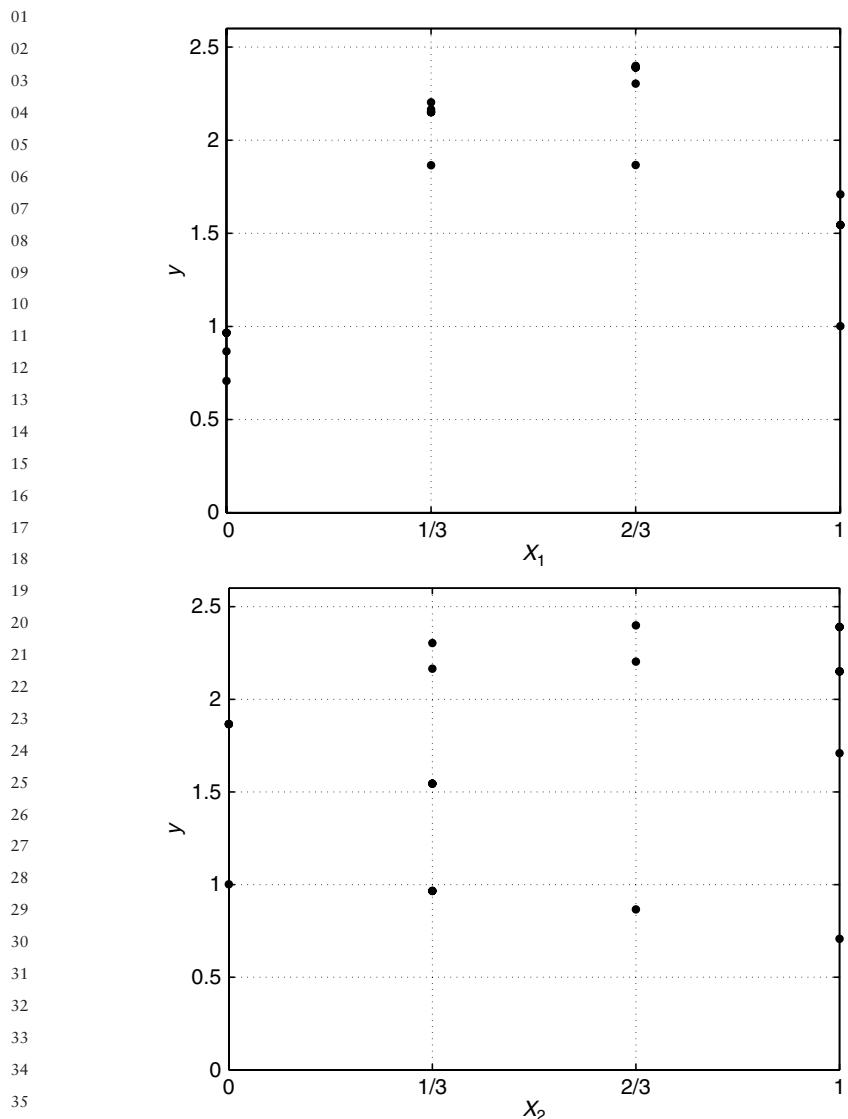


Figure 3.11 Scatterplots of  $y = \sin(\pi X_1) + \cos(\pi X_2/4) + \sqrt{X_1 X_2}$  as a function of  $X_1$  (top plot) and  $X_2$  (bottom plot)

01                   **Table 3.9** Computation of the elementary effects and  
 02                   their absolute values for Exercise 4

		$y(X_i + \Delta, X_j)$	$y(X_i, X_j)$	$EE_i(\mathbf{X})$	$ EE_i(\mathbf{X}) $
$X_1$	$t_1$	2.39	0.71	2.52	2.52
	$t_2$	2.30	0.97	2.01	2.01
	$t_3$	2.40	0.87	2.30	2.30
	$t_4$	1.71	2.15	-0.66	0.66
	$t_5$	1.54	2.17	-0.93	0.93
	$t_6$	1.00	1.87	-1.30	1.3
$X_2$	$t_1$	0.71	0.97	-0.39	0.39
	$t_2$	2.39	2.30	0.13	0.13
	$t_3$	2.40	1.87	0.80	0.80
	$t_4$	1.71	1.54	0.25	0.25
	$t_5$	2.15	2.17	-0.02	0.02
	$t_6$	2.20	1.87	0.51	0.51

17                    $\mu^*$  is instead the mean of the absolute values of these elementary effects:

$$20 \quad \mu^*(X_1) = \frac{2.52 + 2.01 + 2.30 + 0.66 + 0.93 + 1.30}{6} = 1.62$$

$$22 \quad \mu^*(X_2) = \frac{0.39 + 0.13 + 0.80 + 0.25 + 0.02 + 0.51}{6} = 0.35.$$

24                   Both values of  $\mu^*$  and  $\sigma$  show that factor  $X_1$  is unequivocally more  
 25                   important than factor  $X_2$ .

- 26       5. Since the factors are normally distributed, we need to sample the quan-  
 27           tiles and subsequently transform the values using the inverse of the  
 28           normal cumulative distribution function, as explained in Section 3.4. In  
 29           this exercise, quantiles are obtained by cutting the tails of the normal  
 30           distribution at quantiles 5 and 95% and dividing this interval into three  
 31           intervals. We leave to the reader the option of repeating the same exer-  
 32           cise without cutting the tails, and instead apportioning the entire space  
 33           of quantiles into four intervals and using the bin centres, as exemplified  
 34           in Exercise 2.

36                   Table 3.10 reports a sample composed of  $r = 4$  trajectories. The last  
 37           column shows the corresponding values of the output. The trajectories  
 38           are labelled as  $t_i$ ,  $i = 1, 2, 3, 4$ .

39                   Consider, for instance, factor  $X_1$ . Its elementary effects are esti-  
 40           mated as shown in Table 3.11. Note that to estimate  $EE_i(\mathbf{X})$  and  
 41           its absolute value, the rescaling factor is  $\Delta = 2/3$  (i.e. the varia-  
 42           tion of the factor in the space of the quantiles  $[0, 1]$  is used).  
 43           Table 3.12 reports the elementary effects for each trajectory and for  
 44           all the factors.

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 43 02  
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Table 3.10 Sampled trajectories (labeled  $t_1$ ,  $t_2$ ,  $t_3$ , and  $t_4$ ) and corresponding values for the Oakley–O’Hagan function

$t_1$															$Y$
$X_1$	$X_2$	$X_3$	$X_4$	$X_5$	$X_6$	$X_7$	$X_8$	$X_9$	$X_{10}$	$X_{11}$	$X_{12}$	$X_{13}$	$X_{14}$	$X_{15}$	
1.64	-1.64	-1.64	0.39	-0.39	0.39	-1.64	-1.64	-0.39	-0.39	1.64	1.64	-0.39	0.39	1.64	24.90
1.64	-1.64	-1.64	0.39	-0.39	-1.64	-1.64	-1.64	-0.39	-0.39	1.64	1.64	-0.39	0.39	1.64	22.72
1.64	-1.64	-1.64	0.39	-0.39	-1.64	-1.64	-1.64	1.64	-0.39	1.64	1.64	-0.39	0.39	1.64	21.04
1.64	-1.64	-1.64	0.39	-0.39	-1.64	-1.64	0.39	1.64	-0.39	1.64	1.64	-0.39	0.39	1.64	16.01
1.64	-1.64	-1.64	-1.64	-0.39	-1.64	-1.64	0.39	1.64	-0.39	1.64	1.64	-0.39	0.39	1.64	10.40
1.64	-1.64	-1.64	-1.64	-0.39	-1.64	-1.64	0.39	1.64	-0.39	1.64	1.64	-0.39	0.39	1.64	10.04
1.64	-1.64	-1.64	-1.64	-0.39	-1.64	-1.64	0.39	1.64	-0.39	1.64	1.64	-0.39	0.39	1.64	8.60
1.64	0.39	-1.64	-1.64	-0.39	-1.64	-1.64	0.39	1.64	-0.39	1.64	1.64	-0.39	0.39	1.64	13.39
1.64	0.39	-1.64	-1.64	-0.39	-1.64	-1.64	0.39	1.64	-0.39	1.64	1.64	-0.39	0.39	1.64	4.69
1.64	0.39	-1.64	-1.64	-0.39	-1.64	-1.64	0.39	1.64	1.64	1.64	1.64	-0.39	-0.39	-1.64	-0.39
1.64	0.39	-1.64	-1.64	1.64	-1.64	-1.64	0.39	1.64	1.64	1.64	1.64	-0.39	-0.39	-1.64	8.02
1.64	0.39	-1.64	-1.64	1.64	-1.64	-1.64	0.39	1.64	1.64	1.64	1.64	-0.39	-0.39	-1.64	9.98
1.64	0.39	-1.64	-1.64	1.64	-1.64	-1.64	0.39	1.64	1.64	1.64	1.64	-0.39	-0.39	-1.64	3.75
1.64	0.39	-1.64	-1.64	1.64	-1.64	0.39	0.39	1.64	1.64	1.64	1.64	-0.39	-0.39	-1.64	1.33
1.64	0.39	0.39	-1.64	1.64	-1.64	0.39	0.39	1.64	1.64	1.64	1.64	-0.39	-0.39	-1.64	-0.39
-0.39	0.39	0.39	-1.64	1.64	-1.64	0.39	0.39	1.64	1.64	1.64	1.64	-0.39	-0.39	-1.64	-0.39
-0.39	0.39	0.39	-1.64	1.64	-1.64	0.39	0.39	1.64	1.64	1.64	1.64	-0.39	-0.39	-1.64	6.37
-0.39	0.39	0.39	-1.64	1.64	-1.64	0.39	0.39	1.64	1.64	1.64	1.64	-0.39	-0.39	-1.64	9.99

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Table 3.10 (Continued)

$t_2$															Y
$X_1$	$X_2$	$X_3$	$X_4$	$X_5$	$X_6$	$X_7$	$X_8$	$X_9$	$X_{10}$	$X_{11}$	$X_{12}$	$X_{13}$	$X_{14}$	$X_{15}$	
-0.39	-0.39	0.39	0.39	-0.39	-0.39	-0.39	-1.64	0.39	-1.64	0.39	-0.39	-0.39	1.64	1.64	14.04
-0.39	-0.39	0.39	0.39	-0.39	-0.39	-0.39	-1.64	0.39	-1.64	0.39	-0.39	1.64	1.64	1.64	12.86
-0.39	-0.39	0.39	0.39	-0.39	-0.39	1.64	-1.64	0.39	-1.64	0.39	-0.39	1.64	1.64	1.64	15.42
-0.39	-0.39	0.39	0.39	-0.39	-0.39	1.64	-1.64	-1.64	-1.64	0.39	-0.39	1.64	1.64	1.64	14.56
-0.39	1.64	0.39	0.39	-0.39	-0.39	1.64	-1.64	-1.64	-1.64	0.39	-0.39	1.64	1.64	1.64	6.17
-0.39	1.64	0.39	0.39	1.64	-0.39	1.64	-1.64	-1.64	-1.64	0.39	-0.39	1.64	1.64	1.64	0.96
-0.39	1.64	0.39	0.39	1.64	-0.39	1.64	-1.64	-1.64	-1.64	0.39	1.64	1.64	1.64	1.64	2.91
-0.39	1.64	-1.64	0.39	1.64	-0.39	1.64	-1.64	-1.64	-1.64	0.39	1.64	1.64	1.64	1.64	-3.65
-0.39	1.64	-1.64	0.39	1.64	1.64	1.64	-1.64	-1.64	-1.64	0.39	1.64	1.64	1.64	1.64	-6.31
-0.39	1.64	-1.64	0.39	1.64	1.64	1.64	-1.64	-1.64	-1.64	0.39	1.64	1.64	1.64	1.64	-0.70
-0.39	1.64	-1.64	0.39	1.64	1.64	1.64	-1.64	-1.64	-1.64	1.64	1.64	1.64	1.64	-0.39	-11.79
-0.39	1.64	-1.64	0.39	1.64	1.64	1.64	-1.64	-1.64	-1.64	1.64	1.64	1.64	-0.39	-0.39	-16.95
-0.39	1.64	-1.64	0.39	1.64	1.64	1.64	-1.64	-1.64	0.39	-1.64	1.64	1.64	-0.39	-0.39	-15.54
-0.39	1.64	-1.64	0.39	1.64	1.64	1.64	-1.64	0.39	-1.64	1.64	1.64	-0.39	-0.39	-0.39	-3.01
-0.39	1.64	-1.64	-1.64	1.64	1.64	1.64	0.39	-1.64	0.39	-1.64	1.64	1.64	-0.39	-0.39	-2.12
1.64	1.64	-1.64	-1.64	1.64	1.64	1.64	0.39	-1.64	0.39	-1.64	1.64	1.64	-0.39	-0.39	-14.36

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$t_3$

$X_1$	$X_2$	$X_3$	$X_4$	$X_5$	$X_6$	$X_7$	$X_8$	$X_9$	$X_{10}$	$X_{11}$	$X_{12}$	$X_{13}$	$X_{14}$	$X_{15}$	Y
0.39	0.39	-0.39	-0.39	0.39	0.39	-1.64	0.39	-0.39	1.64	-0.39	0.39	-1.64	1.64	-1.64	3.96
0.39	0.39	-0.39	-0.39	0.39	0.39	-1.64	0.39	-0.39	1.64	1.64	0.39	-1.64	1.64	-1.64	2.92
0.39	0.39	-0.39	1.64	0.39	0.39	-1.64	0.39	-0.39	1.64	1.64	0.39	-1.64	1.64	-1.64	9.78
0.39	0.39	-0.39	1.64	0.39	0.39	-1.64	0.39	-0.39	1.64	1.64	-1.64	-1.64	1.64	-1.64	1.96
-1.64	0.39	-0.39	1.64	0.39	0.39	-1.64	0.39	-0.39	1.64	1.64	-1.64	-1.64	1.64	-1.64	-5.53
-1.64	0.39	-0.39	1.64	0.39	0.39	0.39	0.39	-0.39	1.64	1.64	-1.64	-1.64	1.64	-1.64	1.87
-1.64	0.39	1.64	1.64	0.39	0.39	0.39	0.39	-0.39	1.64	1.64	-1.64	-1.64	1.64	-1.64	-0.45
-1.64	-1.64	1.64	1.64	0.39	0.39	0.39	0.39	-0.39	1.64	1.64	-1.64	-1.64	1.64	-1.64	-3.81
-1.64	-1.64	1.64	1.64	0.39	0.39	0.39	-1.64	-0.39	1.64	1.64	-1.64	-1.64	1.64	-1.64	0.78
-1.64	-1.64	1.64	1.64	-1.64	0.39	0.39	-1.64	-0.39	1.64	1.64	-1.64	-1.64	1.64	-1.64	-0.27
-1.64	-1.64	1.64	1.64	-1.64	0.39	0.39	-1.64	1.64	1.64	1.64	-1.64	-1.64	1.64	-1.64	0.17
-1.64	-1.64	1.64	1.64	-1.64	-1.64	0.39	-1.64	1.64	1.64	1.64	-1.64	-1.64	1.64	-1.64	-5.89
-1.64	-1.64	1.64	1.64	-1.64	-1.64	0.39	-1.64	1.64	1.64	1.64	-1.64	-1.64	1.64	-1.64	-0.63
-1.64	-1.64	1.64	1.64	-1.64	-1.64	0.39	-1.64	1.64	1.64	1.64	-1.64	0.39	1.64	-1.64	8.37
-1.64	-1.64	1.64	1.64	-1.64	-1.64	0.39	-1.64	1.64	1.64	1.64	-1.64	0.39	1.64	0.39	5.65
-1.64	-1.64	1.64	1.64	-1.64	-1.64	0.39	-1.64	1.64	1.64	1.64	-1.64	0.39	-0.39	0.39	-1.91

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Table 3.10 (Continued)

$t_4$															
$X_1$	$X_2$	$X_3$	$X_4$	$X_5$	$X_6$	$X_7$	$X_8$	$X_9$	$X_{10}$	$X_{11}$	$X_{12}$	$X_{13}$	$X_{14}$	$X_{15}$	Y
1.64	-0.39	1.64	-0.39	0.39	0.39	-1.64	1.64	-1.64	-1.64	0.39	0.39	-1.64	0.39	0.39	5.05
1.64	-0.39	1.64	-0.39	-1.64	0.39	-1.64	1.64	-1.64	-1.64	0.39	0.39	-1.64	0.39	0.39	3.91
1.64	-0.39	1.64	1.64	-1.64	0.39	-1.64	1.64	-1.64	-1.64	0.39	0.39	-1.64	0.39	0.39	6.81
1.64	-0.39	1.64	1.64	-1.64	0.39	-1.64	1.64	-1.64	0.39	0.39	0.39	-1.64	0.39	0.39	5.58
1.64	1.64	1.64	1.64	-1.64	0.39	-1.64	1.64	-1.64	0.39	0.39	0.39	-1.64	0.39	0.39	11.79
1.64	1.64	1.64	1.64	-1.64	0.39	-1.64	1.64	-1.64	0.39	0.39	0.39	-1.64	0.39	-1.64	5.00
1.64	1.64	1.64	1.64	-1.64	0.39	-1.64	1.64	-1.64	0.39	-1.64	0.39	-1.64	0.39	-1.64	0.77
-0.39	1.64	1.64	1.64	-1.64	0.39	-1.64	1.64	-1.64	0.39	-1.64	0.39	-1.64	0.39	-1.64	1.38
-0.39	1.64	1.64	1.64	-1.64	0.39	-1.64	1.64	-1.64	0.39	-1.64	0.39	-1.64	-1.64	-1.64	-10.16
-0.39	1.64	1.64	1.64	-1.64	0.39	-1.64	1.64	-1.64	0.39	-1.64	0.39	-1.64	-1.64	-1.64	3.51
-0.39	1.64	1.64	1.64	-1.64	0.39	-1.64	1.64	0.39	0.39	-1.64	0.39	0.39	-1.64	-1.64	10.29
-0.39	1.64	1.64	1.64	-1.64	0.39	-1.64	-0.39	0.39	0.39	-1.64	0.39	0.39	-1.64	-1.64	-0.14
-0.39	1.64	1.64	1.64	-1.64	0.39	-1.64	-0.39	0.39	0.39	-1.64	-1.64	0.39	-1.64	-1.64	-9.34
-0.39	1.64	-0.39	1.64	-1.64	0.39	-1.64	-0.39	0.39	0.39	-1.64	-1.64	0.39	-1.64	-1.64	-7.57
-0.39	1.64	-0.39	1.64	-1.64	0.39	0.39	-0.39	0.39	0.39	-1.64	-1.64	0.39	-1.64	-1.64	-7.90
-0.39	1.64	-0.39	1.64	-1.64	-1.64	0.39	-0.39	0.39	0.39	-1.64	-1.64	0.39	-1.64	-1.64	-7.06

01                   **Table 3.11** Estimation of the elementary effects for factor  $X_1$  of  
 02                   Exercise 5

	$y(X_1 + \Delta, X_{\sim 1})$	$y(X_1, X_{\sim 1})$	$EE_1(\mathbf{X})$	$ EE_1(\mathbf{X}) $
$t_1$	2.59	6.37	-5.67	5.67
$t_2$	-14.36	-2.12	-18.36	18.36
$t_3$	1.96	-5.53	11.24	11.24
$t_4$	0.77	1.38	-0.92	0.92

10                   **Table 3.12** Elementary effects for all the factors of Exercise  
 11                   5 using the  $r = 4$  trajectories shown in Table 3.10

	$t_1$	$t_2$	$t_3$	$t_4$
$X_1$	-5.67	-18.36	11.24	-0.92
$X_2$	7.18	-12.58	5.04	9.31
$X_3$	1.89	9.84	-3.47	-2.66
$X_4$	8.42	-1.33	10.29	4.34
$X_5$	2.93	-7.82	1.57	1.71
$X_6$	3.28	-3.99	9.10	-1.25
$X_7$	-3.62	3.85	11.1	-0.5
$X_8$	-7.55	18.8	-6.89	15.65
$X_9$	-2.51	1.30	0.66	10.18
$X_{10}$	5.00	2.11	11.33	-1.83
$X_{11}$	9.34	16.64	-1.56	6.35
$X_{12}$	0.54	2.93	11.72	13.81
$X_{13}$	5.43	-1.78	7.90	20.5
$X_{14}$	2.15	7.74	4.08	17.31
$X_{15}$	13.05	-8.41	13.49	10.19

29                   For instance, the three sensitivity measures for factor  $X_1$  are obtained  
 30                   as follows:

$$31 \quad \mu(X_1) = \frac{-5.67 - 18.36 + 11.24 - 0.92}{4} = -3.42$$

$$34 \quad \mu^*(X_1) = \frac{5.67 + 18.36 + 11.24 + 0.92}{4} = 9.05$$

$$37 \quad \sigma(X_1) = \sqrt{\frac{(-2.24)^2 + (-14.93)^2 + (14.67)^2 + (2.51)^2}{3}} = 12.24.$$

40                   Columns 2–4 of Table 3.13 show the sensitivity analysis results for the  
 41                   Oakley–O’Hagan function for  $r = 4$ . Results for  $r = 10$  are also reported  
 42                   in the table. The last two columns show, for comparative purposes, the  
 43                   analytical values of the total- and first-order sensitivity indices for the  
 44                   factors.

01      **Table 3.13** Sensitivity analysis results for the Oakley–O'Hagan function of  
 02      Exercise 5 using  $r = 4$  and  $r = 10$  trajectories. The last two columns report the  
 03      analytical values of the total- and first-order sensitivity indices

	$r = 4$			$r = 10$			<i>Analytics</i>	<i>Analytics</i>
	$\mu^*$	$\mu$	$\sigma$	$\mu^*$	$\mu$	$\sigma$	$S_T$	$S$
$X_1$	9.05	-3.42	12.24	6.21	0.98	6.77	0.059	0.002
$X_2$	8.53	2.24	10.03	3.35	1.28	4.46	0.063	0.000
$X_3$	4.46	1.40	6.10	6.54	0.77	7.59	0.036	0.001
$X_4$	6.09	5.43	5.14	4.54	0.63	5.49	0.055	0.003
$X_5$	3.51	-0.4	4.98	3.13	-0.67	4.51	0.024	0.003
$X_6$	4.40	1.78	5.72	5.93	3.58	7.76	0.041	0.023
$X_7$	4.77	2.71	6.38	7.18	4.72	8.36	0.058	0.024
$X_8$	12.22	5.00	14.17	5.26	2.38	6.30	0.082	0.027
$X_9$	3.66	2.41	5.44	8.25	7.10	7.87	0.097	0.046
$X_{10}$	5.07	4.15	5.54	2.79	1.04	3.91	0.036	0.015
$X_{11}$	8.47	7.69	7.53	8.82	8.82	5.82	0.151	0.102
$X_{12}$	7.25	7.25	6.50	8.33	8.33	4.12	0.148	0.136
$X_{13}$	8.91	8.02	9.28	10.65	7.95	9.64	0.142	0.102
$X_{14}$	7.82	7.82	6.74	7.10	5.32	6.71	0.141	0.105
$X_{15}$	11.29	7.08	10.43	7.83	7.83	4.01	0.155	0.123

23      In our experiments, the use of  $r = 4$  trajectories has not helped to  
 24      discern the relative importance of the factors; for instance, the most  
 25      important factor according to  $\mu^*$  is  $X_8$ , while according to the analytic  
 26      values of  $ST$  it is only the seventh most important factor. These prob-  
 27      lems with the Oakley–O'Hagan function are mainly due to the fact that  
 28      interactions between all pairs of factors play a relevant role in the model.  
 29      Increasing the number of trajectories to  $r = 10$  allows us to better under-  
 30      stand the sensitivity of the model. Figure 3.12 shows in a barplot the  
 31      value of  $\mu^*$  for the inputs of the Oakley–O'Hagan function. This plot  
 32      highlights that in this model it is not possible to identify a subset of  
 33      factors to be fixed without affecting the output. The high values of  $\sigma$   
 34      confirm that this is related to the presence of non-negligible interactions  
 35      even for factors with low main effects ( $X_1, \dots, X_{10}$ ).

- 36      6. According to the matrix  $G$  and considering the results of the previous  
 37      exercise, factors are grouped so that all inputs with a high main  
 38      effect are in the first group. Table 3.14 reports the trajectories  
 39      obtained for the 15 factors grouped according to the matrix  $G$ . As  
 40      in Exercise 5, since factors are normally distributed quantiles are  
 41      sampled first and then levels are obtained using the inverse cumulative  
 42      distribution function.

43      Table 3.15 shows the absolute values of the elementary effects esti-  
 44      mated for each group using the 10 trajectories. The value of  $\mu^*$  for the

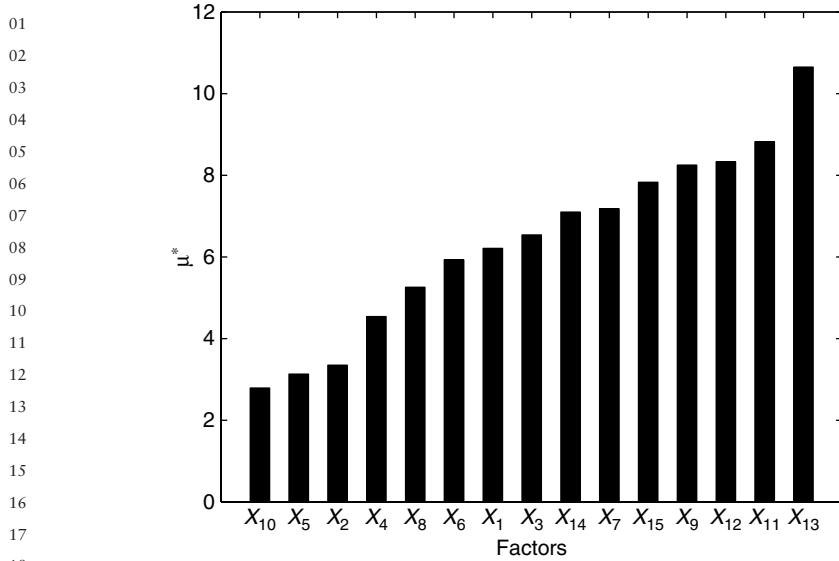


Figure 3.12 Barplot of  $\mu^*$  for the Oakley–O’Hagan function of Exercise 5, using  $r = 10$  trajectories

group (last column) is the average over the 10 estimates. It is clearly verified that the first group is more important than the second. However, it is also confirmed that the factors in  $G_2$  are actually playing a role on the output (see also the values of their  $S_T$  in Table 3.13) and thus cannot be discarded.

7. Since the number of factors is quite high, we do not report the complete sample used for the sensitivity analysis. However, Figure 3.13 shows the histogram of  $y$  for a design with  $p = 4$  levels and  $r = 10$  trajectories (i.e.  $N = 210$  model evaluations). Table 3.16 reports the sensitivity analysis results. Figure 3.14 helps in reading these results by presenting the scatterplot  $\{\mu^*, \sigma\}$ . This is the representation suggested by Morris (1991).

Figure 3.15 presents a horizontal barplot of the values of  $\mu^*$  for the inputs of the function  $y$ . Factors  $X_{11}, \dots, X_{20}$  are seen at a glance to be negligible. In fact, looking at the structure of  $y$ , their coefficients are never large. Factors  $X_8, X_9, X_{10}$  have a strong linear effect (for factors 1–10,  $\beta_i = 20$ ). The linear plus nonlinear influence of  $X_7$ , due to the transformation  $\omega_i = 2(1.1X_i/(X_i + 0.1) - 1/2)$ , is also captured by the high value of the standard deviation. Finally, factors  $X_1, \dots, X_6$  are all identified as influential and to have linear, nonlinear and nonadditive effects.

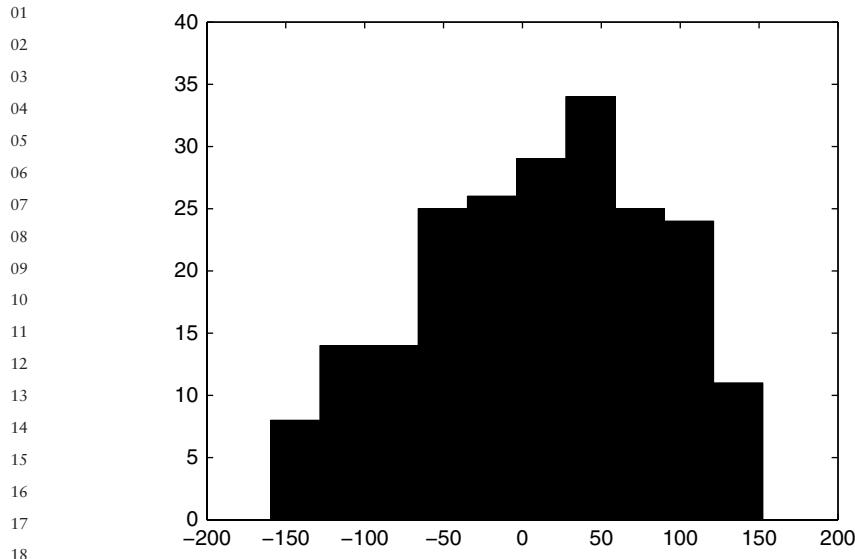
Table 3.14 Trajectories obtained for Exercise 6 (Oakley-O'Hagan function,  $r = 10$ ) in case the two groups described by matrix  $\mathbf{G}$  are considered

X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	X <sub>4</sub>	X <sub>5</sub>	X <sub>6</sub>	X <sub>7</sub>	X <sub>8</sub>	X <sub>9</sub>	X <sub>10</sub>	X <sub>11</sub>	X <sub>12</sub>	X <sub>13</sub>	X <sub>14</sub>	X <sub>15</sub>	Y
0.39	-0.39	-1.64	0.39	-0.39	-0.39	0.39	0.39	-1.64	-0.39	0.39	-1.64	1.64	1.64	1.64	13.85
-1.64	1.64	0.39	-1.64	1.64	1.64	-1.64	-1.64	-1.64	1.64	0.39	-1.64	1.64	1.64	1.64	-10.11
-1.64	1.64	0.39	-1.64	1.64	1.64	-1.64	-1.64	0.39	1.64	-1.64	0.39	-0.39	-0.39	-0.39	1.12
-0.39	-0.39	0.39	-1.64	0.39	-1.64	1.64	1.64	0.39	-1.64	0.39	-0.39	0.39	0.39	0.39	13.37
-0.39	-0.39	0.39	-1.64	0.39	-1.64	1.64	1.64	-1.64	-1.64	-1.64	1.64	-1.64	-1.64	-1.64	-13.33
1.64	1.64	-1.64	0.39	-1.64	0.39	-0.39	-0.39	-1.64	0.39	-1.64	1.64	-1.64	-1.64	-1.64	-12.68
1.64	-1.64	1.64	1.64	1.64	-0.39	-1.64	-1.64	-0.39	-0.39	1.64	1.64	-1.64	1.64	0.39	15.65
1.64	-1.64	1.64	1.64	1.64	-0.39	-1.64	-1.64	1.64	-0.39	-0.39	0.39	0.39	-0.39	-1.64	1.59
-0.39	0.39	-0.39	-0.39	-0.39	1.64	0.39	0.39	1.64	1.64	-0.39	-0.39	0.39	-0.39	-1.64	10.99
-0.39	-1.64	-1.64	0.39	0.39	-0.39	0.39	-0.39	-0.39	1.64	1.64	1.64	1.64	-1.64	1.64	22.92
1.64	0.39	0.39	-1.64	-1.64	1.64	-1.64	1.64	-0.39	-0.39	1.64	1.64	1.64	-1.64	1.64	22.62
1.64	0.39	0.39	-1.64	-1.64	1.64	-1.64	1.64	1.64	-0.39	-0.39	-0.39	0.39	-0.39	-0.39	6.42
1.64	1.64	-1.64	1.64	1.64	-0.39	-0.39	1.64	0.39	1.64	0.39	-0.39	0.39	-0.39	1.64	18.01
1.64	1.64	-1.64	1.64	1.64	-0.39	-0.39	1.64	-1.64	1.64	-1.64	1.64	-1.64	1.64	-0.39	3.82
-0.39	-0.39	0.39	-0.39	-0.39	1.64	1.64	-0.39	-1.64	-0.39	-1.64	1.64	-1.64	1.64	-0.39	9.27
0.39	-1.64	-1.64	-0.39	-1.64	-1.64	-0.39	-1.64	-0.39	-0.39	-0.39	-1.64	0.39	-1.64	0.39	-0.71
0.39	-1.64	-1.64	-0.39	-1.64	-1.64	-0.39	-1.64	1.64	-0.39	1.64	0.39	-1.64	0.39	-1.64	0.62
-1.64	0.39	0.39	1.64	0.39	0.39	1.64	0.39	1.64	1.64	1.64	0.39	-1.64	0.39	-1.64	10.63
-1.64	-1.64	0.39	-1.64	1.64	1.64	1.64	1.64	1.64	-1.64	-0.39	0.39	-1.64	1.64	0.39	16.47
-1.64	-1.64	0.39	-1.64	1.64	1.64	1.64	1.64	-0.39	-1.64	1.64	-1.64	0.39	-0.39	-1.64	2.33
0.39	0.39	-1.64	0.39	-0.39	-0.39	-0.39	-0.39	-0.39	0.39	1.64	-1.64	0.39	-0.39	-1.64	7.41

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Table 3.15 Absolute values of the elementary effects obtained for the two groups in Exercise 6.  $\mu^*$  is the average over the 10 estimates

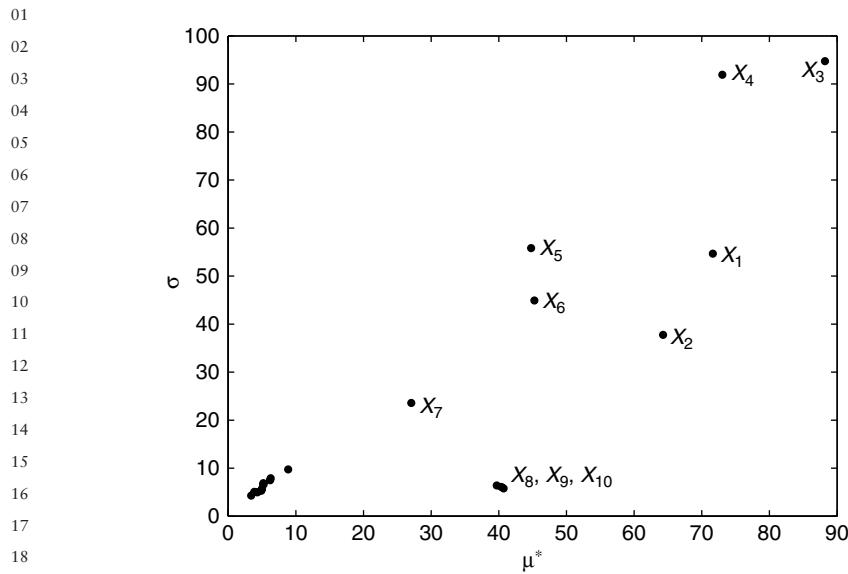
$t_1$	$t_2$	$t_3$	$t_4$	$t_5$	$t_6$	$t_7$	$t_8$	$t_9$	$t_{10}$	$\mu^*$
G <sub>1</sub>	16.86	40.06	21.09	24.3	21.29	1.99	21.2	16.75	5.28	36.16
G <sub>2</sub>	35.95	0.97	14.1	0.45	8.18	15.01	7.62	12.26	7.70	13.75



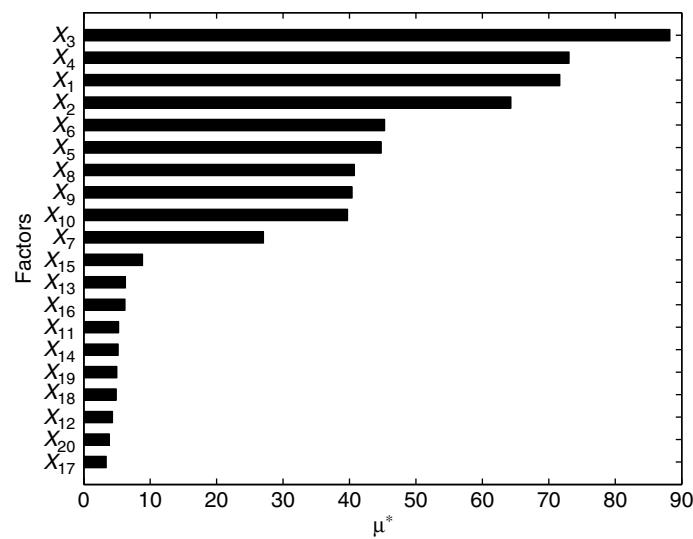
19      **Figure 3.13** Empirical density of the Morris function obtained for Exercise 7 with  
20       $r = 10$  trajectories

22      **Table 3.16** Sensitivity analysis for the Morris function  
23      of Exercise 7 using  $r = 10$  trajectories

	$\mu^*$	$\mu$	$\sigma$
$X_1$	71.644	55.256	54.648
$X_2$	64.290	64.29	37.737
$X_3$	88.207	55.572	94.737
$X_4$	73.038	9.310	91.918
$X_5$	44.777	32.874	55.793
$X_6$	45.280	35.187	44.940
$X_7$	27.039	27.039	23.594
$X_8$	40.716	40.716	5.789
$X_9$	40.385	40.385	6.101
$X_{10}$	39.706	39.706	6.400
$X_{11}$	5.252	1.232	6.608
$X_{12}$	4.324	1.494	4.990
$X_{13}$	6.268	0.922	7.892
$X_{14}$	5.183	0.192	6.845
$X_{15}$	8.842	3.797	9.773
$X_{16}$	6.201	2.183	7.511
$X_{17}$	3.389	-1.335	4.291
$X_{18}$	4.903	-1.540	5.338
$X_{19}$	4.989	-0.766	5.686
$X_{20}$	3.854	-2.407	5.087



**Figure 3.14** Sensitivity analysis results for the Morris function of Exercise 7 using  $r = 10$  trajectories



**Figure 3.15** Horizontal barplot of the value of  $\mu^*$  for the the Morris function of Exercise 7, obtained using  $r = 10$  trajectories

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**Table 3.17** Sample of  $r = 10$  trajectories for the analysis by group of Exercise 8

	$X_1$	$X_2$	$X_3$	$X_4$	$X_5$	$X_6$	$X_7$	$X_8$	$X_9$	$X_{10}$	$X_{11}$	$X_{12}$	$X_{13}$	$X_{14}$	$X_{15}$	$X_{16}$	$X_{17}$	$X_{18}$	$X_{19}$	$X_{20}$	$Y$
$t_1$	0	0	1	1	1/3	1	1	1/3	0	0	1	0	0	1/3	2/3	1/3	1/3	1	0	0	58.28
	0	0	1	1	1/3	1	1	1/3	0	0	1	0	0	1	0	1	1	0	0	0	68.24
	0	0	1	1	1/3	1/3	1/3	1	2/3	0	1	0	2/3	1	0	1	1	1/3	0	0	87.75
	0	0	1	1/3	1/3	1/3	1/3	1	2/3	0	1	0	2/3	1	0	1	1	1/3	2/3	2/3	23.04
	2/3	2/3	1/3	1/3	1	1/3	1/3	1	2/3	2/3	1/3	2/3	2/3	1	0	1	1	1/3	2/3	2/3	63.61
$t_2$	1	1/3	2/3	0	1/3	1/3	2/3	1	1/3	1/3	2/3	1/3	1/3	0	1/3	0	2/3	0	1	1/3	81.50
	1/3	1	0	0	1/3	1/3	2/3	1	1/3	1	0	1	1/3	0	1/3	0	2/3	0	1	1/3	38.17
	1/3	1	0	0	1/3	1/3	2/3	1	1/3	1	0	1	1/3	2/3	1	2/3	0	0	1	1/3	47.28
	1/3	1	0	0	1/3	1	0	1/3	1	1	0	1	1	2/3	1	2/3	0	2/3	1	1/3	43.58
	1/3	1	0	2/3	1	1	0	1/3	1	1	0	1	1	2/3	1	2/3	0	2/3	1/3	1	72.56
$t_3$	1	1	1/3	0	2/3	0	2/3	2/3	1	0	0	2/3	1	1/3	0	1	0	1/3	1/3	1/3	115.15
	1	1	1/3	2/3	0	0	2/3	2/3	2/3	1	0	0	2/3	1	1/3	0	1	0	1	1	116.45
	1	1	1/3	2/3	0	2/3	0	0	0	1	0	0	0	1	1/3	0	1	2/3	1	1	9.06
	1/3	1/3	1	2/3	0	2/3	0	0	0	1/3	2/3	2/3	0	1	1/3	0	1	2/3	1	1	-50.12
	1/3	1/3	1	2/3	0	2/3	0	0	0	1/3	2/3	2/3	0	1/3	1	2/3	1/3	2/3	1	1	-48.06
$t_4$	0	1/3	0	2/3	1/3	2/3	1	0	1	0	0	1	1/3	0	2/3	2/3	2/3	2/3	1	1/3	-33.16
	0	1/3	0	0	1	2/3	1	0	1	0	0	1	1/3	0	2/3	2/3	2/3	2/3	1	-67.02	
	0	1/3	0	0	1	2/3	1	0	1	0	0	1	1/3	2/3	0	0	2/3	1/3	1	-60.14	
	0	1/3	0	0	1	0	1/3	2/3	1/3	0	0	1	1	2/3	0	0	0	0	1/3	1	-132.66
	2/3	1	2/3	0	1	0	1/3	2/3	1/3	2/3	2/3	1/3	1	2/3	0	0	0	0	1/3	1	81.88
$t_5$	1/3	0	2/3	0	0	1/3	2/3	1/3	1/3	0	1/3	2/3	1/3	0	2/3	1	1	1/3	1/3	2/3	-118.82
	1/3	0	2/3	0	0	1	0	1	1	0	1/3	2/3	1	0	2/3	1	1	1	1/3	2/3	-32.49
	1	2/3	0	0	0	1	0	1	1	2/3	1	0	1	0	2/3	1	1	1	1/3	2/3	30.46
	1	2/3	0	2/3	2/3	1	0	1	1	2/3	1	0	1	0	2/3	1	1	1	1	0	62.69
	1	2/3	0	2/3	2/3	1	0	1	1	2/3	1	0	1	2/3	0	1/3	1/3	1	1	0	57.40

$t_6$	1/3	2/3	0	1/3	1/3	0	1	0	1/3	1/3	2/3	1/3	1	2/3	1/3	2/3	1	0	2/3	2/3	-49.84	
	1/3	2/3	0	1	1	0	1	0	1/3	1/3	2/3	1/3	1	2/3	1/3	2/3	1	0	0	0	36.19	
	1	0	2/3	1	1	0	1	0	1/3	1	0	1	1	2/3	1/3	2/3	1	0	0	0	86.51	
	1	0	2/3	1	1	2/3	1/3	2/3	1	1	0	1	1/3	2/3	1/3	2/3	1	2/3	0	0	104.25	
	1	0	2/3	1	1	2/3	1/3	2/3	1	1	0	1	1/3	0	1	0	1/3	2/3	0	0	97.56	
$t_7$	0	1	2/3	1	1	1	1/3	0	0	1/3	2/3	1/3	0	1/3	2/3	1	2/3	1	2/3	1	-13.28	
	0	1	2/3	1	1	1	1/3	0	0	1/3	2/3	1/3	0	1	0	1/3	0	1	2/3	1	-17.35	
	0	1	2/3	1/3	1/3	1	1/3	0	0	1/3	2/3	1/3	0	1	0	1/3	0	1	0	1/3	25.31	
	2/3	1/3	0	1/3	1/3	1	1/3	0	0	1	0	1	0	1	0	1/3	0	1	0	1/3	1.93	
	2/3	1/3	0	1/3	1/3	1/3	1	2/3	2/3	1	0	1	2/3	1	0	1/3	0	1/3	0	1/3	38.27	
$t_8$	1/3	1/3	0	0	0	1/3	1/3	2/3	2/3	2/3	1/3	2/3	2/3	0	2/3	1/3	1	0	1/3	1/3	-103.13	
	1	1	2/3	0	0	1/3	1/3	2/3	2/3	0	1	0	2/3	0	2/3	1/3	1	0	1/3	1/3	69.38	
	1	1	2/3	0	0	1	1	0	0	0	1	0	0	0	2/3	1/3	1	2/3	1/3	1/3	34.50	
	1	1	2/3	0	0	1	1	0	0	0	1	0	0	2/3	0	1	1/3	2/3	1/3	1/3	32.28	
	1	1	2/3	2/3	2/3	1	1	0	0	0	1	0	0	2/3	0	1	1/3	2/3	1	1	-153.14	
$t_9$	1/3	1	1/3	1/3	2/3	2/3	1/3	1	1	0	1	2/3	1/3	2/3	2/3	2/3	0	1			86.29	
	1/3	1	1/3	1/3	2/3	0	0	1	1/3	1	0	1	0	1/3	2/3	2/3	2/3	0	0	1		68.73
	1/3	1	1/3	1/3	2/3	0	0	1	1/3	1	0	1	0	1	0	0	0	0	0	1		60.16
	1	1/3	1	1/3	2/3	0	0	1	1/3	1/3	2/3	1/3	0	1	0	0	0	0	0	1		21.83
	1	1/3	1	1	0	0	0	1	1/3	1/3	2/3	1/3	0	1	0	0	0	0	2/3	1/3		43.05
$t_{10}$	1/3	1/3	1/3	1/3	1/3	1/3	1	1	2/3	0	0	0	0	0	2/3	1	2/3	1	1/3	2/3		38.96
	1/3	1/3	1/3	1	1	1/3	1	1	2/3	0	0	0	0	0	2/3	1	2/3	1	1	1		67.35
	1/3	1/3	1/3	1	1	1/3	0	0	0	0	0	0	0	2/3	1	2/3	1	2/3	1	1		-7.34
	1	1	1	1	1	1	1/3	1/3	0	2/3	2/3	2/3	0	2/3	1	2/3	1	2/3	1/3	1		-205.31
	1	1	1	1	1	1	1/3	1/3	0	2/3	2/3	2/3	2/3	0	1/3	0	1/3	1	0	1		-212.21

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02  
03  
04      **Table 3.18** Absolute values of the elementary effects  
05 for each trajectory and each group of Exercise 8. The  
06 measure  $\mu^*$  (last row) is the average over the 10 runs  
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	$G_1$	$G_2$	$G_3$	$G_4$
$t_1$	60.87	97.07	14.94	29.27
$t_2$	64.99	43.47	13.67	5.55
$t_3$	88.76	1.95	3.09	161.09
$t_4$	321.81	50.79	10.31	108.78
$t_5$	94.42	48.35	7.94	129.50
$t_6$	75.48	129.04	10.04	26.60
$t_7$	35.07	63.99	6.11	54.51
$t_8$	258.76	278.13	3.33	52.32
$t_9$	57.49	31.83	12.86	26.34
$t_{10}$	296.95	42.58	10.36	112.04
$\mu^*$	135.46	78.72	9.26	70.60

- 16  
17 8. Table 3.17 shows the sample for the groups and the corresponding values  
18 for the output. Note that slightly different results might be obtained  
19 since the parameters  $\beta_i, \beta_{i,j}, \beta_{i,j,k}, \beta_{i,j,k,l}$  are all randomly generated.  
20 Table 3.18 reports the absolute values of the elementary effects,  $|EE_i(\mathbf{X})|$ ,  
21 for each group along each of the 10 trajectories. Results confirm that  
22 there are three relevant groups ( $G_1, G_2$  and  $G_4$ ) and one group with low  
23 influence on the output ( $G_3$ ). This is indeed correct since the factors in  
24  $G_3$  ( $X_{14}, X_{15}, X_{16}$  and  $X_{17}$ ) have low main effects and low interactions  
25 (see also Table 3.16 above). Even the relative importance of  $G_1, G_2$  and  
26  $G_3$  reflects the structure of the function  $y$  and the sensitivity analysis  
27 results of the previous exercise.  
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# 4

## Variance-based Methods

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17 HOW IS VARIANCE DECOMPOSITION RELATED TO SENSITIVITY ANALYSIS? WHEN  
18 IS IT WORTH USING VARIANCE-BASED TECHNIQUES INSTEAD OF SOMETHING ELSE?  
19 WHICH MEASURES CAN WE OBTAIN WITH VARIANCE-BASED METHODS? HOW ARE  
20 THESE MEASURES CALCULATED?

21 In this chapter we describe in more detail the variance-based methods  
22 that were introduced in Chapter 1. We first illustrate the settings that can  
23 be useful when dealing with modelling under conditions of uncertainty. We  
24 discuss the importance of a proper sensitivity test for a given setting. We  
25 sketch the historical background of variance-based methods, and discuss  
26 the properties of variance decompositions, from model independence to  
27 the capacity to evaluate the importance of groups of factors. Total effect  
28 indices are also introduced as a means of dealing synthetically with model  
29 complexity. We then illustrate two basic methods of computing the sensi-  
30 tivity indices, the Monte Carlo based design developed by Saltelli (2002)  
31 as well as the Random Balance Designs based on the Fourier Amplitude  
32 Sensitivity Test (FAST-RBD (Tarantola *et al.*, 2006)). Finally, we offer some  
33 examples.

34

35

### 4.1 DIFFERENT TESTS FOR DIFFERENT SETTINGS

37

38 It is common to find cases in the literature in which different sensitivity tests  
39 are applied to the same problem in a nonstructured fashion. This practice  
40 can yield a variety of results – e.g. in terms of ranking the factors in order of  
41

42

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

importance – with no guidance as to which we should believe or privilege. As discussed in Chapter 1, we suggest instead a careful consideration of (a) the output of interest and (b) the concept of ‘importance’, as it applies to the problem at hand. This would in general allow for the identification of the most appropriate setting for a given problem and, in turn, the sensitivity test to be applied. A list of possible settings (Saltelli *et al.*, 2004) is given here:

- The **Factor Prioritization** setting (FP) is used to identify a factor (or group of factors) which, when fixed to its true value, leads to the greatest reduction in the variance of the output. In other words, the identified factor (or group of factors) is that which accounts for most of the output variance. Therefore, this setting allows us (a) to detect and rank those factors which need to be better measured in order to reduce the output variance, as well as (b) to detect the factors that have a better chance of being estimated in a subsequent numerical or experimental estimation process. This latter point is particularly interesting as the analyst can identify the factors to be estimated before any estimation is made or measurements carried out. See Tarantola *et al.* (2000) for an example in the field of physics.
- The **Factor Fixing** setting (FF) is used to identify factors in the model which, left free to vary over their range of uncertainty, make no significant contribution to the variance of the output. The identified factors can then be fixed at any given value within their range of variation without affecting the output variance. This analysis can be performed on groups of factors, especially for large models, to identify noninfluential subsets of factors. Sometimes, factors are set up to represent alternative structures for model components (e.g. simple versus complex) and significant model simplifications can be often achieved when these factors are found to be noninfluential.
- The **Variance Cutting** setting (VC) is used for the reduction of the output variance to below a given tolerance. This may be desirable in risk or reliability analysis, where the analyst is interested in making sure, for example, that the uncertainty of the reliability of a given system component is below a given tolerance. In this setting the analyst wants to guarantee that the uncertainty is brought under a given value by acting on the smallest possible number of factors (see Saltelli and Tarantola, 2002).
- The **Factor Mapping** setting (FM) is used to study which values of the input factors lead to model realizations in a given range of the output space. For example, one may want to highlight model realizations falling above the 95th percentile because these correspond to risky conditions in an industrial plant or to a considerable financial loss (Campolongo *et al.*, 2007). In this setting one investigates which combination of factors leads to the realizations under analysis (Monte Carlo filtering, see Chapter 5).

01 The utility of variance-based sensitivity measures derives from their wide  
02 range of application. Of the four settings just recounted, the first three are  
03 susceptible of variance-based analysis.

## 06 4.2 WHY VARIANCE? 07

08 Most models live through their operational life as ‘deterministic’. Each time  
09 they are ‘interrogated’ they are fed with a deterministic set of values for  
10 the input variables and the output – be it a scalar, a time series or a 2D  
11 map – is investigated for possible inferences. Sensitivity analysis for these  
12 models will generally entail changing one input at a time to test its effect  
13 on the output. In this book we profess a different philosophy of modelling,  
14 in which modellers are willing – and usually eager – to explore their model  
15 over different combinations of values for the uncertain inputs. Variance-  
16 based measures have proven useful in this framework. They study how the  
17 variance of the output depends on the uncertain input factors and can be  
18 decomposed accordingly.  
19

20 But why study the variance? Could a sensitivity measure be built on the  
21 mean? To give an example, in risk analysis the model output may happen  
22 to be itself a mean,<sup>1</sup> and we might be interested in how the mean of the  
23 model output depends on its constituents. A legitimate question would then  
24 be how much each component of a system contributes to the risk that  
25 the system might fail. The answer could be that the risk depends 25% on  
26 component A, 15% on component B, and so on. Decomposing the absolute  
27 level of the risk into system components can be useful to help understanding  
28 which component is worth improving in order to reduce the level of risk in  
29 the system.<sup>2</sup>

30 Another measure encountered in risk analysis is the ‘risk reduction worth’,  
31 which measures the amount by which the risk associated with a system  
32 could be reduced if a model element were perfect, i.e. without risk of failure  
33 (see Borgonovo and Apostolakis, 2001).

34 The two examples just illustrated are based on a deterministic output –  
35 risk – and how the risk level can be modified by eliminating the uncertainty  
36 in the input. We are in principle against such an elimination of uncertainty;  
37 we prefer rather to retain the uncertain factors as an ingredient of sensitivity  
38 analysis. Even when we study how the mean of the output changes when

40     <sup>1</sup> For example, a risk may happen to be estimated as the product of the probability of a given  
41 outcome and the consequence of that outcome, averaged over a set of possible outcomes.

42     <sup>2</sup> Risk analysts use, for example, the Fussell–Vesely measure of importance in probabilistic  
43 safety assessments. This measure is defined as the fraction of risk that is contributed by the  
44 failure of a model element (Borgonovo and Apostolakis, 2001).

01 a factor is fixed – we denoted this in Chapter 1 as  $E(Y|X_i = x_i^*)$  – we  
 02 would then take the variance of this measure over all possible values  $x_i^*$ ,  
 03 i.e.  $V(E(Y|X_i))$ . Taking the mean of  $E(Y|X_i = x_i^*)$  would have been of scant  
 04 use – it would have led us back to the overall (unconditioned) mean. In  
 05 other words, in a Monte Carlo framework variance emerges naturally if  
 06 one wants to preserve the factors' uncertainty.

07 Returning to our example of risk analysis, note that ‘risk’ has been  
 08 expressed as a crisp figure (e.g. a rate of failure, or the expected incidence  
 09 of health effects), which may distract from the fact that risk is in itself an  
 10 average. A practitioner might be interested in how the average is arrived at,  
 11 in the form of the risk distribution tails and in details such as the topology  
 12 of the low probability high-consequence regions and in the key assumptions  
 13 shaping these regions. These issues are addressed by the methods presented  
 14 in this book.

15 A key issue in sensitivity analysis is how to quantify the uncertainty of a  
 16 model prediction – variance clearly being just one of the possible options.  
 17 Depending on the problem at hand, we might be interested in the model  
 18 prediction falling in the upper or lower 5th percentile of the distribution or  
 19 in any particular interval of interest in the distribution, as in Monte Carlo  
 20 filtering.

21 Methods have been developed which look at the entire distribution of  
 22 the output and at how this is modified, on average, if a factor is fixed  
 23 (Borgonovo, 2006).

24 We recommend using variance as a summary measure of uncertainty  
 25 whenever the application allows it. This is in order to exploit the statistical  
 26 properties of variance described in this chapter to investigate how factors  
 27 contribute to the variance.

28 Interesting features of variance-based methods are:

- 30 • model independence: the sensitivity measure is model-free;
- 31 • capacity to capture the influence of the full range of variation of each  
   input factor;
- 33 • appreciation of interaction effects among input factors;
- 34 • capacity to tackle groups of input factors: uncertain factors might pertain  
   to different logical types, and it might be desirable to decompose the  
   uncertainty according to these types.

37 The drawback of variance-based measures is their computational cost, as  
 38 we shall discuss later in the chapter, and this is the reason why much recent  
 39 research aims to find efficient numerical algorithms for their computation.  
 40 Techniques for computation are offered both in this chapter and the next.

42 Sensitivity measures based on the decomposition of the variance of the  
 43 model output are relatively recent in the literature. A brief summary of their  
 44 development follows.

### 01           4.3 VARIANCE-BASED METHODS. A BRIEF HISTORY

02  
 03 Variance-based methods for sensitivity analysis were first employed by  
 04 chemists in the early 1970s (Cukier *et al.*, 1973). Cukier and colleagues  
 05 not only proposed conditional variances for a sensitivity analysis based on  
 06 first-order effects, but were already aware of the need to treat higher-order  
 07 terms and of the underlying variance decomposition theorems (Cukier *et al.*,  
 08 1978). Their method, known as FAST (Fourier Amplitude Sensitivity Test),  
 09 although quite effective, enjoyed limited success among practitioners, not  
 10 least because of the difficulty in encoding it. The method did not allow the  
 11 computation of higher-order indices, although this was much later made  
 12 possible by extensions developed by other investigators (see Saltelli *et al.*,  
 13 1999).

14 Also much later, Hora and Iman (1986) introduced the ‘uncertainty  
 15 importance’ of a factor  $X_i$ ,<sup>3</sup> defined as the expected reduction in the vari-  
 16 ance of the model output  $Y$  achieved by fixing  $X_i$  at a given value within  
 17 its range of uncertainty:

$$18 \quad 19 \quad I_i = \sqrt{\text{Var}(Y) - E[\text{Var}(Y|X_i)]}. \quad (4.1)$$

20 Later, the same authors (Iman and Hora, 1990) proposed a new statistic  
 21 based on estimating the following quantity:

$$23 \quad 24 \quad \frac{\text{Var}_{X_i}[E(\log Y|X_i)]}{\text{Var}[\log Y]}. \quad (4.2)$$

26 From Chapter 1 it is clear that this is the first-order variance term relative  
 27 to  $\log Y$ . This measure has the advantage of robustness,<sup>4</sup> although it is not  
 28 easy to convert results of sensitivity analysis pertaining to  $\log Y$  back to  $Y$ .  
 29 Transformations of  $Y$  for sensitivity analysis are presented in Chapter 5.

30 A visual inspection of sensitivity results has been suggested by Sacks *et al.*  
 31 (1989). They proposed a decomposition of the response

$$33 \quad Y = f(X_1, X_2, \dots, X_k) \quad (4.3)$$

34 into a set of functions of increasing dimensionality, whose plots are them-  
 35 selves used as measures of sensitivity (as will be discussed in detail in

38  
 39 <sup>3</sup> We refer to  $X_i$  as the  $i$ th element of  $\mathbf{X}$ , though the formulas presented in this chapter are  
 40 appropriate also if  $X_i$  corresponds to a subset of model inputs.

41 <sup>4</sup> The range of variation of  $\log Y$  can be much smaller than that of  $Y$  and hence its estimate  
 42 can be obtained – *ceteris paribus* – at a lower sample size. For the same reason formulas  
 43 similar to (4.2) were proposed on the rank of  $Y$ , e.g. replacing the values of  $Y$  with the integer  
 44 corresponding to 1 for the highest  $Y$  value and with  $N$  (the size of the sample) for the lowest  
 (Saltelli *et al.*, 1993).

Chapter 5). Although these authors do not use the variance, the functions they consider are the same as in Sobol's functional development.

The Russian mathematician I. M. Sobol' was inspired by the work of Cukier, and generalized it to provide a straightforward Monte Carlo-based implementation of the concept, capable of computing sensitivity measures for arbitrary groups of factors.

Given a square integrable function  $f$  over  $\Omega^k$ , the  $k$ -dimensional unit hypercube,

$$\Omega^k = \{X | 0 \leq x_i \leq 1; i = 1, \dots, k\}, \quad (4.4)$$

Sobol' considers an expansion of  $f$  into terms of increasing dimensions:

$$f = f_0 + \sum_i f_i + \sum_i \sum_{j>i} f_{ij} + \dots + f_{12\dots k} \quad (4.5)$$

in which each individual term is also square integrable over the domain of existence and is a function only of the factors in its index, i.e.  $f_i = f_i(X_i)$ ,  $f_{ij} = f_{ij}(X_i, X_j)$  and so on. This decomposition is not a series decomposition, as it has a finite number of terms. Of the  $2^k$  terms, one is constant ( $f_0$ ),  $k$  are first-order functions ( $f_i$ ),

$$\binom{k}{2}$$

are second-order functions ( $f_{ij}$ ), and so on. This expansion, called high-dimensional model representation (HDMR), is not unique, meaning that, for a given model  $f$ , there could be infinite choices for its terms. Sobol' proved that, if each term in the expansion above has zero mean, i.e.  $\int f(x_i) dx_i = 0$ , then all the terms of the decomposition are orthogonal in pairs, i.e.  $\int f(x_i) f(x_j) dx_i dx_j = 0$ . As a consequence, these terms can be univocally calculated using the conditional expectations of the model output  $Y$ .

In particular,

$$f_0 = E(Y) \quad (4.6)$$

$$f_i = E(Y|X_i) - E(Y) \quad (4.7)$$

$$f_{ij} = E(Y|X_i, X_j) - f_i - f_j - E(Y) \quad (4.8)$$

An analytic example of this decomposition is offered in Exercise 5.

As mentioned in Chapter 1 (see Conditional Variances – second path), the conditional expectation  $E(Y|X_i)$  can be calculated empirically by cutting the  $X_i$  domain into slices and averaging the values of  $(Y|X_i)$  within the same slice  $X_i$ . In this way, if the scatterplot has a pattern, the conditional expectation  $E(Y|X_i)$  has a large variation across  $X_i$  values and the factor  $X_i$  is revealed to be important. Hence, the variance of the conditional expectation can be

01 considered as a summary measure of sensitivity. In fact, the variances of  
 02 the terms in the decomposition above are the measures of importance being  
 03 sought. In particular,  $V(f_i(X_i))$  is  $V[E(Y|X_i)]$ ; when we divide this by the  
 04 unconditional variance  $V(Y)$ , we obtain the first-order sensitivity index. In  
 05 short:

$$06 \quad S_i = \frac{V[E(Y|X_i)]}{V(Y)}. \quad (4.9)$$

09 The first-order index represents the main effect contribution of each input  
 10 factor to the variance of the output. The same quantity has been described  
 11 by different investigators as an ‘importance measure’ (see Hora and Iman,  
 12 1986; Ishigami and Homma, 1996; Iman and Hora, 1990; Saltelli *et al.*,  
 13 1993; Homma and Saltelli, 1996), and as a ‘correlation ratio’ (see Krzykacz-  
 14 Hausmann, 1990; McKay, 1996).

15 Sobol’ also proposed a comparable definition of  $S_i$  (Sobol’, 1996) which  
 16 is based on the correlation between the model  $Y$  and the conditional expec-  
 17 tation  $E(Y|X_i)$ :

$$18 \quad S_i = \text{Corr}(Y, E(Y|X_i)). \quad (4.10)$$

#### 21 4.4 INTERACTION EFFECTS

24 How can Sobol’s variance decomposition help in investigating the existence  
 25 of interaction effects? Two factors are said to interact when their effect on  $Y$   
 26 cannot be expressed as a sum of their single effects. Interactions may imply,  
 27 for instance, that extreme values of the output  $Y$  are uniquely associated  
 28 with particular combinations of model inputs, in a way that is not described  
 29 by the first-order effects  $S_i$  just mentioned. Interactions represent important  
 30 features of models, and are more difficult to detect than first-order effects.  
 31 For example, by using regression analysis tools it is fairly easy to estimate  
 32 first-order indices, but not interactions (remember the relationship  $S_i = \beta_{X_i}^2$   
 33 discussed in Chapter 1 for linear models and orthogonal inputs, where  $\beta_{X_i}$   
 34 is the standardized regression coefficient for factor  $X_i$ ).

35 A useful feature of decomposition (4.7 and 4.8) is that

$$36 \quad V_i = V(f_i(X_i)) = V[E(Y|X_i)]$$

38 and

$$41 \quad V_{ij} = V(f_{ij}(X_i, X_j)) = V(E(Y|X_i, X_j)) - V(E(Y|X_i)) - V(E(Y|X_j)).$$

43 In this equation,  $V(E(Y|X_i, X_j))$  measures the joint effect of the pair  $(X_i, X_j)$   
 44 on  $Y$ , and, from now on we will denote the joint effect by  $V_{ij}^c$ . The term

01      $V(f_{ij})$  is the joint effect of  $X_i$  and  $X_j$  minus the first-order effects for the  
 02     same factors.  $V(f_{ij})$  is known as a second-order, or two-way, effect (Box  
 03     *et al.*, 1978). Analogous formulas can be written for higher-order terms,  
 04     enabling the analyst to quantify the higher-order interactions.

05     By condensing the notation of the variances, i.e.  $V(f_i) = V_i$ ,  $V(f_{ij}) = V_{ij}$ ,  
 06     and so on, and by square integrating each term of the decomposition (4.5)  
 07     over  $\Omega^k$ , we can write the so-called ANOVA-HDMR decomposition:<sup>5</sup>

$$09 \quad V(Y) = \sum_i V_i + \sum_i \sum_{j>i} V_{ij} + \dots + V_{12\dots k}. \quad (4.11)$$

11     Dividing both sides of the equation by  $V(Y)$ , we obtain

$$14 \quad \sum_i S_i + \sum_i \sum_{j>i} S_{ij} + \sum_i \sum_{j>i} \sum_{l>j} S_{ijl} + \dots + S_{12\dots k} = 1 \quad (4.12)$$

16     which we already know from Chapter 1.

17     We recall that the number of these terms increases exponentially with the  
 18     number of input factors.

20     Exercise 5, part 2, provides an example of the computation of partial  
 21     variances and sensitivity indices for the same analytic case used for the  
 22     functional decomposition in Section 4.3.

## 25     4.5 TOTAL EFFECTS

27     Total effects are a direct consequence of Sobol's variance decomposition  
 28     approach and estimation procedure, although they were explicitly intro-  
 29     duced and made computationally affordable by other investigators (see  
 30     Homma and Saltelli, 1996; Saltelli, 2002).

31     The total effect index accounts for the total contribution to the output  
 32     variation due to factor  $X_i$ , i.e its first-order effect plus all higher-order  
 33     effects due to interactions.

34     For a three-factor model, for example, the total effect of  $X_1$  is the sum  
 35     of all the terms in Equation (4.12) where the factor  $X_1$  is considered:

$$37 \quad S_{T1} = S_1 + S_{12} + S_{13} + S_{123}. \quad (4.13)$$

---

40     <sup>5</sup> This is because of the orthogonality properties between any pair of terms in the expansion  
 41     (see Exercise 5, part 3). Note that this variance decomposition holds only when the input  
 42     factors  $X_i$  are independent (i.e. orthogonal). When the input factors are not independent of  
 43     one another, the quantities  $V_i$ ,  $V_{ij}^c$ ,  $V_{ijl}^c$  retain their meaning but are no longer related to one  
 44     another via (4.11).

In this example, the total index is composed of four terms. Total indices are useful in sensitivity analysis, as they give information on the nonadditive features of the model. As mentioned, for a purely additive model  $\sum_{i=1}^k S_i = 1$ , while for a given factor  $X_j$  a significant difference between  $S_{Tj}$  and  $S_j$  signals important interaction involving that factor. The total indices could be calculated in principle by computing all the terms in the decomposition (4.12), but there are as many as  $2^k - 1$  of these. There are techniques that enable us to estimate total indices at the same cost of first-order indices (such as the Sobol' technique, see Homma and Saltelli (1996)), thus circumventing the so-called ‘curse of dimensionality’. We customarily compute the set of all  $S_i$  plus the set of all  $S_{Ti}$  to obtain a fairly good description of the model sensitivities at a reasonable cost. We will see how to compute these indices in the next section.

The total effect measure provides the educated answer to the question: ‘Which factor can be fixed anywhere over its range of variability without affecting the output?’ The condition  $S_{Ti} = 0$  is necessary and sufficient for  $X_i$  to be a noninfluential factor. If  $S_{Ti} \cong 0$ , then  $X_i$  can be fixed at any value within its range of uncertainty without appreciably affecting the value of the output variance  $V(Y)$ . The approximation error that is made when this model simplification is carried out depends on the value of  $S_{Ti}$  (see Sobol' *et al.*, 2007). Total indices are suitable for the factor fixing setting.

We recall from Chapter 1 that the unconditional variance can be decomposed into main effect and residual:

$$V(Y) = V(E(Y|X_i)) + E(V(Y|X_i)). \quad (4.14)$$

Another way to find the total index is to decompose the output variance  $V(Y)$  again, in terms of main effect and residual, conditioning this time with respect to all the factors but one, i.e.  $X_{\sim i}$ :

$$V(Y) = V(E(Y|X_{\sim i})) + E(V(Y|X_{\sim i})). \quad (4.15)$$

The measure  $V(Y) - V(E(Y|X_{\sim i})) = E(V(Y|X_{\sim i}))$  is the remaining variance of  $Y$  that would be left, on average, if we could determine the true values of  $X_{\sim i}$ . The average is calculated over all possible combinations of  $X_{\sim i}$ , since  $X_{\sim i}$  are uncertain factors and their ‘true values’ are unknown. Dividing by  $V(Y)$  we obtain the total effect index for  $X_i$ :

$$S_{Ti} = \frac{E[V(Y|X_{\sim i})]}{V(Y)} = 1 - \frac{V[E(Y|X_{\sim i})]}{V(Y)}. \quad (4.16)$$

## 01           4.6 HOW TO COMPUTE THE SENSITIVITY INDICES 02

03     In this section we describe the Monte-Carlo based numerical procedure for  
04     computing the full set of first-order and total-effect indices for a model of  
05      $k$  factors.

06     This procedure is the best available today for computing indices based  
07     purely on model evaluations. Additional procedures are described in the  
08     next chapter, based on emulators, i.e. on the ability to generate estimates  
09     of model output at untried points without rerunning the simulation model.  
10     The method offered here is attributable to Saltelli (2002) and represents an  
11     extension of the original approach provided by Sobol' (1990) and Homma  
12     and Saltelli (1996).

13     At first sight, it might seem that the computational strategy for the  
14     estimation of conditional variances such as  $V(E(Y|X_i))$  and  $V(E(Y|X_i, X_j))$   
15     would be the cumbersome, brute-force computation of the multidimen-  
16     sional integrals in the space of the input factors. To obtain, for example,  
17      $V(E(Y|X_i))$ , one would first use a set of Monte Carlo points to estimate  
18     the inner expectation for a fixed value of  $X_i$ , and then repeat the proce-  
19     dure many times for different  $X_i$  values to estimate the outer variance. To  
20     give an indication, if 1000 points were used to get a good estimate of the  
21     conditional mean  $E(Y|X_i)$ , and the procedure were repeated 1000 times to  
22     estimate the variance, then we would need  $10^6$  points just for one sensitivity  
23     index.

24     This is in fact not necessary, as the computation can be accelerated via  
25     existing short cuts. In the following, we describe the instrument proposed  
26     by Saltelli:

- 27     • Generate a  $(N, 2k)$  matrix of random numbers ( $k$  is the number of inputs)  
28       and define two matrices of data ( $A$  and  $B$ ), each containing half of the  
29       sample (see 4.17 and 4.18).  $N$  is called a base sample; to give an order  
30       of magnitude,  $N$  can vary from a few hundreds to a few thousands.  
31       Sobol' recommends using sequences of quasi-random numbers (Sobol',  
32       1967, 1976). The software to generate these sequences is freely available  
33       (SIMLAB, 2007).

$$40 \quad A = \begin{bmatrix} x_1^{(1)} & x_2^{(1)} & \dots & x_i^{(1)} & \dots & x_k^{(1)} \\ x_1^{(2)} & x_2^{(2)} & \dots & x_i^{(2)} & \dots & x_k^{(2)} \\ \dots & \dots & \dots & \dots & & \dots \\ x_1^{(N-1)} & x_2^{(N-1)} & \dots & x_i^{(N-1)} & \dots & x_k^{(N-1)} \\ x_1^{(N)} & x_2^{(N)} & \dots & x_i^{(N)} & \dots & x_k^{(N)} \end{bmatrix} \quad (4.17)$$

$$B = \begin{bmatrix} x_{k+1}^{(1)} & x_{k+2}^{(1)} & \cdots & x_{k+i}^{(1)} & \cdots & x_{2k}^{(1)} \\ x_{k+1}^{(2)} & x_{k+2}^{(2)} & \cdots & x_{k+i}^{(2)} & \cdots & x_{2k}^{(2)} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ x_{k+1}^{(N-1)} & x_{k+2}^{(N-1)} & \cdots & x_{k+i}^{(N-1)} & \cdots & x_{2k}^{(N-1)} \\ x_{k+1}^{(N)} & x_{k+2}^{(N)} & \cdots & x_{k+i}^{(N)} & \cdots & x_{2k}^{(N)} \end{bmatrix}. \quad (4.18)$$

- Define a matrix  $C_i$  formed by all columns of  $B$  except the  $i$ th column, which is taken from  $A$ :

$$C_i = \begin{bmatrix} x_{k+1}^{(1)} & x_{k+2}^{(1)} & \cdots & x_i^{(1)} & \cdots & x_{2k}^{(1)} \\ x_{k+1}^{(2)} & x_{k+2}^{(2)} & \cdots & x_i^{(2)} & \cdots & x_{2k}^{(2)} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ x_{k+1}^{(N-1)} & x_{k+2}^{(N-1)} & \cdots & x_i^{(N-1)} & \cdots & x_{2k}^{(N-1)} \\ x_{k+1}^{(N)} & x_{k+2}^{(N)} & \cdots & x_i^{(N)} & \cdots & x_{2k}^{(N)} \end{bmatrix}. \quad (4.19)$$

- Compute the model output for all the input values in the sample matrices  $A$ ,  $B$ , and  $C_i$ , obtaining three vectors of model outputs of dimension  $N \times 1$ :

$$y_A = f(A) \quad y_B = f(B) \quad y_{C_i} = f(C_i). \quad (4.20)$$

We anticipate that these vectors are all we need to compute the first- and total-effect indices  $S_i$  and  $S_{Ti}$ , for a given factor  $X_i$ . Because there are  $k$  factors, the cost of this approach is  $N + N$  runs of the model for matrices  $A$ ,  $B$ , plus  $k$  times  $N$  to estimate  $k$  times the output vector corresponding to matrix  $C_i$ . The total cost is hence  $N(k+2)$ , much lower than the  $N^2$  runs of the brute-force method.

Our recommended method estimates first-order sensitivity indices as follows:

$$S_i = \frac{V[E(Y|X_i)]}{V(Y)} = \frac{y_A \cdot y_{C_i} - f_0^2}{y_A \cdot y_A - f_0^2} = \frac{(1/N) \sum_{j=1}^N y_A^{(j)} y_{C_i}^{(j)} - f_0^2}{(1/N) \sum_{j=1}^N (y_A^{(j)})^2 - f_0^2} \quad (4.21)$$

where

$$f_0^2 = \left( \frac{1}{N} \sum_{j=1}^N y_A^{(j)} \right)^2 \quad (4.22)$$

is the mean, and the symbol  $(\cdot)$  denotes the scalar product of two vectors.

Similarly, the method estimates total-effect indices as follows:

$$S_{Ti} = 1 - \frac{V[E(Y|\mathbf{X}_{\sim i})]}{V(Y)} = 1 - \frac{y_B \cdot y_{C_i} - f_0^2}{y_A \cdot y_A - f_0^2} = 1 - \frac{(1/N) \sum_{j=1}^N y_B^{(j)} y_{C_i}^{(j)} - f_0^2}{(1/N) \sum_{j=1}^N (y_B^{(j)})^2 - f_0^2}. \quad (4.23)$$

01 Why do these formulas work? We offer here a ‘hand waving’ explanation  
 02 of (4.21). In the scalar product  $y_A \cdot y_{C_i}$  values of  $Y$  computed from  $A$  are  
 03 multiplied by values of  $Y$  for which all factors but  $X_i$  are resampled while  
 04 the values of  $X_i$  remain fixed. If  $X_i$  is noninfluential, then high and low  
 05 values of  $y_A$  and  $y_{C_i}$  are randomly associated. If  $X_i$  is influential, then high  
 06 (or low) values of  $y_A$  will be preferentially multiplied by high (or low) values  
 07 of  $y_{C_i}$  increasing the value of the resulting scalar product. We leave to the  
 08 reader the task of understanding (4.23). (Hint: the scalar product  $y_B \cdot y_{C_i}$   
 09 gives the first-order effect of non- $X_i$ .)

10 Note that the accuracy of both  $f_0$  and  $V(Y)$  can be improved by using  
 11 both  $y_A$  and  $y_B$  points rather than just  $y_A$  in Equations (4.21) and (4.23) (see  
 12 Saltelli, 2002). This will improve the accuracy of the estimates for  $S_i$  and  
 13  $S_{Ti}$ , although the factors’ ranking will remain unchanged. Error estimates  
 14 for Equations (4.21) and (4.23) can be obtained by bootstrapping data  
 15 points from vectors  $y_A$ ,  $y_B$  and  $y_{C_i}$ . Alternatively, the error in the numerical  
 16 estimates can be evaluated using the probable error associated with the  
 17 crude Monte Carlo estimate.

18 The probable error is the error which will not be exceeded by 50 percent  
 19 of the cases, and corresponds to 0.6745<sup>6</sup> times the standard error.

20 For example, the probable error in  $V_{X_i}[E(Y|X_i)]$  (that will not be exceeded  
 21 by the error in the estimate with 50% probability) is:

$$22 \\ 23 P.E. = \frac{0.6745}{\sqrt{N}} \sqrt{\sum_{j=1}^N (y_A^{(j)} y_{C_i}^{(j)})^2 - \left( \sum_{j=1}^N y_A^{(j)} y_{C_i}^{(j)} \right)^2}.$$

26 Before using the sensitivity measures in our case studies, let us recall  
 27 some of the properties of sensitivity indices that will prove useful in the  
 28 interpretation of the results:

- 30 • Whatever the strength of the interactions in the model,  $S_i$  indicates by  
 31 how much one could reduce, on average, the output variance if  $X_i$  could  
 32 be fixed; hence, it is a measure of main effect.
- 33 • Whatever the interactions in the model,  $S_{i_1, i_2, \dots, i_s}^c$  indicates by how  
 34 much the variance could be reduced, on average, if one could fix  
 35  $X_{i_1}, X_{i_2}, \dots, X_{i_s}$ . We recall that ‘ $c$ ’ denotes the joint effect.
- 36 • By definition,  $S_{Ti}$  is greater than  $S_i$ , or equal to  $S_i$  in the case that  $X_i$  is  
 37 not involved in any interaction with other input factors. The difference

40  
 41 <sup>6</sup> The probability  $P_\delta$  that a random sample from a normally distributed universe will have a  
 42 mean  $m$  within a distance  $|\delta|$  of the mean  $\mu$  of the universe is  $P_\delta = 2\Phi(|\delta|)$  where  $\Phi(z)$  is the  
 43 standard normal distribution function and  $\delta$  is the observed value of  $z = \frac{\bar{X} - \mu}{\sigma/\sqrt{N}}$ .

44 The value  $\delta^*$  of  $\delta$  such that  $P_\delta = \frac{1}{2}$ , is given by  $\delta^* = \sqrt{2} \cdot \text{erf}^{-1}\left(\frac{1}{2}\right) = 0.6745$ .

- 01       $S_{T_i} - S_i$  is a measure of how much  $X_i$  is involved in interactions with any  
 02      other input factor.  
 03      •  $S_{T_i} = 0$  implies that  $X_i$  is noninfluential and can be fixed anywhere in its  
 04      distribution without affecting the variance of the output.  
 05      • The sum of all  $S_i$  is equal to 1 for additive models and less than 1  
 06      for nonadditive models. The difference  $1 - \sum_i S_i$  is an indicator of the  
 07      presence of interactions in the model.  
 08      • The sum of all  $S_{T_i}$ s is always greater than 1. It is equal to 1 if the model  
 09      is perfectly additive.
- 10
- 11
- 12

## 4.7 FAST AND RANDOM BALANCE DESIGNS

13      The classic Fourier Amplitude Sensitivity Test (FAST) method (Cukier *et al.*,  
 14      1978) is based on selecting  $N$  design points over a particular space-filling  
 15      curve in the  $k$ th dimensional input space, built so as to explore each factor  
 16      with a different (integer) frequency  $(\omega_1, \omega_2, \dots, \omega_k)$ . A quite complex algo-  
 17      rithm is used to set the frequencies such that they are free of interferences  
 18      up to a given order  $M$  ( $M = 6$  is usually considered sufficient). The computa-  
 19      tional model is run at each design point and the Fourier spectrum is  
 20      calculated on the model output at specific frequencies  $(\omega_i, 2\omega_i, \dots, M\omega_i)$   
 21      to estimate the sensitivity index of factor  $X_i$ . It is important that none of  
 22      the higher harmonics of  $\omega_1, \omega_2, \dots, \omega_k$  interfere until order  $M$ , so that the  
 23      Fourier spectrum at a given frequency corresponds uniquely to factor  $X_i$ .  
 24      The design points are selected as follows:

25

26

$$X_i(s_j) = G_i(\sin \omega_i s_j), \quad \forall i = 1, 2, \dots, k, \quad \forall j = 1, 2, \dots, N \quad (4.24)$$

27

28

29

30      where  $X_i$  is the  $i$ th input factor, the functions  $G_i$  are chosen according to  
 31      the desired pdf of  $X_i$ ,  $s_j$  is the parametric variable varying in  $(-\pi, \pi)$  which  
 32      is sampled over its range using  $N$  points, and  $\omega_i$  are the frequencies.

33

34      In Random Balance Designs (RBD) (Tarantola *et al.*, 2006)  $N$  points are  
 35      selected over a curve in the input space using a frequency equal to 1 for each  
 36      factor. The curve covers only a subset of the input space. Then independent  
 37      random permutations are applied to the coordinates of the  $N$  points in  
 38      order to generate the design points. The computational model is evaluated  
 39      at each design point. Subsequently, the model outputs are reordered such  
 40      that the design points are in increasing order with respect to factor  $X_i$ .  
 41      The Fourier spectrum is calculated on the model output at the frequency  
 42      1 and at its higher harmonics (2, 3, 4, 5, 6) and yields the estimate of  
 43      the sensitivity index of factor  $X_i$ . The same model outputs are reordered  
 44      with respect to each other factor (and the Fourier spectra are calculated

accordingly) to obtain all the other sensitivity indices. The design points are chosen as follows:

$$X_i(s_{ij}) = G_i(\sin \omega s_{ij}), \quad \forall i = 1, 2, \dots, k, \quad \forall j = 1, 2, \dots, N \quad (4.25)$$

where  $(s_{i1}, s_{i2}, \dots, s_{iN})$  denotes the  $i$ th random permutation of the  $N$  points. Equation (4.25) provides a different random permutation for each factor  $X_i$ .

For RBD the model is evaluated  $N$  times over the sample of size  $N$ :

$$Y(s_j) = f(X_1(s_{1j}), X_2(s_{2j}), \dots, X_k(s_{kj})) \quad \forall j = 1, 2, \dots, N. \quad (4.26)$$

The values of model output  $Y(s_j)$ ,  $j = 1, \dots, N$  are then reordered ( $Y^R(s_j)$ ) such that the corresponding values of  $X_i(s_{ij})$  are ranked in increasing order. The sensitivity of  $Y$  to  $X_i$  is quantified by the Fourier spectrum of the reordered model output:

$$F(\omega) = \left| \frac{1}{\pi} \sum_{j=1}^N Y^R(s_j) \exp(-i\omega s_j) \right|^2 \quad (4.27)$$

evaluated at  $\omega = 1$  and its higher harmonics (2, 3, 4, 5, 6). In the discrete case:

$$\widehat{V}_i = V[E(Y|X_i)] = \sum_{l=1}^M F(\omega)|_{\omega=l} = \sum_{l=1}^M R(l). \quad (4.28)$$

This is an estimate of the main effect  $V_i$ . The procedure is repeated for all factors, whereby the same set of model outputs is simply reordered according to  $X_i(s_{ij})$  and (4.27) and (4.28) are used to estimate  $V_i$ ,  $i = 2, \dots, k$ .

Here we provide the basic *Matlab*<sup>®</sup> code to compute a generic sensitivity index according to the RBD method:

```
s0=[-pi:2*pi/N:pi]';
s=s0(randperm(N))'; % Performs a random permutation of the integers
from 1 to N
x=.5+asin(sin(1*s))/pi; % (see (4.25))
[dummy,index]=sort(s); % orders the elements of s in ascending order
Y=model(x)
yr=y(index);
spectrum=(abs(fft(yr))).^2/N; % fft is the fast Fourier transform
V1=2*sum(spectrum(2:M+1)); % (see 4.28)
V=sum(spectrum(2:N));
S1=V1/V;
Random Balance Designs have a number of advantages with respect to
FAST:
```

- 01     • the absence of a lower limit for the size  $N$  of the design points (FAST  
02     has the problem of aliasing, so a minimum sample size is required and  
03     this minimum size increases with the dimensionality  $k$ );  
04     • the nonnecessity to have an algorithm to search for frequencies free of  
05     interferences;  
06     • better accuracy in the estimates, which are not influenced by interferences;  
07     • the possibility to select larger values of the order  $M$  without affecting  
08     the sample size  $N$ .  
09     • contrary to the method of Saltelli, each model run contributes to the  
10     estimation of all the first-order indices.

12     The disadvantage of the RBD method is that it allows the computation of  
13     first-order terms only; we can use the sum of these to check if the model  
14     is additive. If the sum is noticeably smaller than 1 we must use another  
15     algorithm to compute interactions or total-effect terms. The main advantage  
16     of RBD is that it is relatively easy to implement, and the sample size  $N$ ,  
17     being independent of the number of factors  $k$ , can lead to a considerable  
18     saving in computer time for expensive models.  
19

#### 20 21 22 23     4.8 PUTTING THE METHOD TO WORK: THE 24         INFECTION DYNAMICS MODEL 25

26     Let us consider an infective process at its early stage, where  $I$  is the number  
27     of infected individuals at time  $t$  and  $S$  is the number of individuals suscep-  
28     tible to infection at time  $t$ .  
29

30     We assume that the infection is propagated through some kind of contact  
31     between individuals who, especially at the early stage, do not take any  
32     precaution to avoid contagion.

33     It is reasonable to assume that the number of contacts per unit time is  
34     proportional to the number of individuals in each group (i.e. to  $I \times S$ ) via a  
35     contact coefficient  $k < 1$ . Also, the number of infections is proportional to  
36     the number of contacts through an ‘infection coefficient’ ( $\gamma < 1$ ), which is  
37     the likelihood that the infection is passed on during a given contact.

38     Depending on the dangerousness of the infection, the infected individuals  
39     will end up in either of two ways: by recovering or by dying. It is presumed  
40     that recovery and death rates ( $r$  and  $\delta$ ) are proportional to the number of  
41     infected individuals.

42     The number of susceptible individuals decreases with the number of infec-  
43     tions, but can increase with new births  $b$ , proportional to  $S$ , or migration  
44     which happens at a constant rate  $m$ .

Two equations describe the dynamics of  $I$  and  $S$ , representing the model of the infection process:

$$\frac{dI}{dt} = \gamma kIS - rI - \delta I \quad (4.29)$$

$$\frac{dS}{dt} = -\gamma kIS + bS + m. \quad (4.30)$$

Let us investigate the evolution of the infection at its early stage  $t \sim 0$ , when we presuppose that the number of the susceptible individuals is much larger than that of the infected ( $S(t) >> I(t)$ ), and that  $S$  is changing slowly ( $S(t) \sim S_0 = \text{const}$ ).

Equation (4.29) becomes linear and homogeneous:

$$\frac{dI}{dt} = (\gamma kS_0 - r - \delta)I. \quad (4.31)$$

The solution is  $I = I_0 \cdot \exp(Y)$ , where  $Y = \gamma kS_0 - r - \delta$ . If  $Y > 0$  the infection spreads, while if  $Y < 0$  the infection dies out.

Suppose that  $S_0 = 1000$  (a small village), and that factors are distributed as follows:

- Infection coefficient  $\gamma \sim U(0, 1)$ . The infection is at an early stage, and no information is available about how it is acting.
- Contact coefficient  $k \sim \text{beta}(2, 7)$ . This distribution describes the probability of a person to come into contact with other individuals. In other words, the probability of meeting all the inhabitants of the village (and of meeting nobody) is low, while the probability of meeting an average number of persons is higher.
- Recovery rate  $r \sim U(0, 1)$ . We assume this to be uniform, as we do not know how it behaves at the beginning of the propagation.
- Death rate  $\delta \sim U(0, 1)$ , for the same reason as  $r$ .

Let us calculate the sensitivity indices for the four factors using the method described in Section 4.6. The total number of model runs is  $N(k+2)=7680$  ( $N = 1280$  and  $k = 4$ ).

Let us analyse the sensitivity indices shown in Table 4.1. Negative signs are due to numerical errors in the estimates. Such negative values can often be encountered for the Saltelli method when the analytical sensitivity indices are close to zero (i.e. for unimportant factors). Increasing the sample size of the analysis reduces the probability of having negative estimates. FAST and RBD estimates are always positive, by construction.

The most influential factors are  $\gamma$  and  $k$ , while factors  $r$  and  $\delta$  are noninfluential as their total indices are negligible. The infection is likely to

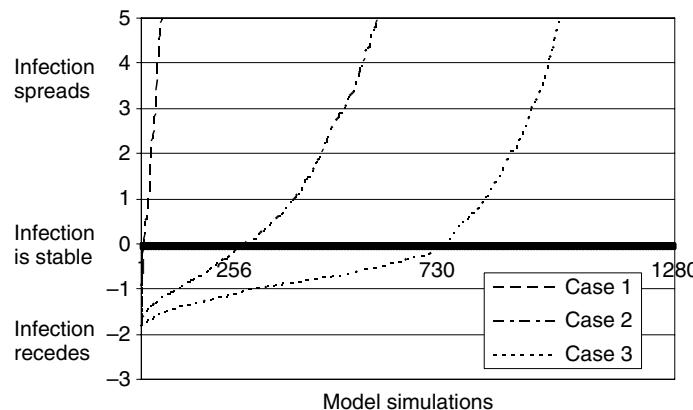
01                   **Table 4.1** First-order and total-effect sensitivity indices obtained  
 02                   with the method of Saltelli with  $k \sim \text{beta}(2, 7)$

03                   Factor	04                   First-order indices	05                   Total-order indices
05                   Infection ( $\gamma$ )	0.49	0.69
06                   Contact ( $k$ )	0.41	0.61
07                   Recovery ( $r$ )	-0.00	-0.00
08                   Death ( $\delta$ )	-0.00	-0.00

10                   spread proportionally to the number of contacts between people; unlike  $\gamma$ ,  
 11                   which depends on the virus strength,  $k$  is a controllable factor. This means  
 12                   that if the number of contacts could be reduced, the variability in the output  
 13                   would also be reduced.

14                   The sum of first-order effects is approximately 0.89, while the sum of  
 15                   the total indices is 1.29; as these two sums are both different from 1, there  
 16                   must be interactions among factors in the model. Moreover, given that both  
 17                   factors  $\gamma$  and  $k$  have total indices greater than their first orders, we conclude  
 18                   that they are taking part in interactions.

19                   With the model outputs calculated at the 1280 points sampled above,  
 20                   we perform uncertainty analysis (see Figure 4.1, case 1). The picture shows  
 21                   that the infection propagates in almost all cases (in 99.7% of the cases the  
 22                   sign of the model predictions is positive).



38                   **Figure 4.1** Uncertainty analysis for the three cases of the infection dynamics exercise.  
 39                   On the Y axis we plot the output variable of interest (if  $Y$  is positive the  
 40                   infection propagates, if it is negative the infection recedes and if it is zero – the  
 41                   X axis – the number of infected individuals is stable), and on the X axis the total  
 42                   number of model runs. Model outputs for each case are sorted in increasing order,  
 43                   so that each plot is a monotonic curve. As almost all model runs for the first case  
 44                   correspond to positive  $Y$ 's, many of which can be of the order of a hundred, the Y  
 axis is cut at +5 to visualize the plot around zero

Assume that, in consequence of this epidemic spread, some measures are taken in order to reduce the propagation of the disease. Following these new measures, which warn the inhabitants to avoid contacts, we assume that  $k$  is now distributed as  $k \sim \text{beta}(0.5, 10)$  (see Figure 4.2) and we repeat the sensitivity analysis to see how the relative importance of the factors has been modified. The results are reported in Table 4.2.

We observe that, in this new configuration, factor  $k$  becomes more important in controlling the spread of the infection.

This causes us to wonder whether the restriction is adequate to reduce the propagation of the infection. By looking at the output of the model, we see that the infection recedes in 20% of cases, while in 80% of cases it propagates (see Figure 4.1, case 2): that is a significant improvement with respect to the initial situation, but stronger measures could still be taken.

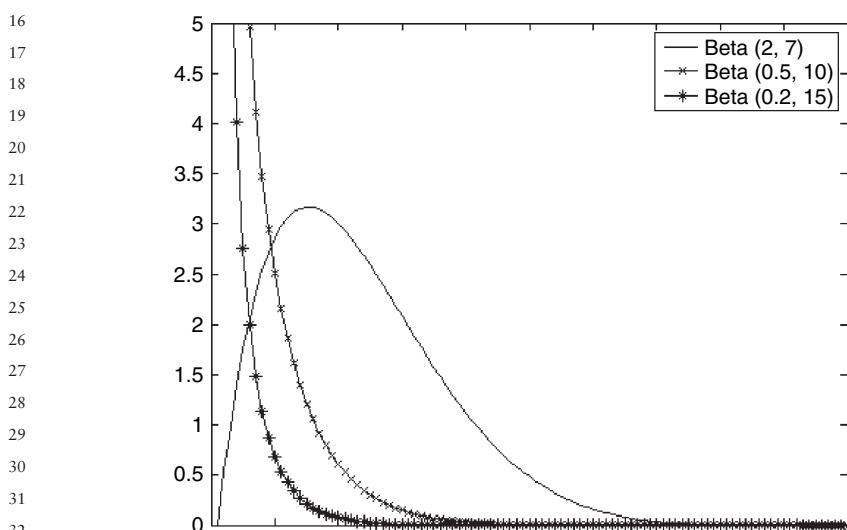


Figure 4.2 Beta distribution with different parameters

Table 4.2 First-order and total effect sensitivity indices obtained with the method of Saltelli with  $k \sim \text{beta}(0.5, 10)$

Factor	First-order indices	Total-order indices
Infection ( $\gamma$ )	0.14	0.36
Contact ( $k$ )	0.76	0.98
Recovery ( $r$ )	-0.00	-0.00
Death ( $\delta$ )	-0.00	-0.00

01 Assume that we implement additional restrictions on contact between  
 02 persons, which means further squeezing the distribution of  $k$  to the left-hand  
 03 side of its uncertainty range ( $k \sim \text{beta}(0.2, 15)$ , see Figure 4.2).

04 We observe in Table 4.3 that factor  $k$  becomes even more important,  
 05 while factor  $\gamma$  has less influence in controlling the spread of the infection.  
 06 The uncertainty analysis shows that in 57% of cases the infection recedes  
 07 (see Figure 4.1, case 3).

08 The present example is quite academic, yet it shows how information  
 09 obtained from sensitivity analysis (e.g. that the amount of contact between  
 10 people is the most important factor in determining the spread of the disease)  
 11 can help to inform decisions (e.g. designing measures to reduce people's  
 12 contact in order to control the infection's propagation).

13 We test the RBD method described in Section 4.7 on the same case study  
 14 selecting  $N = 1280$ , i.e. the same sample size that was employed for the  
 15 method of Saltelli. In the RBD method each model run contributes to the  
 16 estimation of all the sensitivity indices, while in the method of Saltelli it  
 17 contributes to the estimation of one single first-order index (and its related  
 18 total effect). In summary, RBD has better convergency properties than the  
 19 method of Saltelli, in the sense that, for a given sample size, RBD estimates  
 20 are more accurate (Tarantola *et al.*, 2006). We report the results for the  
 21 three configurations of  $k$  in Table 4.4.

22 RBD produces indices for important factors (i.e. infection and contact)  
 23 which are similar to those obtained with the method of Saltelli. Although  
 24 the nonrelevant factors (recovery and death) are somewhat overestimated  
 25  
 26

27 **Table 4.3** First-order and total-effect sensitivity indices obtained  
 28 with the method of Saltelli with  $k \sim \text{beta}(0.2, 15)$

Factor	First-order indices	Total-order indices
Infection ( $\gamma$ )	0.05	0.32
Contact ( $k$ )	0.77	1.05
Recovery ( $r$ )	-0.00	-0.00
Death ( $\delta$ )	0.00	0.00

37 **Table 4.4** RBD method first-order sensitivity indices

Factor	$k \sim \text{beta}(2, 7)$	$k \sim \text{beta}(0.5, 10)$	$k \sim \text{beta}(0.2, 15)$
Infection ( $\gamma$ )	0.43	0.13	0.05
Contact ( $k$ )	0.41	0.58	0.65
Recovery ( $r$ )	0.01	0.01	0.01
Death ( $\delta$ )	0.01	0.01	0.01

01 by RBD, this is a minor problem, since they can anyhow be identified as  
 02 noninfluential.

## 05 4.9 CAVEATS

07 Variance-based methods are powerful in quantifying the relative importance  
 08 of input factors or groups. The main drawback of variance-based methods  
 09 is the cost of the analysis, which, in the case of computationally intensive  
 10 models, can become prohibitive even when using the approach described  
 11 above.

12 With Saltelli's method,  $N(k+2)$  runs for a full set of  $S_i$  and  $S_{Ti}$  require  
 13 that for a model with 15 factors we need to execute the model at least  
 14 17 000 times, taking  $N = 1000$ . Using random balance designs with just  
 15  $N$  model executions we can compute the full set of  $S_i$ , but the  $S_{Ti}$  would  
 16 remain unknown.

17 In terms of computational time, thousands or tens of thousands of model  
 18 executions can be either trivial or unfeasible, depending on the model at  
 19 hand. A viable alternative for computationally expensive models is the  
 20 screening method discussed in Chapter 3. The elementary effect test is a  
 21 good proxy for the total sensitivity indices.

22 If the model is both expensive to run and rich in factors we recommend  
 23 using the elementary effect method to reduce the number of factors and  
 24 then running a variance-based analysis on a reduced set of factors.

## 27 4.10 EXERCISES

### 29 Exercise 1

31 Let us consider the model  $Y = \sum_{j=1}^k X_j$  where  $k=3$ ,  $X_j \sim U(\bar{x}_j - \sigma_j, \bar{x}_j +$   
 32  $\sigma_j)$ ,  $\bar{x}_j = 3^{j-1}$  and  $\sigma_j = 0.5\bar{x}_j$ .

33 Calculate the first-order sensitivity indices for the  $k$  factors.

34 First we calculate the expected value and the variance for the model.

$$36 Y = X_1 + X_2 + X_3$$

$$37 \bar{X}_1 = 1$$

$$39 \bar{X}_2 = 3$$

$$40 \bar{X}_3 = 9$$

$$42 \sigma_1 = 0.5$$

$$43 \sigma_2 = 1.5$$

01                    $\sigma_3 = 4.5$   
 02                    $X_1 \sim U(0.5, 1.5)$   
 03                    $X_2 \sim U(1.5, 4.5)$   
 04                    $X_3 \sim U(4.5, 13.5)$   
 05  
 06                    $E(Y) = E(X_1) + E(X_2) + E(X_3) = 1 + 3 + 9 = 13.$   
 07

08                   Next we compute the variance as  
 09

10                    $V(X_i) = E(X_i)^2 - E^2(X_i) = p(X_i) \int_a^b X_i^2 dx_i - E^2(X_i).$       (4.32)  
 11  
 12

13                   So in our case we will have  
 14  
 15                    $V(X_1) = \int_{0.5}^{1.5} X_1^2 dx_1 - 1 = \frac{1}{12}$   
 16  
 17                    $V(X_2) = \frac{1}{3} \int_{1.5}^{4.5} X_2^2 dx_2 - 9 = \frac{3}{4}$   
 18  
 19                    $V(X_3) = \frac{1}{9} \int_{4.5}^{13.5} X_3^2 dx_3 - 81 = \frac{27}{4}$   
 20  
 21                    $V(Y) = V(X_1) + V(X_2) + V(X_3) = \frac{1}{12} + \frac{3}{4} + \frac{27}{4} = \frac{91}{12}.$   
 22  
 23

24                   We compute the variance of the conditional expectation  $V_{X_j}[E(Y|X_j)]$  and  
 25                   the expected residual variance  $E_{X_j}[V(Y|X_j)].$   
 26

27                    $V_{X_1}[E(Y|X_1)] = V(X_1) = \frac{1}{12}$   
 28  
 29                    $V_{X_2}[E(Y|X_2)] = V(X_2) = \frac{9}{12}$   
 30  
 31                    $V_{X_3}[E(Y|X_3)] = V(X_3) = \frac{81}{12}$   
 32  
 33                    $E_{X_1}[V(Y|X_1)] = V(Y) - V_{X_1}[E(Y|X_1)] = \frac{91}{12} - \frac{1}{12} = \frac{90}{12}$   
 34  
 35                    $E_{X_2}[V(Y|X_2)] = V(Y) - V_{X_2}[E(Y|X_2)] = \frac{91}{12} - \frac{9}{12} = \frac{82}{12}$   
 36  
 37                    $E_{X_3}[V(Y|X_3)] = V(Y) - V_{X_3}[E(Y|X_3)] = \frac{91}{12} - \frac{81}{12} = \frac{10}{12}.$   
 38  
 39

40                   Now we have all what we need to find the first-order indices:  
 41

42                    $S_1 = \frac{V_{X_1}[E(Y|X_1)]}{V(Y)} = \frac{1/12}{91/12} = \frac{1}{91}$   
 43  
 44

$$S_2 = \frac{V_{X_2}[E(Y|X_2)]}{V(Y)} = \frac{9/12}{91/12} = \frac{9}{91}$$

$$S_3 = \frac{V_{X_3}[E(Y|X_3)]}{V(Y)} = \frac{81/12}{91/12} = \frac{81}{91}.$$

The model is additive, which means that there are no interactions among factors.

### Exercise 2

Consider now the model  $Y = X_1 + X_2$  where  $X_1, X_2$  are normally distributed. We also know that  $\bar{x}_1 = 1, \bar{x}_2 = 2$  and  $\sigma_1 = 2, \sigma_2 = 3$ .

Compute the expected value and the variance for model Y.

$$E(Y) = E(X_1) + E(X_2) = 1 + 2 = 3.$$

In this case, as factors are normally distributed, we can calculate the variance in an easier way:

$$V(Y) = V(X_1) + V(X_2) = \sigma_1^2 + \sigma_2^2 = 4 + 9 = 13. \quad (4.33)$$

Calculate the first-order sensitivity indices for the two factors:

$$S_1 = \frac{V_{X_1}[E(Y|X_1)]}{V(Y)} = \frac{4}{13}$$

$$S_2 = \frac{V_{X_2}[E(Y|X_2)]}{V(Y)} = \frac{9}{13}.$$

Also in this case the model is additive, without interactions among factors.

### Exercise 3

Two input factors are normally distributed in the model

$$Y = X_1 \times X_2,$$

with parameters  $\mu_1 = 1, \mu_2 = 2, \sigma_1 = 3$  and  $\sigma_2 = 2$ .

Calculate the first- and second-order indices for the inputs and comment on the level of additivity of the model.

$$V(Y) = \mu_{X_1}^2 \sigma_{X_2}^2 + \mu_{X_2}^2 \sigma_{X_1}^2 + \sigma_{X_1}^2 \sigma_{X_2}^2 = 76.$$

$$S_{X_1} = \frac{\mu_{X_2}^2 \sigma_{X_1}^2}{V(Y)} = \frac{9}{19}$$

$$S_{X_2} = \frac{\mu_{X_1}^2 \sigma_{X_2}^2}{V(Y)} = \frac{1}{19}$$

$$S_{X_1, X_2} = \frac{\sigma_{X_1}^2 \sigma_{X_2}^2}{V(Y)} = \frac{9}{19}.$$

Factor  $X_1$  is the most influential in determining the output variance (its first-order index is high). Factor  $X_2$  has a low first-order index and is thus apparently less important.

Yet the interaction effect  $S_{X_1, X_2}$  is as high as the first-order effect of factor  $X_1$ . This means that the output variance is significantly driven by the two factors' interaction, even if factor  $X_2$  appears to be noninfluential. This shows that ignoring interactions could lead to serious type II errors.<sup>7</sup>

#### Exercise 4

A model has eight input factors, but for computational cost's reasons we need to reduce the number of factors to five.

The model is

$$Y = \sum_{i=1}^8 X_i$$

where  $X_i$  are normally distributed as follows:

$$\begin{aligned} X_1 &\sim N(0, 1) \\ X_2 &\sim N(2, 2) \\ X_3 &\sim N(1, 3) \\ X_4 &\sim N(1, 5) \\ X_5 &\sim N(3, 1) \\ X_6 &\sim N(4, 1) \\ X_7 &\sim N(1, 2) \\ X_8 &\sim N(5, 5) \end{aligned}$$

1. Calculate the first-order sensitivity indices and identify the three least important factors, in order to exclude them from the model.
2. Recalculate the first orders for the remaining five factors and find out which are the most influential: if we decide to fix them at a given value in their range of variation, by what amount will the variance of the output be reduced?

---

<sup>7</sup> That is, ignoring the influence of an influential factor. This is typically the most serious, nonconservative error. On the other hand type I error means considering a noninfluential factor as influential.

01       1. We first calculate the output variance of the model:

02  
03        $V(Y) = \sum_{i=1}^8 V(X_i) = 1 + 4 + 9 + 25 + 1 + 1 + 4 + 25 = 70.$

04  
05

06       Now it is easy to derive the first-order sensitivity indices for all input  
07       factors:

08        $S_1 = \frac{V_{X_1}[E(Y|X_1)]}{V(Y)} = \frac{1}{70} = 0.01$   
09  
10  
11        $S_2 = \frac{V_{X_2}[E(Y|X_2)]}{V(Y)} = \frac{4}{70} = 0.06$   
12  
13        $S_3 = \frac{V_{X_3}[E(Y|X_3)]}{V(Y)} = \frac{9}{70} = 0.13$   
14  
15  
16        $S_4 = \frac{V_{X_4}[E(Y|X_4)]}{V(Y)} = \frac{25}{70} = 0.36$   
17  
18  
19        $S_5 = \frac{V_{X_5}[E(Y|X_5)]}{V(Y)} = \frac{1}{70} = 0.01$   
20  
21  
22        $S_6 = \frac{V_{X_6}[E(Y|X_6)]}{V(Y)} = \frac{1}{70} = 0.01$   
23  
24        $S_7 = \frac{V_{X_7}[E(Y|X_7)]}{V(Y)} = \frac{4}{70} = 0.06$   
25  
26  
27        $S_8 = \frac{V_{X_8}[E(Y|X_8)]}{V(Y)} = \frac{25}{70} = 0.36.$   
28

29       The three least influential factors are  $X_1, X_5$  and  $X_6$ , each one  
30       accounting for 1% of the output variance.

31       2. We discard the nonimportant factors from the model and we repeat  
32       the calculations with only the five remaining factors. We now have a  
33       new output variance:  
34

35        $V(Y) = \sum_{i=1}^5 V(X_i) = 4 + 9 + 25 + 4 + 25 = 67,$   
36  
37

38       and new elementary effects for the inputs:  
39

40        $S_1 = \frac{V_{X_1}[E(Y|X_1)]}{V(Y)} = \frac{4}{67} = 0.06$   
41  
42  
43        $S_2 = \frac{V_{X_2}[E(Y|X_2)]}{V(Y)} = \frac{9}{67} = 0.14$   
44

$$S_3 = \frac{V_{X_3}[E(Y|X_3)]}{V(Y)} = \frac{25}{67} = 0.37$$

$$S_4 = \frac{V_{X_4}[E(Y|X_4)]}{V(Y)} = \frac{4}{67} = 0.06$$

$$S_5 = \frac{V_{X_5}[E(Y|X_5)]}{V(Y)} = \frac{25}{67} = 0.37.$$

We see that the two most influential factors are  $X_3$  and  $X_5$ , each one determining 37% of the output variance.

If we decide to fix those two factors at a given value in their range of variation, we will have only three factors varying, i.e. factors  $X_1, X_2$  and  $X_4$ . In such a situation, the model will have a lower variance:

$$V(Y) = \sum_{i=1}^3 V(X_i) = 4 + 9 + 4 = 17.$$

We conclude that, in this example, by fixing the two most important factors the output variance decreases from 76 to 17, with a reduction of 75%.

## Exercise 5

- Calculate the expansion of  $f$  into terms of increasing dimensionality (4.5) for the function (Ishigami and Homma, 1996):

$$f(X_1, X_2, X_3) = \sin X_1 + a \sin^2 X_2 + b X_3^4 \sin X_1. \quad (4.34)$$

The input probability density functions are assumed as follows:<sup>8</sup>

$$p_i(X_i) = \frac{1}{2\pi},$$

when  $-\pi \leq X_i \leq \pi$  and

$$p_i(X_i) = 0,$$

when  $X_i < -\pi, X_i > \pi$  for  $i = 1, 2, 3$ .

---

<sup>8</sup> Note that this does not contradict the assumption that all factors are uniformly distributed within the unit hypercube  $\Omega$ . It is always possible to map the hypercube to the desired distribution, and the sensitivity measure relative to the hypercube factors is identical to the measure for the transformed factors.

We calculate the decomposition of the function as (4.5) for  $k = 3$ :

$$\begin{aligned} f(X_1, X_2, X_3) &= f_0 + f_1(X_1) + f_2(X_2) + f_3(X_3) + f_{12}(X_1, X_2) \\ &\quad + f_{13}(X_1, X_3) + f_{23}(X_2, X_3) + f_{123}(X_1, X_2, X_3). \end{aligned}$$

Thus

$$\begin{aligned} f_0 &= E(Y) = \int \int \int f(X_1, X_2, X_3) p(X_1) p(X_2) p(X_3) dx_1 dx_2 dx_3 \\ &= \frac{1}{(2\pi)^3} \int \int \int (\sin X_1 + a \sin^2 X_2 + b X_3^4 \sin X_1) dx_1 dx_2 dx_3 \\ &= \frac{1}{(2\pi)^3} \left[ \int \sin X_1 dx_1 + \int a \sin^2 X_2 dx_2 + \int \int b X_3^4 \sin X_1 dx_1 dx_3 \right] \\ &= \dots = \frac{a}{2}. \end{aligned}$$

So  $f_0 = a/2$ .

The  $f_i(X_i)$  terms are easily obtained:

$$\begin{aligned} f_1(X_1) &= \int \int f(X_1, X_2, X_3) p(X_2) p(X_3) dx_2 dx_3 - f_0 \\ &= \frac{1}{(2\pi)^2} \left[ (2\pi)^2 \sin X_1 + a \int \int \sin^2 X_2 dx_2 dx_3 \right. \\ &\quad \left. + b \sin X_1 \int \int X_3^4 dx_2 dx_3 \right] - \frac{a}{2} \\ &= \dots = \frac{1}{(2\pi)^2} \left[ (2\pi)^2 \sin X_1 + 2a\pi^2 + \frac{4}{5}b \sin X_1 \pi^6 \right] - \frac{a}{2} \\ &= \sin X_1 + \frac{1}{5}b\pi^4 \sin X_1 = \left( 1 + \frac{1}{5}b\pi^4 \right) \sin X_1. \end{aligned}$$

$$\begin{aligned} f_2(X_2) &= \int \int f(X_1, X_2, X_3) p(X_1) p(X_3) dx_1 dx_3 - f_0 \\ &= \frac{1}{(2\pi)^2} \left[ \int \int \sin X_1 dx_1 dx_3 + (2\pi)^2 a \sin^2 X_2 \right. \\ &\quad \left. + b \int \int X_3^4 \sin X_1 dx_1 dx_3 \right] - \frac{a}{2} \\ &= \dots = a \sin^2 X_2 - \frac{a}{2}. \end{aligned}$$

$$\begin{aligned} f_3(X_3) &= \int \int f(X_1, X_2, X_3) p(X_1) p(X_2) dx_1 dx_2 - f_0 \\ &= \frac{1}{(2\pi)^2} \left[ \int \int \sin X_1 dx_1 dx_2 + a \int \int \sin X_2^2 dx_1 dx_2 \right] \end{aligned}$$

$$\begin{aligned}
 & + bX_3^4 \int \int \sin X_1 dx_1 dx_2 \Big] - \frac{a}{2} \\
 & = \dots = 0.
 \end{aligned}$$

The  $f_{ij}(X_i, X_j)$  terms are computed as

$$\begin{aligned}
 f_{12}(X_1, X_2) &= \int f(X_1, X_2, X_3) p(X_3) dx_3 - f_1(X_1) - f_2(X_2) - f_0 \\
 &= \sin X_1 + a \sin X_2^2 + b \sin X_1 \frac{1}{2\pi} \int X_3^4 dx_3 - f_1(X_1) - f_2(X_2) \\
 &\quad - f_0 = 0. \\
 f_{13}(X_1, X_3) &= \int f(X_1, X_2, X_3) p(X_2) dx_2 - f_1(X_1) - f_3(X_3) - f_0 \\
 &= \sin X_1 + a \frac{1}{2\pi} \int \sin X_2^2 dx_2 + bX_3^4 \sin X_1 - f_1(X_1) - f_3(X_3) - f_0 \\
 &= \dots = \left( bX_3^4 - \frac{1}{5}b\pi^4 \right) \sin X_1. \\
 f_{23}(X_2, X_3) &= \int f(X_1, X_2, X_3) p(X_1) dx_1 - f_2(X_2) - f_3(X_3) - f_0 \\
 &= \frac{1}{2\pi} \int \sin X_1 dx_1 + a \sin X_2^2 + bX_3^4 \sin X_1 dx_1 \\
 &\quad - f_2(X_2) - f_3(X_3) - f_0 \\
 &= 0
 \end{aligned}$$

$f_{123}$  is obtained by difference and is equal to zero.

2. Calculate the variances of the terms for the function, according to Equation (4.11).

First we calculate the unconditional variance of the function:

$$\begin{aligned}
 V(f(X)) &= \int [f(X_1, X_2, X_3) - E(f(X))]^2 p(X_1) p(X_2) p(X_3) dx_1 dx_2 dx_3 \\
 &= \frac{1}{(2\pi)^3} \int \int \int (\sin^2 X_1 + a^2 \sin^4 X_2 + b^2 X_3^8 \sin^2 X_1 \\
 &\quad + 2a \sin X_1 \sin^2 X_2 + 2bX_3^4 \sin^2 X_1 \\
 &\quad + 2abX_3^4 \sin X_1 \sin^2 X_2 + \frac{a}{4} dx_1 dx_2 dx_3 \\
 &\quad + a \sin X_1 - a^2 \sin^2 X_2 - abX_3^4 \sin X_1) \\
 &= \frac{1}{(2\pi)^3} \left( \frac{1}{2} + \frac{3}{8}a^2 + \frac{b^2}{18}\pi^8 + \frac{a^2}{4} + \frac{b}{5}\pi^4 - \frac{a^2}{2} \right) (2\pi)^3 \\
 &= \frac{1}{2} + \frac{a^2}{8} + \frac{b\pi^4}{5} + \frac{b^2\pi^8}{18}.
 \end{aligned}$$

01 We now calculate the variances of Equation (4.11), showing the  
 02 passages for factor  $X_1$ :

$$\begin{aligned} 03 \quad V_1 &= \int f_1^2(X_1) dx_1 = \int \left( \sin X_1 + \frac{1}{5} b \pi^4 \sin X_1 \right)^2 dx_1 \\ 04 \quad &= \int \left[ \sin^2 X_1 + \frac{2}{5} b \pi^4 \sin X_1^2 + \frac{1}{25} b^2 \pi^8 \sin^2 X_1 \right] dx_1 = \\ 05 \quad &= \dots = \frac{1}{2} + \frac{b \pi^4}{5} + \frac{b^2 \pi^8}{50}. \end{aligned}$$

11 The sensitivity index for factor  $X_1$  can be calculated as  
 12

$$\begin{aligned} 13 \quad S_1 &= \frac{V_1}{V} = \frac{1/2 + b \pi^4/5 + b^2 \pi^8/50}{1/2 + a^2/8 + b \pi^4/5 + b^2 \pi^8/18} \\ 14 \quad & \end{aligned}$$

15 For the other factors we have  
 16

$$\begin{aligned} 17 \quad V_2 &= \frac{a^2}{8} \\ 18 \quad V_3 &= 0 \\ 19 \quad V_{12} &= 0 \\ 20 \quad V_{13} &= \frac{b^2 \pi^4}{18} - \frac{b^2 \pi^8}{50} \\ 21 \quad V_{23} &= 0 \\ 22 \quad V_{123} &= 0 \\ 23 \quad & \end{aligned}$$

28 Again the fact that  $V_{13} \neq 0$  even if  $V_3 = 0$  is of particular interest, as  
 29 it shows how an apparently noninfluential factor (i.e. with no main  
 30 effect) may reveal itself to be influential through interacting with other  
 31 parameters.

- 32 3. Show that the terms in the expansion of the function (4.34) are orthogonal.  
 33

34 Let us show, for example, that  $f_1(X_1)$  is orthogonal to  $f_2(X_2)$ :

$$\begin{aligned} 35 \quad \int \int f_1(X_1) f_2(X_2) dx_1 dx_2 &= \left( 1 + \frac{1}{5} b \pi^4 \right) \int \int \sin x_1 \left( a \sin^2 x_2 - \frac{a}{2} \right) \\ 36 \quad &= \left( 1 + \frac{1}{5} b \pi^4 \right) \int \sin x_1 \int \left( a \sin^2 x_2 - \frac{a}{2} \right) dx_2, \\ 37 \quad & \end{aligned}$$

41 which is equal to zero given that  $\int \sin x_1 = 0$ . The reader can verify, as  
 42 a useful exercise, that the same holds for all other pairs of terms.

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WHERE WE DISCUSS ANOTHER CLASS OF QUESTIONS RELEVANT TO MODELLERS:  
HOW ARE THE MODEL OUTPUT VALUES PRODUCED? WHO IS MOST RESPONSIBLE TO

DRIVE MODEL OUTPUT INTO SPECIFIC RANGES? CAN WE REPLACE THE ORIGINAL

COMPLEX MODEL WITH A CHEAPER ONE, WHICH IS OPERATIONALLY EQUIVALENT?

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# 5

## Factor Mapping and Metamodelling

With Peter Young

### 5.1 INTRODUCTION

In previous chapters we have dealt with sensitivity settings like Factor Prioritization (FP) and Factor Fixing (FF) and their associated methodologies. We saw in Chapter 4, for example, that variance-based techniques are able to provide unambiguous and rigorous answers to the questions posed in such settings; in particular, variance-based main effects suit factor prioritization, while total effects address the factor fixing setting. In the latter case, we also saw in Chapter 3 that elementary effect tests can provide excellent and cheap proxies for total effects, and can be used to screen models with a medium-to-large number of input factors. In Chapter 2, we discussed how to deal with models with very large numbers of input factors, exploiting sophisticated experimental designs.

We now turn to a different type of setting, which arises on foot of various questions often encountered in mathematical and computational modelling.

Modellers often need to address prototypical questions such as: ‘Which factor or group of factors are most responsible for producing model outputs

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

01 within or outside specified bounds? Which parameters determine uniqueness  
02 or instability or runaway conditions in a dynamic model?' For example, if  
03  $Y$  were a dose of contaminant, we might be interested in how much (how  
04 often) a threshold level for this contaminant is being exceeded; or  $Y$  might  
05 have to fulfil a set of constraints, based on the information available on  
06 observed systems. The latter situation is typical in calibration.

07 Another typical question is whether it is possible to represent in a  
08 direct way (graphically, analytically, etc.) the relationship between input  
09 factors and output  $Y = f(X_1, \dots, X_k)$ . Computing  $Y$  usually requires solving  
10 systems of nonlinear differential equations and the relationship  $f(\cdot)$  can only  
11 be evaluated numerically, its form remaining unknown. Sensitivity analysis  
12 techniques discussed in previous chapters allow for ranking the importance  
13 of the various input factors in terms of influence on the variation of  $Y$ .  
14 In addition, some sort of direct representation of  $Y = f(X_1, \dots, X_k)$  would  
15 make the model's properties even more transparent.

16 In this chapter we will discuss techniques that can help to provide answers  
17 to such questions. We assign all these methods to the Factor Mapping  
18 setting, in which specific points/portions of the model output realizations,  
19 or even the entire domain, are mapped backwards onto the space of the  
20 input factors.

## 23 5.2 MONTE CARLO FILTERING (MCF)

24 WHICH FACTOR OR GROUP OF FACTORS ARE MOST RESPONSIBLE FOR PRODUCING  
25 MODEL OUTPUTS WITHIN OR OUTSIDE SPECIFIED BOUNDS? WHICH PARAME-  
26 TERS DETERMINE UNIQUENESS OR INSTABILITY OR RUNAWAY CONDITIONS IN A  
27 DYNAMIC MODEL?

28 Let us first consider the case where the analyst is interested in targeted  
29 portions (extreme values, ceilings, thresholds, etc.) of the space of  $Y$ -  
30 realizations. In this situation, it is natural to partition the model realizations  
31 into 'good' and 'bad'. This leads very naturally to Monte Carlo filtering  
32 (MCF), in which one runs a Monte Carlo experiment producing realizations  
33 of the output(s) of interest corresponding to different sampled points in  
34 the input factors' space. Having done this, one 'filters' the realizations, i.e.  
35 the elements of the Monte Carlo sample that fall within the 'good' realiza-  
36 tions are flagged as 'behavioural', while the remaining ones are flagged as  
37 'nonbehavioural'. Regionalized Sensitivity Analysis (RSA, see Young *et al.*,  
38 1978; Hornberger and Spear, 1981; Spear *et al.*, 1994; Young *et al.* 1996;  
39 Young 1999a and references cited therein) is an MCF procedure that aims  
40 to identify which factors are most important in leading to realizations of  $Y$   
41 that are either in the 'behavioural' or 'nonbehavioural' regions. In typical  
42 cases, RSA can answer this question by examining, for each factor, the  
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01 subsets corresponding to ‘behavioural’ and ‘nonbehavioural’ realizations. It  
 02 is intuitive that, if the two subsets are dissimilar to one another (as well as,  
 03 one would expect, to the initial marginal distribution of the factor), then  
 04 that factor is influential.

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### 07 5.2.1 Implementation of Monte Carlo Filtering

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In Monte Carlo filtering a multiparameter Monte Carlo simulation is performed, sampling model parameters  $(X_1, \dots, X_k)$  from prior ranges and propagating parameter values through the model. Then, based on a set of constraints targeting the desired characteristics, a categorization is defined for each MC model realization, as either within or outside the target region. The terms behavioural ( $B$ ) or nonbehavioural ( $\bar{B}$ ) are current in the literature.

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The  $[B - \bar{B}]$  categorization is mapped back onto the input’s structural parameters, each of which is thus also partitioned into a  $B$  and  $\bar{B}$  subsample. Given a full set of  $N$  Monte Carlo runs, one obtains two subsets:  $(X_i|B)$  of size  $n$  and  $(X_i|\bar{B})$  of size  $\bar{n}$ , where  $n + \bar{n} = N$ . In general, the two subsamples will come from different unknown probability density functions,  $f_n(X_i|B)$  and  $f_{\bar{n}}(X_i|\bar{B})$ .

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In order to identify the parameters that are most responsible for driving the model into the target behaviour, the distributions  $f_n$  and  $f_{\bar{n}}$  are compared for each parameter. If for a given parameter  $X_i$  the two distributions are significantly different, then  $X_i$  is a key factor in driving the model’s behaviour and there will be clearly identifiable subsets of values in its predefined range that are more likely to fall under  $B$  than under  $\bar{B}$ . If the two distributions are not significantly different, then  $X_i$  is unimportant and any value in its predefined range is likely to fall into either  $B$  or  $\bar{B}$ .

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This comparison can be made by applying standard statistical tests, such as the Smirnov two-sample test (two-sided version). In the Smirnov test the  $d_{n,\bar{n}}$  statistic is defined for the cumulative distribution functions of  $X_i$  by

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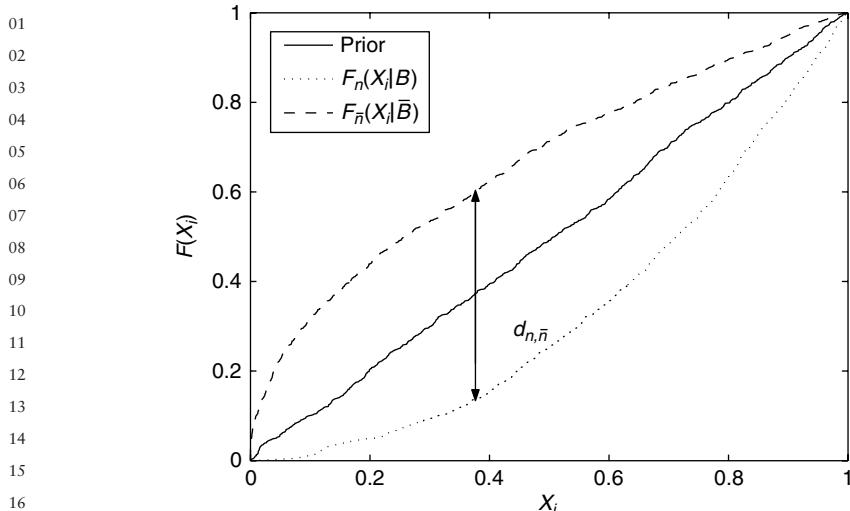
$$d_{n,\bar{n}}(X_i) = \sup \|F_n(X_i|B) - F_{\bar{n}}(X_i|\bar{B})\|$$

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and the question answered by the test is: ‘At what significance level  $\alpha$  does the computed value of  $d_{n,\bar{n}}$  determine the rejection of the null hypothesis  $f_n(X_i|B) = f_{\bar{n}}(X_i|\bar{B})$ ?’

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The smaller  $\alpha$  (or equivalently the larger  $d_{n,\bar{n}}$ ), the more important the parameter is in driving the behaviour of the model. The procedure is exemplified in Figure 5.1 for a parameter  $X_i$ , uniformly distributed in the range  $(0, 1)$  and displaying a significant difference between the  $B$  and  $\bar{B}$  subsets. In order to identify the portion of  $X_i$  values more likely to fall



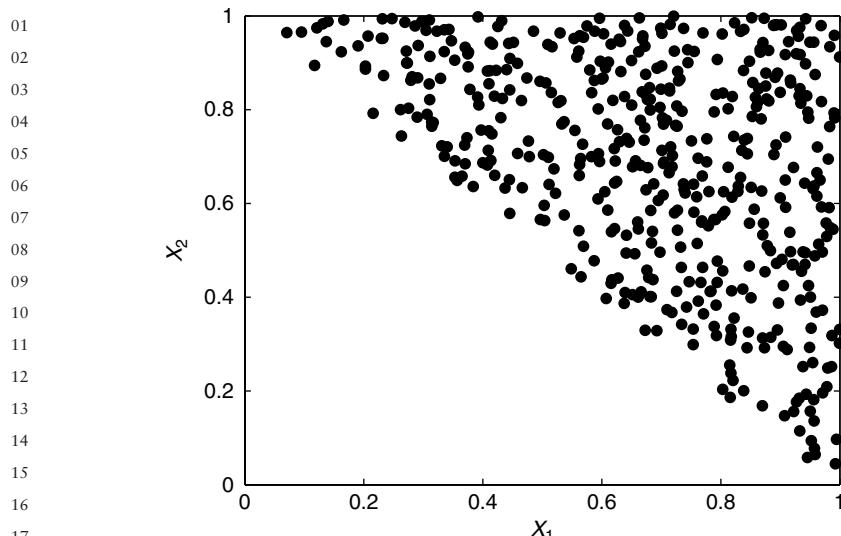
**Figure 5.1** Graphical representation of the Smirnov test for an important parameter  $X_i$ . The vertical bar is the  $d_{n,\bar{n}}$  statistic. Model realizations under the  $B$  category are more likely when  $X_i$  falls on the right of its predefined range

under  $B$ , the shape of the cumulative distribution  $F_n(X_i|B)$  has to be examined. The latter is steeper on the right-hand side of the graph (or, equivalently, it has shifted downwards), indicating that  $X_i$  values on the right of its predefined range are more likely to produce a behavioural model realization.

The  $B$  and  $\bar{B}$  subsets can be further probed through bidimensional projections, in order to detect significant patterns. The standard procedure consists of computing the correlation coefficients  $\rho_{ij}$  between all parameters under the  $B$  or  $\bar{B}$  subsets, and plotting the bidimensional projections of the sample for the couples having  $|\rho_{ij}|$  larger than a significance threshold. This usually makes it possible to ‘visualize’ relationships between parameters.

For example, let us consider a simple model given by the equation  $Y = X_1 + X_2$ , with  $X_i \in (0, 1)$ . Let us define the model’s target behaviour as  $Y > 1$ . Then, an MCF procedure can identify a significant negative correlation between  $X_1$  and  $X_2$  in the  $B$  subset, and the corresponding triangular pattern can be visualized through the projection of the  $B$  sample shown in Figure 5.2. From this pattern, one can deduce a constraint  $X_1 + X_2 > 1$  to fulfil the target behaviour.

The same procedure can evidently be applied in more typical cases where the constraint on the factors is not evident from the form of the mathematical model, i.e. when the model is a computer code.



**Figure 5.2** Bidimensional projection of the  $B$  subsample for the simple model  $Y = X_1 + X_2$  (target behaviour  $Y > 1$ ). The triangular pattern clearly indicates the relationship  $X_1 + X_2 > 1$  for the target behaviour. The correlation coefficient between  $X_1$  and  $X_2$  in the MC sample is  $\rho_{12} = -0.45$

### 5.2.2 Pros and Cons

Similarly to variance-based methods, RSA has many global properties: (a) the whole range of values of the input factors is considered, and (b) all factors are varied at the same time. Smirnov analysis considers univariate marginal distributions and it relates not only to main effects of variance-based methods, but can also highlight certain types of interaction effects (see the Exercises below). Higher-order analysis can only be performed for two-way interactions that are detectable through correlation analysis, but no procedure is provided for more complex interaction structure. Spear *et al.* (1994), reviewing their experience with RSA, highlighted two key drawbacks:

1. A low success rate: practice has shown that the fraction of  $B$  is barely larger than 5% over the total simulations for large models (with number of factors  $k > 20$ ), implying a lack of statistical power;
2. Difficulty in uncovering correlation and interaction structures of the  $B$  subset (see also Beck's review, 1987):
  - the Smirnov test is sufficient to ascertain whether a factor under analysis is important. However, it does not provide a necessary condition

01 for importance, i.e. its nonsignificance does not ensure that a factor  
02 is noninfluential;

- 03 • many types of interaction structures induced by the classification are  
04 not detected by the univariate  $d_{n,\bar{n}}$  statistic: e.g. factors combined  
05 as products or quotients may compensate (see Exercise 6 below, for  
06  $c = 0$ );  
07 • the interaction structure is often far too complex for correla-  
08 tion analysis to be effective, i.e. bivariate correlation analysis is  
09 not revealing in many cases (see Saltelli *et al.*, 2004, Example 2,  
10 pp. 159–161).

11 Such characteristics of RSA imply that no complete assessment can be  
12 performed with RSA, since for those factors proving unimportant in the  
13 Smirnov test, further inspection is needed (e.g. by applying other global SA  
14 tools) to verify that they are not involved in interactions. Only after this  
15 subsequent inspection can the relevance of an input factor be fully assessed.  
16 In order to address these limitations of RSA and to better understand the  
17 impact of uncertainty and interaction in the high-dimensional parameter  
18 spaces of models, Spear *et al.* (1994) developed the computer-intensive  
19 Tree-Structured Density Estimation technique (TSDE), which allows for the  
20 characterization of complex interactions in that portion of the parameter  
21 space which gives rise to successful simulations. In TSDE, the  $B$  subsample  
22 is analysed by clustering regions of input factors characterized by high point  
23 density. This is based on a sequence of recursive binary splits of the  $B$   
24 sample into two subdomains (similarly to peaks and tails of histograms) of  
25 complementary characteristics:

- 26 • small regions of relatively high density;  
27 • larger sparsely populated regions.

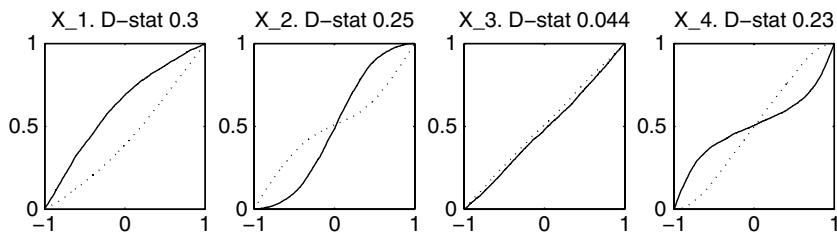
28 The TSDE procedure relies on the assumption that any nonrandom density  
29 pattern indicates an influence of input factors on the model output. Interest-  
30 ing applications of TSDE in environmental sciences can be found in Spear  
31 (1997), Grieb *et al.* (1999) and Pappenberger *et al.* (2006). In the latter  
32 reference it is shown how factor mapping can be used to identify areas  
33 of desirable and undesirable model behaviour, which aids the modelling  
34 process. Helton *et al.* (2006) also provide mapping techniques on scatter-  
35 plots, based on the same assumptions as TSDE.

36 Our experience suggests that such extended RSA techniques for mapping  
37  $B$  subsets can be revealing *when they work*, but, in spite of their higher  
38 coding and computational complexity, they may still be characterized by  
39 lack of statistical power in discriminating the significance of such density  
40 patterns in a robust manner. Hence, we limit our discussion here to  
41 the Smirnov test and correlation analysis, due to the simplicity of their

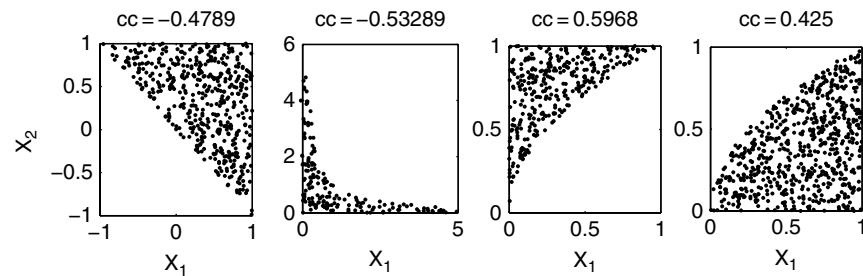
01 implementation and their ease of interpretation. Later on we will present  
 02 more powerful mapping techniques when discussing metamodeling.  
 03  
 04

### 05 5.2.3 Exercises

- 06
- 07 1. Interpret the plots below, which represent the Smirnov test for a set  
 08 of input factors. The behavioural set is indicated by dotted lines, the  
 09 nonbehavioural by solid lines. Think of some functional forms that could  
 10 produce such results. The D-stat above each plot indicates the value of  
 11 the Smirnov statistic.



- 22
- 23 2. Interpret the plots below, showing the bidimensional projections of  
 24 behavioural subsets. Think of an analytic form of the types of interaction  
 25 that produce the behavioural sets.



- 37 3. Consider the model  $Y = Z_1 + Z_2$ , with

$$Z_1 \sim N(0, 1)$$

$$Z_2 \sim N(0, 3).$$

42 Discuss the mapping problem  $Y > 0$  analytically and using the MCF  
 43 techniques.

- 01     4. For the same model as in Exercise 3, map the highest 5% quantile for Y  
 02     onto the input space.  
 03     5. For the same model as in Exercise 3, map the highest 5% quantile for Y  
 04     when

05                  $Z_1 \sim N(0, 1)$

06                  $Z_2 \sim N(0, 1).$

- 09     6. Consider the model  $Y = X_1 \cdot X_2$ , with  $X_i \sim N(0, 2)$  and discuss the cases  
 10      $Y > -1$ ,  $Y > 0$ ,  $Y > 1$ .  
 11     7. Consider the model  $Y = X_1 \cdot X_2 \cdot X_3$ , with  $X_i \sim U(0, 2)$  and discuss the  
 12     case  $Y < 1$ .

14  
 15     5.2.4 Solutions

- 17     1. Three input factors out of four have a significant effect on the  
 18     behavioural properties of the model. Only  $X_3$  has a negligible effect.

20     The dotted cumulative distribution curve for  $X_1$  is steepest on the  
 21     right-hand side (it has shifted downwards), so high values of  $X_1$  are more  
 22     likely to produce behavioural model realizations. This kind of result  
 23     suggests a monotonic mapping between  $X_1$  and  $Y$ , e.g. a simple linear  
 24     relationship.

25     Input factor  $X_2$ , on the other hand, has two different behavioural  
 26     regions: the dotted line has two separate sections of steepness, one for  
 27     the smallest values and one for the largest. This implies that the extreme  
 28     values of  $X_2$  (either smallest or largest) are more likely to produce  
 29     behavioural realizations of  $Y$ . This kind of result suggests a nonmono-  
 30     tonic mapping between  $X_2$  and  $Y$ , e.g. a quadratic form. Also, interaction  
 31     effects can lead to the same type of Smirnov test (see Exercise 6 below).

32     For  $X_4$  we have the opposite situation with respect to  $X_2$ : the dotted  
 33     line is steeper in the central part of the support, implying that the  
 34     extreme values of  $X_4$  have to be avoided in order to produce behavioural  
 35     model realizations. This kind of result suggests a nonmonotonic mapping  
 36     between  $X_4$  and  $Y$ , e.g. a quadratic form with *opposite* concavity with  
 37     respect to  $X_2$ .<sup>1</sup>

- 38     2. The first shape is characterized by a negative correlation between  $X_1$   
 39     and  $X_2$  in producing behavioural model realizations. Negative corre-  
 40     lations suggest that the two input factors act through sum or product

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43     <sup>1</sup> The true model used for this example was  $Y = 4X_1 + (4X_2^2 - 1) - X_3^3 - (2X_4^4 - 1)$  with  
 44      $X_i \sim U[-1, 1]$ .

relationships. In this case, a plausible description for the behavioural set is given by  $X_1 + X_2 > 0$ , i.e. an additive relationship.

The second shape is also characterized by a negative correlation, suggesting action through sum/product. In this case, the shape resembles a hyperbola, suggesting a plausible functional form as  $X_1 \cdot X_2 < const.$

The third shape is characterized by a positive correlation, implying that the action is now through difference/quotient. Possible relationships are  $a \cdot X_1 - b \cdot X_2^2 < 0$  or  $X_1/X_2^2 < const.$

The fourth shape is again with positive correlation, but flipped with respect to the previous one, so plausible relationships are  $a \cdot X_1 - b \cdot X_2^2 > 0$  or  $X_1/X_2^2 > const.$

3. The behavioural criterion  $Y > 0$  is fulfilled by parameter combinations in the upper-right half plane delimited by the line  $Z_1 = -Z_2$  (i.e.  $Z_1 > -Z_2$ ). If we also consider the input factor distributions (Gaussian), we know that normal samples will fall into the range  $\pm 1.96 \cdot \sigma$  with 95% probability, where  $\sigma$  is the standard deviation of the Gaussian distribution. So, the behavioural samples will be mainly concentrated (with 95% probability) in the upper part of an ellipse with vertical major axis of height 5.88 and horizontal minor axis of width 1.96, cut by the line  $Z_1 = -Z_2$ . Moreover, since  $Z_2$  has a wider variance than  $Z_1$ , it will also be clear that  $Z_2$  drives the sign of  $Y$  more powerfully, i.e. extreme values of  $Z_2$  will be able to drive the sign of  $Y$  regardless of the actual values of  $Z_1$ .

We now perform the analysis applying the MCF approach (we give MATLAB commands as an example).

- (a) Generate a sample of 1000 elements from two normal distributions of standard deviation 1 and 3:

```
30     x1 = randn(1000,1);
31
32     x2 = randn(1000,1).*3;
```

- (b) generate the output:

```
36     y = x1+x2;
```

- (c) look for behavioural elements of the sample:

```
40     ib = find(y>0);
```

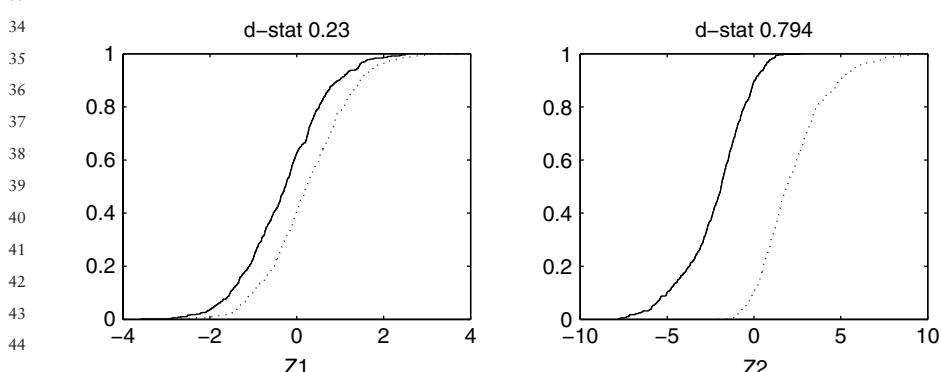
and for the nonbehavioural:

```
44     in = find(y<=0);
```

```

01 (d) compute the Smirnov statistics (e.g. the outputs d1 and d2 of the
02 MATLAB Statistical Toolbox function kstest2):
03 [h1, p1, d1] = kstest2(x1(ib),x1(in));
04
05 [h2, p2, d2] = kstest2(x2(ib),x2(in));
06
07 (e) plot the empirical cumulative density plots (e.g. using MATLAB
08 Statistical Toolbox function cdfplot):
09
10 figure,
11
12 subplot(2,2,1)
13
14 h=cdfplot(x1(ib));
15
16 set(h,'linestyle',':');
17
18 hold on, cdfplot(x1(in))
19
20 gca, title(['d-stat ',num2str(d1)]), xlabel('Z1'),
21 ylabel('')
22
23 subplot(2,2,2)
24
25 h=cdfplot(x2(ib));
26
27 set(h,'linestyle',':');
28
29 hold on, cdfplot(x2(in))
30
31 gca, title(['d-stat ',num2str(d2)]), xlabel('Z2'),
32 ylabel('')
33

```

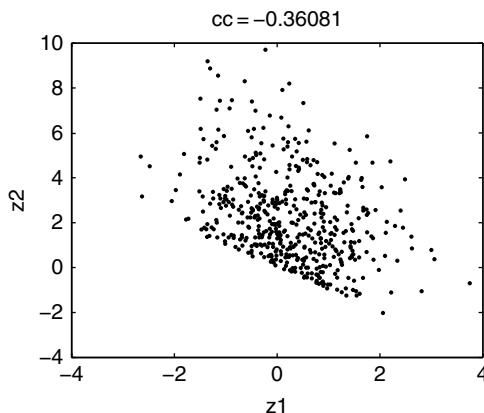


From the Smirnov analysis we can see that, while both input factors have a significant effect on the behavioural realizations of  $Y$ ,  $Z_2$  has the greater impact on the sign of  $Y$  (it has a far larger Smirnov statistic). As already mentioned, this is due to the larger variance of  $Z_2$  with respect to  $Z_1$ , which allows sufficiently large values of  $Z_2$  to force a positive sign in  $Y$ , regardless of the values of  $Z_1$ . The behavioural/nonbehavioural subsets for  $Z_2$  are therefore almost disjoint (they overlap only in the range  $[-1.5, 1.5]$  within a full support of  $[-9, 9]$ ), while for  $Z_1$  the two subsets have a much larger degree of overlap.

(f) compute the correlation coefficient under the behavioural subset:

```

11 cc = corrcoef(x1(ib),x2(ib))
12
13 and plot the bidimensional projection of the behavioural sample,
14 which fills the half plane  $Z_1 + Z_2 > 0$ , as expected.
15
16 plot(x1(ib),x2(ib),'.' )
17
18 xlabel('z1'), ylabel('z2'),
19 title(['cc= ', num2str(cc(2,1))])
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4. The output  $Y$  is the sum of two normally distributed variables, so  $Y \sim N(0, \sqrt{10})$ . The 5% upper tail of a Gaussian distribution is located at a distance from the mean of  $1.65 \cdot \sigma$ . Hence the upper 5% tail of the output probability is given by the set  $Y > Y^{95}$ , where  $Y^{95} = 1.65 \cdot \sqrt{10} = 5.22$ . So the behavioural set of the input factors is given by the upper half plane delimited by the line  $Z_1 + Z_2 = Y^{95}$ .

01 Performing the same analysis applying MCF techniques requires the  
 02 use of the same sample used in Exercise 3 and recomputing the new  
 03 behavioural set.

04 (a) Sort the output values:

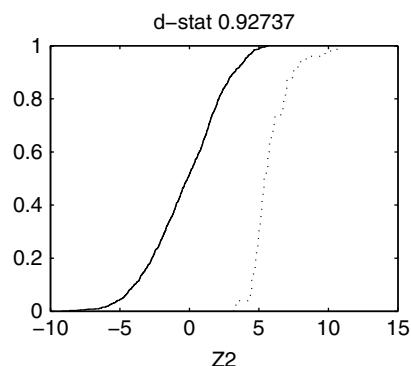
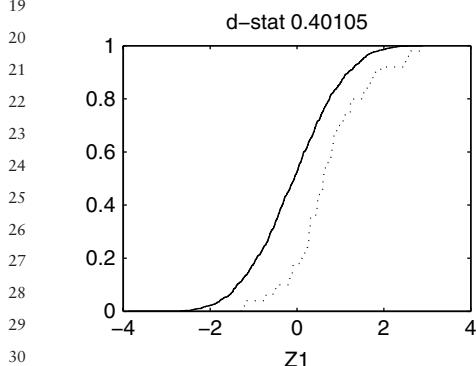
05     `[ys, is]=sort(y);`

06 (b) define the behavioural (upper 5%) and nonbehavioural sets (the rest  
 07 of the sample)

08     `ib = is(951:1000);`

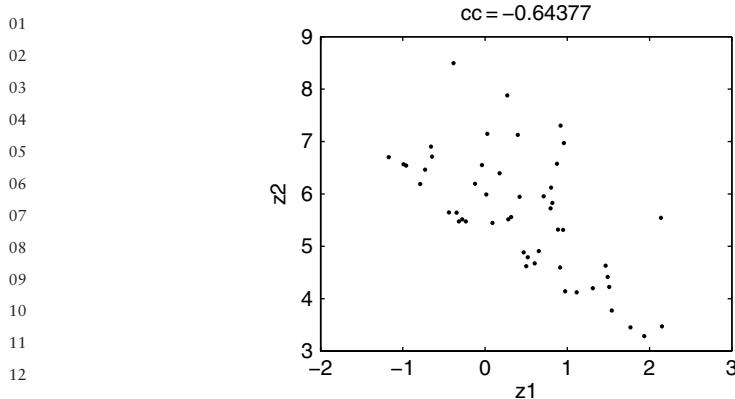
09     `in = is(1:950);`

10 (c) compute the Smirnov statistics and plot the cumulative distributions  
 11 as in the previous exercise:



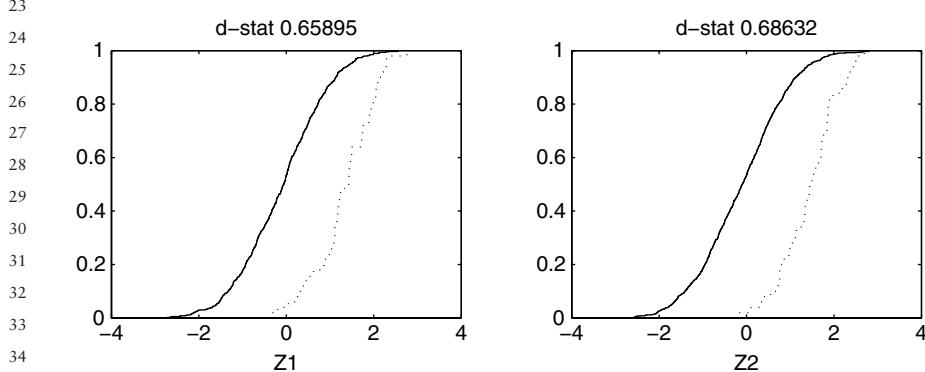
32  
 33 Again we can see that the behavioural and nonbehavioural subsets  
 34 of  $Z_2$  are almost disjoint and sufficiently large values of  $Z_2$  are  
 35 capable of driving  $Y$  into the upper 5% quantile, whatever the value  
 36 of  $Z_1$ .

37 (d) compute the correlation coefficient of the behavioural set and plot  
 38 the bidimensional projection of the input factor behavioural sample,  
 39 which fills the half plane  $Z_1 + Z_2 > Y^{95}$ , as expected. This plot also  
 40 confirms the Smirnov analysis by showing that  $Z_2$  values have to  
 41 remain significantly positive to drive  $Y$  to its upper values, while  $Z_1$   
 42 values can range almost symmetrically around zero (see scatterplot  
 43 on top of next page).



5. In this case, the two input factors have the same variance, so we can expect an equal impact on the extreme values of  $Y$ . In analytic terms,  $Y$  now has a Gaussian distribution  $N(0, \sqrt{2})$ . Hence the upper 5% quantile is given by  $Y > Y^{95} = 1.65 \cdot \sqrt{2} = 2.33$ .

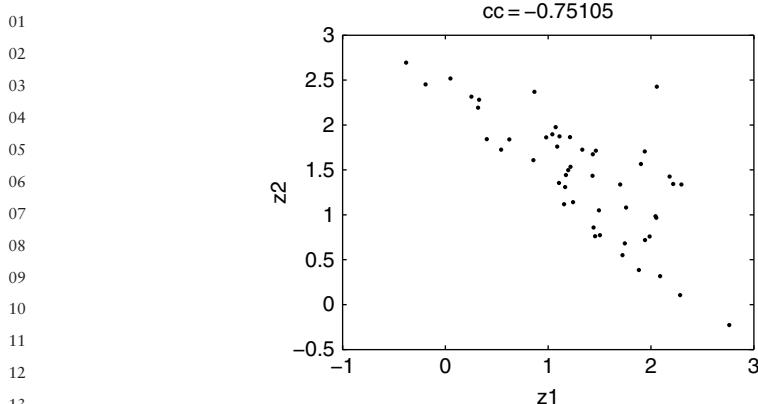
Performing the MCF analysis, we first obtain the Smirnov statistics and plot the cumulative distributions, which clearly display the similarity of the effects of the two input factors on  $Y$ .



We can subsequently perform the correlation analysis and plot the bidimensional projection of the behavioural sample, which also confirms the equivalent effect of  $Z_1$  and  $Z_2$  on  $Y$  (see scatterplot on top of next page).

6. Analytically, the problems can be formalized as  $Y > c$ , with  $c = -1, 0, 1$ . This implies that  $X_1 \cdot X_2 > c$ .

For  $c = -1$ , the behavioural condition is fulfilled for the portion of the  $(X_1, X_2)$  plane *between* the two branches of the hyperbola  $X_1 = -1/X_2$ .



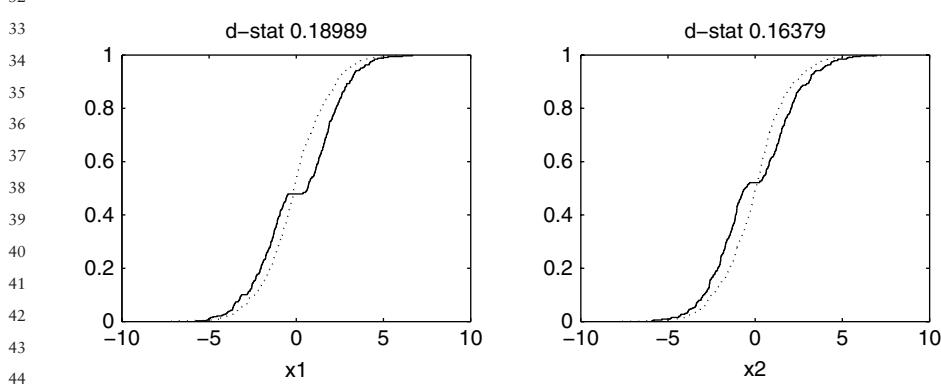
15 This also implies that the central part of the support of each input factor  
16 will be more likely to produce behavioural Y-realizations.

17 For  $c = 0$ , the behavioural condition is fulfilled if  $X_1$  and  $X_2$  have the  
18 same sign, i.e. all positive values of both  $X_1$  and  $X_2$  or all negative values  
19 of both  $X_1$  and  $X_2$ . This also implies that any value in the support of  
20 one input factor has an equal probability of producing a behavioural or  
21 nonbehavioural run, conditional on the value of the other one. Therefore,  
22 the Smirnov test would not highlight any significant effect of  $X_1$  and  $X_2$ .

23 For  $c = 1$ , the behavioural condition is fulfilled for the two portions of  
24 the  $(X_1, X_2)$  plane *outside* the two branches of the hyperbola  $X_1 = 1/X_2$ .  
25 This also implies that the lower/upper part of the support of each input  
26 factor will be more likely to produce behavioural Y-realizations.

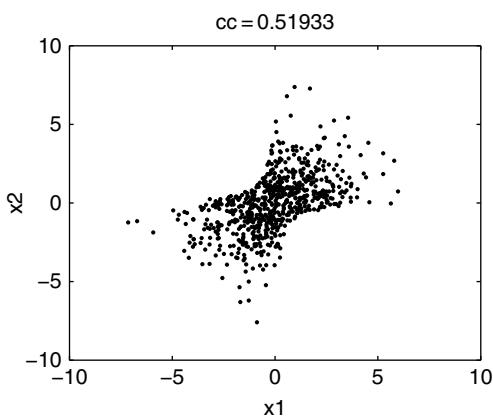
27 The MCF analysis can be implemented in a completely identical  
28 manner to the examples before.

- 29
- 30 •  $c = -1$ . We first compute the Smirnov statistics and plot the cumulative distributions.
- 31



Analysing the steepness of the cumulative distributions under  $B$  and  $\bar{B}$  shows that the behavioural distribution is concentrated (steeper) in the central part of the initial support, while the nonbehavioural is concentrated (steeper) in two disjoint subsets in the lower and upper part of the initial support.

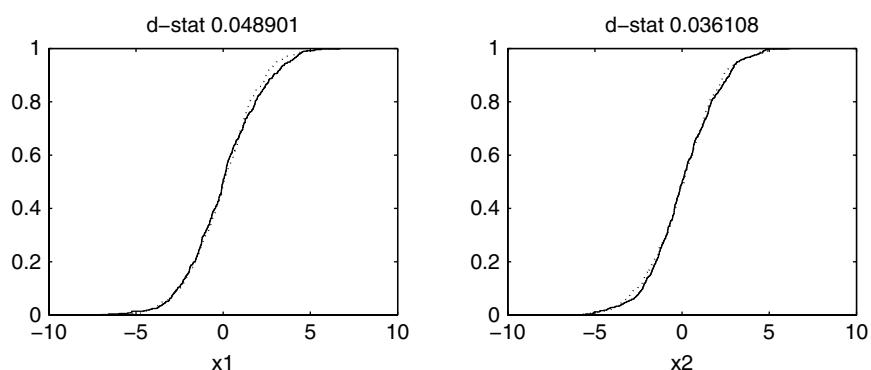
We then compute the correlation coefficient and plot the bidimensional projection of the behavioural subset.



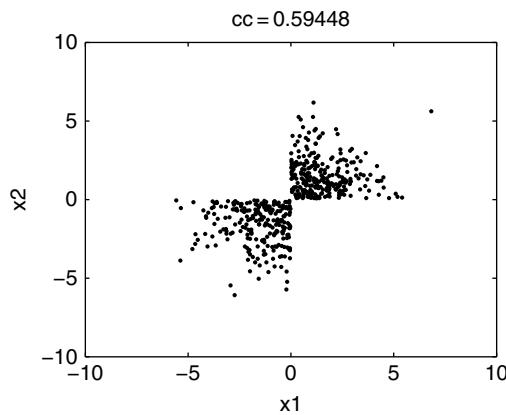
This shows neatly the portion of space between the two branches of hyperbola  $X_1 = -1/X_2$  that produces behavioural  $Y$ -realizations.

- $c = 0$ . We first compute the Smirnov statistics and plot the cumulative distributions.

This shows that the two subsets have the same distribution, i.e. any value in the original support for each input factor is equally likely to produce behavioural or nonbehavioural realizations.

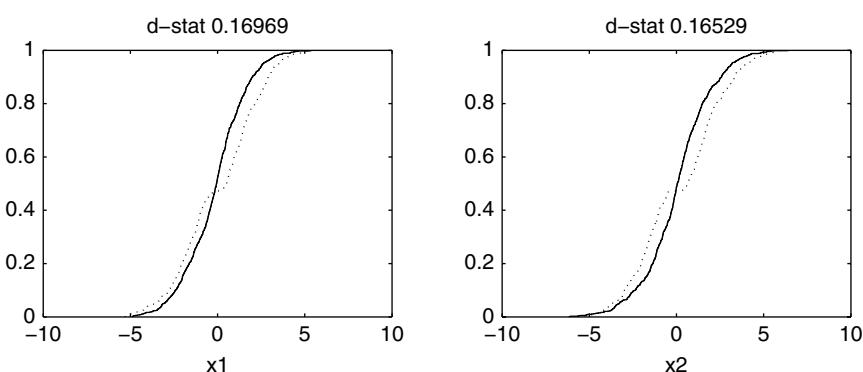


01 We then compute the correlation coefficient and plot the bidimensional  
 02 projection of the behavioural subset.  
 03



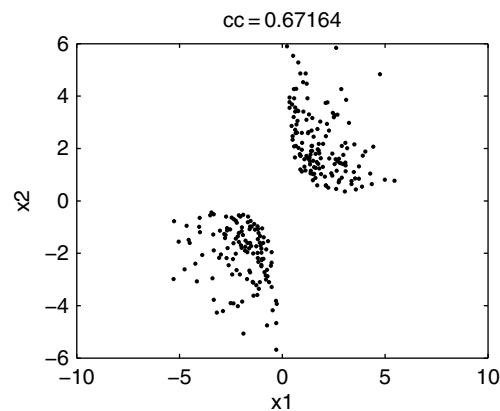
18 This allows us to understand the interaction mechanism between  $X_1$  and  
 19  $X_2$  that produces behavioural realizations.  
 20

- 21 •  $c = 1$ . We first compute the Smirnov statistics and plot the cumulative  
 22 distributions.



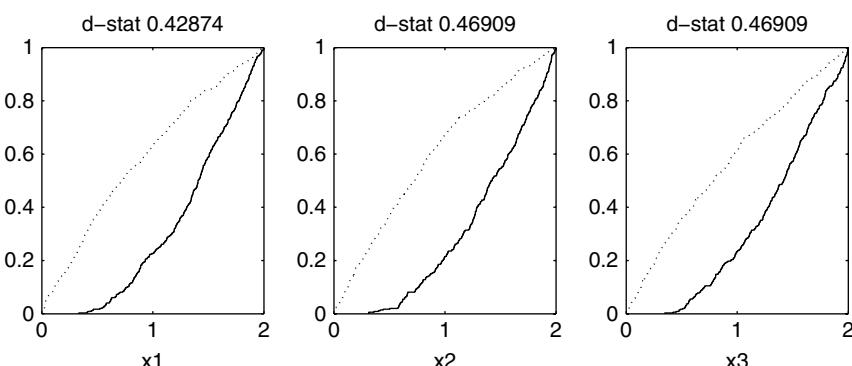
38 This shows that values of the input factors concentrated in the  
 39 lower/upper part of each support are more likely to produce behavioural  
 40 runs, while the central values of the original support are excluded from  
 41 the behavioural set (the dotted cumulative lines are flat around the zero  
 42 values of  $Z_i$ , implying a zero density of points of the behavioural subset  
 43 in the central part of each support).  
 44

01 We then compute the correlation coefficient and plot the bidimensional  
 02 projection of the behavioural subset.



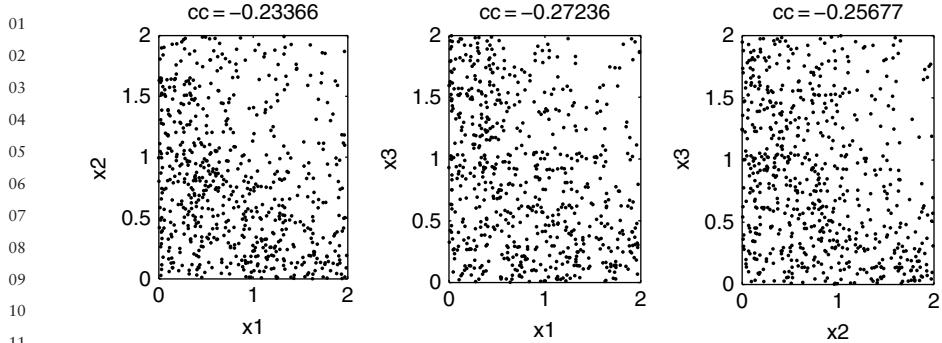
19 This shows the two disjoint portions of the  $(X_1, X_2)$  plane outside the  
 20 two branches of the hyperbola  $X_1 = 1/X_2$  that produce the behavioural  
 21 Y-realizations.

22 7. We first compute the Smirnov statistics and plot the cumulative distri-  
 23 butions.



39 This shows that, to maintain the output realization smaller than 1, all  
 40 factors must be sufficiently small. The behavioural distribution is there-  
 41 fore steepest towards the smallest values of the original supports of  $X_i$ .

42 We then compute the correlation coefficient and plot the bidimensional  
 43 projection of the behavioural subset.



The negative correlation coefficients indicate that the effect of input factors on  $Y$  is through sums/products. Moreover, these plots show nicely that the upper-right regions, combining large values of all the input factors, have to be avoided to ensure that  $Y < 1$ .

### 5.2.5 Examples

We now show a few examples of the use of MCF to characterize the stability behaviour of dynamic models. We will give an example for a chemical reactor (continuous time model) and for a macroeconomic model (discrete time model). Finally, we will also consider, in the light of MCF techniques, the infection dynamics model previously analysed in Chapter 4.

#### 5.2.5.1 Stability analysis of a controlled chemical reactor

Let us consider a continuous stirred tank reactor (CSTR) where a first-order exothermic irreversible reaction  $A \rightarrow B$  takes place in liquid phase.

The behaviour of the CSTR can be expressed in terms of mass and heat (enthalpy) balance equations. Mass balance reads as

$$V \frac{dC_A}{d\bar{t}} = Q(C_{A0} - C_A) - k(T)C_A \cdot V \quad (5.1)$$

where  $\bar{t}$  is time [s],  $V$  is the reactor volume [ $m^3$ ];  $C_A$  is the concentration of  $A$  in the reactor and at its outlet [ $kmol/m^3$ ];  $C_{A0}$  is the concentration of  $A$  at the inlet;  $Q$  is the volumetric flow rate [ $m^3/s$ ] at the input and output of the reactor,  $k(T)$  is the kinetic ‘constant’ [1/s] of the first-order chemical reaction  $A \rightarrow B$ , which is expressed as a function of temperature  $T$  [K]:

$$k(T) = k_0 \exp\left(-\frac{E}{RT}\right),$$

01 where  $k_0$  is the Arrhenius factor [1/s],  $E$  is the activation energy [kJ/kmol]  
 02 and  $R$  is the gas constant [kJ/(kmol K)].

03 The mass balance equation (5.1) tells us that the rate of change of the  
 04 amount of reactant  $A$ , given by the left-hand side term  $V(dC_A/d\bar{t})$ , equals the  
 05 flow of  $A$  at the inlet,  $Q \cdot C_{A0}$ , minus the flow of  $A$  at the outlet,  $Q \cdot C_A$ , and  
 06 minus the amount of  $A$  that is transformed into  $B$  per time unit,  $k(T) \cdot C_A V$ .

07 The heat balance reads as

$$08 \quad 09 \quad 10 \quad V\rho c_p \frac{dT}{d\bar{t}} = Q\rho c_p(T_0 - T) - \Delta H_r k(T) C_A V - UA(T - T_c) \quad (5.2)$$

11 where  $\rho$  is the density of the reacting mixture [kg/m<sup>3</sup>],  $c_p$  is the specific  
 12 heat of the mixture [kJ/(kg K)],  $T_0$  is the temperature of liquid entering  
 13 the reactor [K],  $T$  is the temperature of the liquid in the reactor and at its  
 14 outlet,  $T_c$  is the temperature of the reactor's coolant,  $(-\Delta H_r)$  is the reaction  
 15 enthalpy [kJ/kmol],  $U$  is the overall heat transfer coefficient between the  
 16 inside of the reactor and the coolant [kJ/(s m<sup>2</sup> K)] and  $A$  is the heat transfer  
 17 area [m<sup>2</sup>].

18 The heat balance equation (5.2) tells us that the rate of change of enthalpy  
 19 in the reactor,  $V\rho c_p(dT/d\bar{t})$ , equals the flow of enthalpy at the inlet,  $Q\rho c_p T_0$ ,  
 20 minus the flow of enthalpy at the outlet,  $Q\rho c_p T$ , plus the heat generated  
 21 by the exothermic reaction,  $(-\Delta H_r) k(T) C_A V$ , minus the heat removed by  
 22 the coolant,  $UA(T - T_c)$ .

23 The CSTR is controlled, in order to keep the temperature, and the asso-  
 24 ciated quantity of product  $B$ , at the desired set-point  $T_s$ . The controlled  
 25 variable is the temperature  $T$  and the manipulated variable is the coolant  
 26 temperature  $T_c$ . The controller follows a standard proportional-integral (PI)  
 27 design, implying the following control rule for the coolant temperature:

$$28 \quad 29 \quad 30 \quad 31 \quad (T_c - T_{cs}) = -k_p(T - T_s) - k_I \int_0^t (T - T_s) d\bar{t} \quad (5.3)$$

32 where  $T_{cs}$  is the coolant temperature at the set-point,  $k_p$  is the proportional  
 33 control gain and  $k_I$  is the integral control gain [1/s]. The control rule (5.3)  
 34 tells us that the coolant 'error' ( $T_c - T_{cs}$ ) is proportionally adjusted, with  
 35 opposite sign, with respect to the temperature error ( $T - T_s$ ) and with respect  
 36 to the integral of the temperature error. In other words, the coolant temper-  
 37 ature will go down as the temperature error ( $T - T_s$ ) and its integral go up.  
 38 The control gains  $k_p$  and  $k_I$  tell us by *how much* the coolant temperature is  
 39 adjusted by the controller for a given temperature error and integral of the  
 40 error: the higher the gains, the greater the change in the coolant. Finally,  
 41 the integral action ensures that the desired set-point is the unique steady  
 42 state of the reactor.

43 Economists or econometricians will be familiar with Taylor rules: in  
 44 monetary policy, for example, the controlled variable is inflation and

the manipulated variable is the nominal interest rate. When the economy is ‘overheated’ (i.e. with high inflation), the Central Bank *increases* the nominal interest rate to ‘cool’ the economy. In the case of the CSTR, the PI regulator *decreases* coolant temperature to cool an overheated reactor.

The controlled CSTR is therefore described by the following system of differential equations, in dimensionless form:

$$\frac{d\xi}{dt} = -\xi + Da(\vartheta)(1 - \xi) \quad (5.4)$$

$$\frac{d\vartheta}{dt} = \vartheta_0 + N[\vartheta_{cs} - k_p(\vartheta - \vartheta_s) - k_I\tau\varphi] - (1 + N)\vartheta + Da(\vartheta)(1 - \xi) \quad (5.5)$$

$$\frac{d\varphi}{dt} = \vartheta - \vartheta_s \quad (5.6)$$

where (notation of Pellegrini and Biardi, 1990)

$$\xi = \frac{C_{A0} - C_A}{C_{A0}} \quad (\text{conversion of } A)$$

$$\tau = \frac{V}{Q} \quad (\text{residence time [s]})$$

$$t = \frac{\tilde{t}}{\tau} \quad (\text{dimensionless time})$$

$$N = \frac{UA}{Q\rho c_p} \quad (\text{dimensionless heat transfer coefficient})$$

$$\vartheta = \frac{T - T_s}{\Delta T_a} \quad (\text{dimensionless temperature})$$

$$\Delta T_a = \frac{-\Delta H_r C_{A0}}{\rho c_p} \quad (\text{adiabatic temperature rise [K]})$$

$$Da(\vartheta) = k_0 \tau \exp\left(-\frac{E}{R(T_s + \Delta T_a \vartheta)}\right) \quad (\text{Damkoehler number})$$

$$\varphi = \int_0^t (\vartheta - \vartheta_s) dt \quad (\text{dimensionless integral of the error})$$

The adiabatic temperature rise indicates the temperature increase that would be caused in the reactor if the entire amount of input *A* were converted into *B* under adiabatic conditions (i.e. without any heat exchange). The Damkoehler number indicates the average number of ‘reaction events’ that occur during the residence time.

The behaviour of this dynamical system, which can present complex dynamic features, from instability of the steady state to chaotic behaviour, has been intensively studied (see Pellegrini and Biardi, 1990; Giona and Paladino, 1994; Paladino *et al.*, 1995; Paladino and Ratto, 2000).

Our aim in the present example is to study the stability conditions of the controlled CSTR. The local stability analysis of the reactor in the neighbourhood of the unique steady state ( $\xi_s, \vartheta_s, \varphi_s$ ) is performed by analysing the Jacobian:

$$J = \begin{pmatrix} -(1 + a_{21}) & a_{12} & 0 \\ -a_{21} & -(k_p N + N + 1) + a_{12} & -k_I \tau \\ 0 & 1 & 0 \end{pmatrix} \quad (5.7)$$

01 where

02

$$03 \quad a_{12} = \xi_s \frac{E\Delta T_a}{R(T_s + \Delta T_a \vartheta_s)^2} > 0 \quad (5.8)$$

04

$$05 \quad a_{21} = Da(\vartheta_s) > 0 \quad (5.9)$$

06  
07 and  $\xi_s = Da(\vartheta_s)/(1 + Da(\vartheta_s))$ .

08 The steady state is stable if all three eigenvalues of  $J$  have negative  
09 real parts. This ensures that, as the operating conditions are moved away  
10 from the set-point (i.e. the steady state), the reactor will return to steady  
11 state. Many authors have demonstrated that this system presents a Hopf  
12 bifurcation locus. At the Hopf locus the steady state becomes unstable  
13 and the dynamic behaviour of the reactor is characterized by persistent  
14 oscillations (limit cycle). This is, of course, unacceptable and must be  
15 avoided.

16 Although the Hopf bifurcation locus can be computed analytically (Giona  
17 and Paladino, 1994), here we analyse the stability conditions by applying  
18 the MCF techniques described in this chapter. This will allow us to confront  
19 the results of the MCF analysis with the analytic results. The problem can  
20 be formalized in the MCF framework as follows:

- 21
- 22 • the input factors are the control gains and the uncertain physicochemical  
23 parameters of the CSTR model;
  - 24 • the outputs are the eigenvalues of the Jacobian;
  - 25 • the filtering criterion is:
    - 26 – behaviour  $B$  if all eigenvalues have negative real parts;
    - 27 – nonbehaviour  $\bar{B}$  otherwise.

28 The nominal conditions of the CSTR are defined as follows:

29

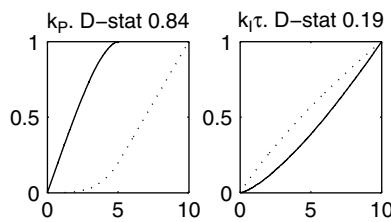
$k_0 = 133600 s^{-1}$	$E/R = 8000 K$	$\tau = 3600 s$	$\Delta T_a = 200 K$
$T_0 = 298.42 K$	$T_s = 430 K$	$T_{es} = 373.16$	
$\vartheta_s = 0$	$\xi_s = 0.8$	$N = 0.5$	

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Such nominal conditions, depending on the values of the various  
physicochemical parameters, are subject to a degree of uncertainty.

Let us first analyse the stability of this system under the nominal conditions,  
by varying only the control gains  $k_p$  and  $k_I\tau$ . As anticipated, this  
analysis can be performed analytically. We analyse here the Hopf bifurcation  
locus in the  $(k_p, k_I\tau)$  plane using the MCF approach. The analysis  
requires the following steps:

- 01     • Sample the control gains uniformly in the range [0, 10];
- 02     • Compute the eigenvalues of the Jacobian;
- 03     • Check the stability condition;
- 04        – the set of control gains providing stable eigenvalues (negative real parts) is the behavioural set;
- 05        – the set of control gains providing unstable eigenvalues (nonnegative real parts) is the nonbehavioural set;
- 06
- 07
- 08
- 09     • Perform the Smirnov analysis;
- 10
- 11
- 12

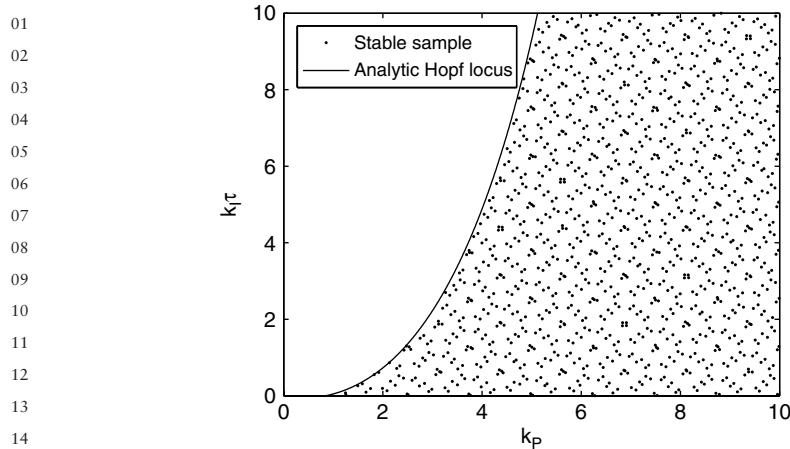


22     Looking at the plot for  $k_p$ , we can see that the nonbehavioural cumulative  
 23 distribution (solid line) has a limit threshold at about  $k_p^* = 5$ , above  
 24 which only stable solutions are present; this implies that sufficiently large  
 25 values of the proportional control gain ( $k_p > k_p^*$ ) are able to stabilize  
 26 the reactor, whatever the value of the integral control gain. The latter  
 27 gain, on the other hand, is more likely to produce a stable reactor for  
 28 small values. However, the two cumulative distributions for  $k_I\tau$  have the  
 29 same support, i.e. both ranges of the stable and unstable sets span the  
 30 entire support [0, 10], implying that no clear threshold of stability can  
 31 be identified.

- 32     • Plot the behavioural sample on the  $(k_p, k_I\tau)$  plane.  
 33        This shows the boundary of stability that exactly corresponds to the  
 34        analytic solution (solid line). Note also that the patterns in the scatterplot  
 35        are due to the Sobol' quasi-random sequences used for the example.
- 36

37     We now check the stability analysis for robustness, by allowing physico-  
 38 chemical parameters to be uncertain. These uncertainties are given by  
 39        normal distributions, with the following characteristics:

- 41     •  $(k_0, E/R)$ : assuming an estimate of kinetic coefficients, they are likely to  
 42        be strongly correlated (Bard, 1974) and with much greater uncertainty  
 43        for  $k_0$  than for  $E/R$ . So we take a standard deviation of 35% for  $k_0$ ,
- 44

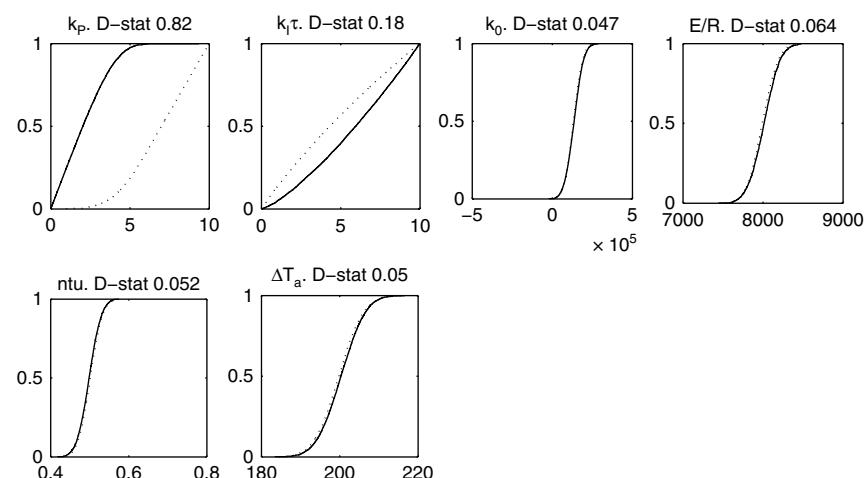


2% for  $E/R$  and a correlation coefficient of 0.96 (Paladino and Ratto, 2000).

- ( $N$ ): the heat transfer coefficient has a standard deviation of 5%, i.e.  $\sim N(0.5, 0.025)$ .
- ( $\Delta T_a$ ): the adiabatic temperature difference has a standard deviation of 5 K, i.e.  $\sim N(200, 5)$ .

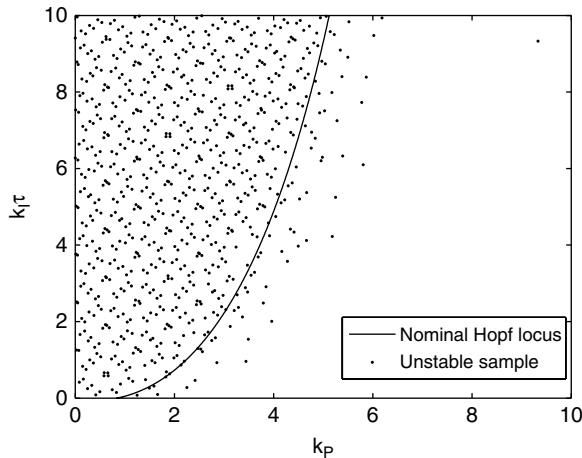
We then proceed with the MCF analysis, as described below.

- First we perform the Smirnov test.



The sensitivity behaviour is still dominated by the control gains. In particular, sufficiently large values of  $k_p$  are still able to stabilize the reactor, whatever the values of  $k_l\tau$  and all the uncertainties in the physicochemical parameters. This is very important, since it allows us to design a stable control, i.e. robust against uncertainties. Looking very carefully at the physicochemical parameters, we can also see that, as expected, the reactor has a very slight tendency towards instability if:

- the heat transfer coefficient decreases;
  - the adiabatic temperature difference increases;
  - the kinetic parameters increase.
- We then plot the bidimensional projection of the unstable sample  $\bar{B}$  onto the  $(k_p, k_l\tau)$  plane.



This shows that unstable behaviour can be present beyond the Hopf locus computed at the nominal values of the physicochemical parameters, implying that safe values for control gains have to be chosen according to uncertainty considerations. Constraining gains as  $k_p > 6$  and  $0 < k_l\tau < 4$  may be a good starting point.

#### 5.2.5.2 Stability analysis of a small macroeconomic model

Let us consider a simple macroeconomic model: a Phillips curve. As usual in economics, this is a discrete-time dynamic model (typically with a quarterly sampling interval). Let  $c_t$  and  $\pi_t$  denote output gap and inflation,

01 respectively. In macroeconomic theory, the output gap denotes the cyclical  
 02 component of GDP (gross domestic product) with respect to the long-term  
 03 trend. In general terms, it is a quantity linked to the business cycle. We can  
 04 write the hybrid Phillips curve as

05

06

$$\pi_t = \omega_b \pi_{t-1} + \omega_f E_t \pi_{t+1} + \beta c_t + a_{\pi t} \quad (5.11)$$

07

08

$$c_t = 2A \cos(2\pi/\tau) c_{t-1} - A^2 c_{t-2} + a_{c,t} \quad (5.12)$$

09

10

11

12 where  $E_t$  denotes the expectation taken at period  $t$ ,  $0 < (\omega_b, \omega_f) < 1$ ,  $A$  and  
 13  $\tau$  are the amplitude and period of  $c_t$  and  $a_{\pi,t}, a_{c,t}$  are white noises.

14 The Phillips curve links the inflation dynamics to the output gap, in such  
 15 a way that periods of economic expansion (i.e. with a positive output gap)  
 16 are typically associated with an increase in inflation and vice versa. More-  
 17 over, the hybrid Phillips curve also says that inflation in the current period  
 18 is linked with some persistence  $\omega_b$  to the rate of inflation in the previous  
 19 period and to the expected level of inflation in the following period, with a  
 20 weight  $\omega_f$ . This leads on to the theory of rational expectation behaviour of  
 21 economic agents. In contrast to standard (physical) dynamic systems, the  
 22 occurrence of a unique, stable solution in macroeconomic rational expec-  
 23 tations models requires that there be an equal number of explosive eigen-  
 24 values and forward-looking variables. In discrete-time dynamic models,  
 25 stable roots have absolute values less than 1, while explosive ones are  
 26 larger than 1. In this case, the Phillips curve has one lag  $\pi_{t-1}$  and one  
 27 lead  $E_t \pi_{t+1}$ , so we need exactly one stable and one explosive eigenvalue.  
 28 To help explain the stability conditions of economic rational expectations  
 29 models to non-economists, we can say that the fact that the current level of  
 30 inflation depends on both past and future levels, makes the system like a  
 31 two-point boundary system (similar to certain types of differential equations  
 32 in space describing advection-dispersion mechanisms). Hence, this implies  
 33 the presence of initial and terminal conditions, corresponding to backward-  
 34 looking and forward-looking components, respectively. Likewise in physical  
 35 systems, backward-looking behaviour propagates the initial conditions into  
 36 the future. This propagation is stable if it is associated to stable eigenvalues,  
 37 thus assuring that the dynamic system will asymptotically converge to the  
 38 steady state. The forward-looking components, on the other hand, prop-  
 39 agate the terminal conditions into the past, i.e. in a symmetrical manner,  
 40 reversing the orientation of the time axis. It intuitively makes sense that,  
 41 if the orientation of time is reversed, explosive roots looking ‘towards the  
 42 future’ become stable roots looking ‘towards the past’; therefore, in order  
 43 to ensure stability of the propagation into the past of forward-looking  
 44 components, such components need to be associated to explosive roots.

The eigenvalues of this simple model can be computed analytically:

$$\begin{aligned} r_b &= \frac{1/\omega_f - \sqrt{1/\omega_f^2 - 4\omega_b/\omega_f}}{2} \\ &= \frac{1 - \sqrt{1 - 4\omega_b\omega_f}}{2\omega_f} \\ r_f &= \frac{1 + \sqrt{1 - 4\omega_b\omega_f}}{2\omega_f}. \end{aligned} \quad (5.13)$$

The restriction  $1 - 4\omega_b\omega_f \geq 0$  ensures that the roots are real. The stability condition is verified if

$$\omega_f < (1 - \omega_b) \quad (5.14)$$

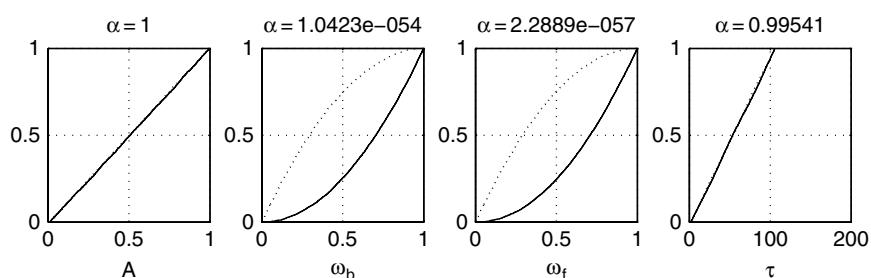
or

$$\omega_f = (1 - \omega_b) \quad \text{and} \quad \omega_b > 0.5.$$

We apply the Monte Carlo filtering technique to identify the stable behaviour. The support for the model coefficients is defined as

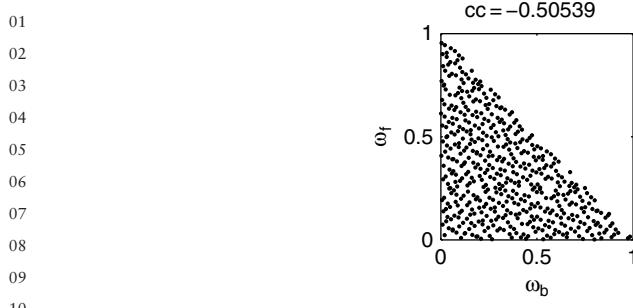
$$A \sim U[0, 1], \quad \omega_b \sim U[0, 1], \quad \omega_f \sim U[0, 1], \quad \tau \sim U[0, 100].$$

We first perform the Smirnov test for the separation of the  $B$  and  $\bar{B}$  subsets.



The occurrence of stable or unstable behaviour is clearly attributable to the coefficients  $\omega_b$  and  $\omega_f$ . Moreover, the shape of the dotted curves (corresponding to  $B$ ) indicates that stable behaviour will more probably occur for smaller  $\omega_b$  and  $\omega_f$  values.

We subsequently perform a correlation analysis of the stable sample and plot the significant correlation selected: the bidimensional projection of the  $B$  subset onto the  $(\omega_b, \omega_f)$  plane.



19     The dots in this plot clearly indicate the first stability condition  $\omega_f <$   
 20      $(1 - \omega_b)$  in (5.14). The second condition in (5.14) is just one limit case, and  
 21     tells us simply that only the half part  $\omega_b > 0.5$  of the stability boundary line  
 22      $\omega_f = (1 - \omega_b)$  provides stable behaviour. This is, of course, hardly visible in  
 23     the plot.

#### 5.2.5.3 Mapping propagation of the infection in the simple infection dynamics model

Let us consider the model presented in Chapter 4. We want to map the conditions under which infection propagates. Recalling the solution to the model shown in Chapter 4, we have

$$I = I_0 \exp(Yt)$$

with

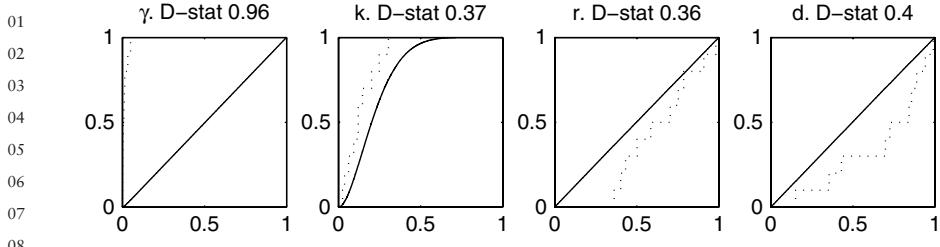
$$Y = \gamma k S_0 - r - d$$

which states that the infection dies out if  $Y < 0$  and propagates if  $Y > 0$ . So, our MCF problem is to map  $Y < 0$ , i.e. the stable eigenvalue of the infection propagation dynamics.

We sample input factors from the same distributions used in Chapter 4 for the three different scenarios of parameter  $k$ .

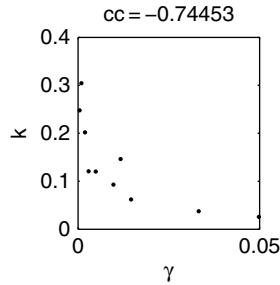
- $k \sim \text{beta}(2, 7)$ . In this case, the probability that the infection will die out is very small (only 1% of the MC sample). Performing the Smirnov analysis we obtain the picture on the top of next page.

This shows that all input factors have a nonnegligible effect in driving the propagation of the infection. However,  $\gamma$  is predominant, based on which it is clear that the infection can die out only for a very narrow range of  $\gamma$  values, in the lowest part of its range. Moreover, we can also

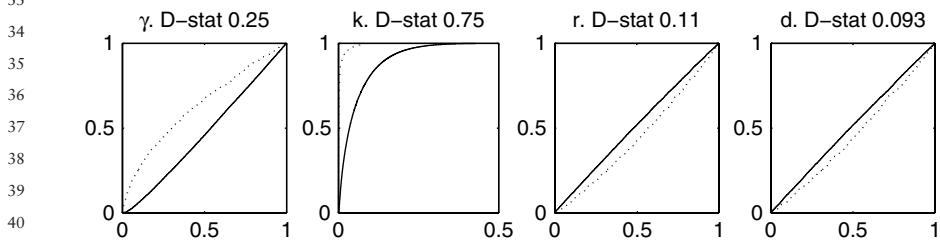


see that smaller values of  $k$  and larger values of  $r$  and  $d$  tend to limit propagation of the infection.

The correlation analysis reveals a negative correlation between  $\gamma$  and  $k$  under the behavioural subset, which reflects the product interaction between these two factors. Note also that  $\gamma$ -values in this behavioural scatterplot are constrained in the range  $[0, 0.05]$  out of a full sample in the range  $[0, 1]$ .



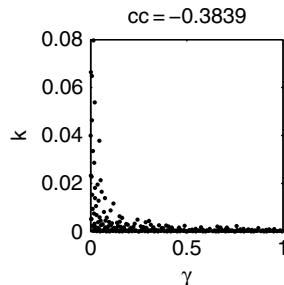
- $k \sim \text{beta}(0.5, 10)$ . Changing the prior distribution of  $k$  raises the probability that the infection will die out to about 20%. Performing the Smirnov analysis produces the following modified picture for the model parameters:



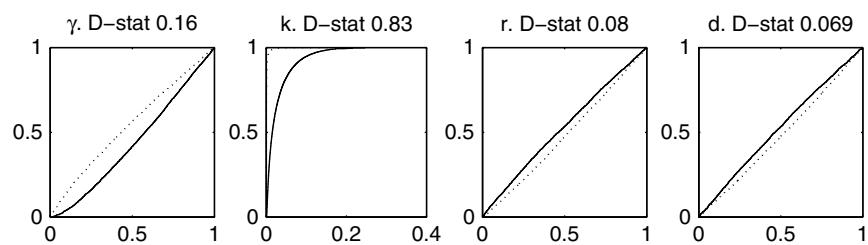
Now the importance of  $k$  has increased, and we can see that the behavioural runs are linked merely to  $k$ , falling in the lowest part of its

01 range. Moreover, small  $\gamma$  values and large  $r$  and  $d$  values also tend to  
 02 produce a declining infection dynamics.

03 The correlation analysis confirms the negative correlation between  $\gamma$   
 04 and  $k$ , while the hyperbola shape linked to the product interaction of  
 05 these two parameters in the model is now more sharply visible.



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- $k \sim \text{beta}(0.2, 15)$ . In this case, the probability of a declining infection dynamics rises to 57%. The Smirnov analysis indicates that  $k$  is now the dominant factor in driving the behaviour of the infection dynamics model, leaving a minor role to the remaining parameters:
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31 The correlation analysis still produces a negative correlation between  $\gamma$   
 32 and  $k$  with the hyperbola boundary between the  $B$  and  $\bar{B}$  subsets.

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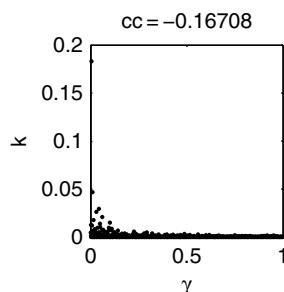
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01           **5.3 METAMODELLING AND THE**  
02           **HIGH-DIMENSIONAL**  
03           **MODEL REPRESENTATION**

04  
05           **IS IT POSSIBLE TO REPRESENT IN A DIRECT WAY THE RELATIONSHIP BETWEEN**  
06           **INPUT FACTORS AND THE MODEL OUTPUT? CAN SUCH A DIRECT AND COMPUTA-**  
07           **TIONALLY CHEAPER APPROXIMATION BE USED IN PLACE OF THE ORIGINAL MODEL?**  
08           **HOW CAN WE ESTIMATE SUCH AN APPROXIMATION?**

09  
10          Let us now consider the problem of representing in a clear and immediate  
11          way the relationship  $Y = f(X_1, \dots, X_k)$ , whose form is usually unknown  
12          to the analyst. This is essentially a problem of model approximation or  
13          metamodelling, whereby the analyst aims to identify a simple relationship  
14          between  $X_i$ 's and  $Y$  that fits the original model well and is less computa-  
15          tionally demanding.

16          There is a vast literature on this subject. Local approximation methods  
17          take the value of  $f$  and its derivatives at a base point  $\mathbf{X}_0$  and construct  
18          a function that matches the properties of  $f$  at  $\mathbf{X}_0$  and in the nearby  
19          region (Taylor series). Interpolation methods look at 'nice' functions that  
20          go through a set of data points spanning the entire domain of the  $Y =$   
21           $f(\cdot)$  mapping. The approximation is then identified by fixing  $p$  parameters  
22          (e.g. the coefficients of the polynomials) using  $p$  data points (Lagrange,  
23          Chebyshev interpolation). Tensor products of orthogonal polynomials or  
24          complete polynomials are usually applied to span the space of func-  
25          tions in  $R^k$  and to interpolate  $Y = f(X_1, \dots, X_k)$ . Regression/smoothing  
26          methods differ from interpolation in that a set of  $N > p$  data points is  
27          used to identify the approximating function. For univariate functions  $f$ ,  
28          the interpolation, regression and smoothing approaches can be extended by  
29          applying piecewise polynomials, constructing functions that are only piece-  
30          wise smooth. Splines (cubic splines are the most popular) are a powerful  
31          and widely used approach to piecewise polynomial interpolation and regres-  
32          sion/smoothing (in the latter case they are called smoothing splines). Splines  
33          are smooth where the polynomial pieces connect. In the multivariate case,  
34          radial basis function (RBF) networks can be seen as the equivalent of  
35          univariate piecewise interpolation, regression and smoothing approaches  
36          (RBFs are also classified under the heading of kernel regression smoothing  
37          methods).

38          Before proceeding with the description of the methodologies, we would  
39          like to draw attention to some additional properties of the approximating  
40          functions, which also uncover fundamental links between metamodelling  
41          and the theory of variance-based sensitivity analysis discussed in previous  
42          chapters.

01 Let  $g(\cdot)$  be the generic function approximating the true model  $Y =$   
 02  $f(X_1, \dots, X_k)$  and let us assume a quadratic loss function  $E[(Y - g(\cdot))^2]$  as a  
 03 measure of ‘fit’ for  $g$ .

04 If we were to approximate  $f$  with a function of *one single* parameter  $X_i$ ,  
 05 what function  $g_i^*(X_i)$  would produce minimum loss?

06 It is well known, from any standard text on statistics, that the univariate  
 07 function

$$08 \quad g_i^* = E[Y|X_i], \quad (5.15)$$

10 i.e. the conditional expectation of  $Y$  given  $X_i$ , is the minimum loss approx-  
 11 imation to  $f$ . The expression (5.15) tells us that at any  $p$ -location  $X_i =$   
 12  $x_{i,p}$ , the value of  $g^*$  is obtained by integrating (averaging)  $Y$  over all the  
 13 remaining  $[X_1, \dots, X_{i-1}, X_{i+1}, \dots, X_k]$  input factors.

14 Equation (5.15) can be generalized to any subset of the input factors  $\mathbf{X}_I$ ,  
 15 indexed by  $I = (i_1, \dots, i_l)$ , as

$$17 \quad g_I^* = E[Y|\mathbf{X}_I]. \quad (5.16)$$

19 Equations (5.15) and (5.16) obviously link to the ANOVA-HDMR  
 20 decomposition of  $f$  discussed in Chapter 4:  
 21

$$22 \quad f(X_1, X_2, \dots, X_k) = f_0 + \sum_i f_i + \sum_i \sum_{j>i} f_{ij} + \dots + f_{12\dots k}, \quad (5.17)$$

25 where the connection between the  $f_i$  terms of the HDMR and the minimum  
 26 loss approximating functions  $g^*(\cdot)$  is made explicit by

$$28 \quad f_0 = E(Y)$$

$$29 \quad f_i(X_i) = E(Y|X_i) - f_0 = g_i^* - f_0 \quad (5.18)$$

$$31 \quad f_{ij}(X_i, X_j) = E(Y|X_i, X_j) - f_i(X_i) - f_j(X_j) - f_0 = g_{i,j}^* - f_i(X_i) - f_j(X_j) - f_0.$$

33 Each term of the ANOVA-HDMR decomposition tells the analyst how  
 34 much, on average,  $Y$  can be moved with respect to its mean level  $f_0$  by  
 35 acting on single input factors or groups of them. Moreover, the quantity  
 36  $V(g_I^*(\mathbf{X}_I))/V(Y) = \text{corr}(g_I^*(\mathbf{X}_I), Y)$  is well known in statistics as the ‘correla-  
 37 tion ratio’ or ‘nonparametric  $R$ -squared’, and provides the fraction of the  
 38 variability of  $Y$  that is explained with the *best* predictor based on  $\mathbf{X}_I$ . The  
 39 equivalence between nonparametric  $R$ -squared and variance-based sensi-  
 40 tivity indices is obvious and this closes the parallel between the problem of  
 41 estimating and measuring the explanatory power of covariates in regression  
 42 and variance-based sensitivity analysis.

43 Coming back to the metamodeling problem, kernel regression methods  
 44 can be shown to provide, under certain regularity conditions, consistent

estimators of  $g^*(\cdot)$ , which are asymptotically normal at the  $\sqrt{N}$  rate (see Doksum and Samarov, 1995, and references cited therein), i.e. as  $N \rightarrow \infty$ ,

$$E \int (\hat{g}(\mathbf{X}_I) - g^*(\mathbf{X}_I))^2 d\mathbf{X}_I = o(N^{-1/2}).$$

The metamodeling approach that we follow in this book can be classified under kernel regression smoothing methods. However, due to its recursive implementation, our approach differs with respect to other *en-bloc* methods. This has some advantages, such as the estimation of ‘smoothing parameters’ (‘hyper-parameters’) with maximum likelihood and greater flexibility in managing nonlinearities in  $f(\cdot)$ .

### 5.3.1 Estimating HDMRs and Metamodels

In the literature on sensitivity analysis there has been a growing interest in metamodeling and smoothing techniques. Storlie and Helton (2008) have reviewed smoothing methods for sensitivity analysis, from smoothing splines to various types of univariate and multivariate kernel regression approaches. Li *et al.* (2002, 2006) developed the so-called Random Sampling HDMR, which involves approximating the truncated HDMR expansion up to order three, based on orthogonal polynomials. Pappenberger and Stauch (2007) use spline smoothing to estimate sensitivity indices. Using the State-Dependent Regression (SDR) approach of Young (2001), Ratto *et al.* (2004, 2007) have developed a nonparametric approach which is very similar to smoothing splines and kernel regression approaches, but which is based on recursive filtering and smoothing estimation (the Kalman Filter, KF, combined with Fixed Interval Smoothing, FIS). Such a recursive least-squares implementation has some fundamental advantages: (a) it is couched with optimal maximum likelihood estimation, thus allowing for an objective estimation of the smoothing hyper-parameters, and (b) it allows for greater flexibility in adapting to local discontinuities, heavy nonlinearity and heteroscedastic error terms (see below). All such methods can be assigned to the regression/smoothing class of approximation approaches.

An example of interpolating metamodels, on the other hand, is given by Gaussian emulators (see Oakley and O'Hagan, 2004, and the references cited therein, for a detailed description) and kriging metamodels (Kleijnen, 2007a,b). Kriging metamodels are similar to Gaussian, except that they do not rely on Bayesian interpretation. While *theoretically* appealing, Gaussian emulators can be prone to the curse of dimensionality and to the smoothness assumptions of the function under analysis. This is because, instead of trying to identify the best predictors of Y based on a subset

of input factors or on low-order ANOVA-HDMR terms, Gaussian emulators try to interpolate and predict the  $f(\cdot)$  mapping by applying a Gaussian kernel of the same  $k$ -dimensionality as the input parameter space. Therefore, as  $k$  increases, the number of ‘hyperparameters’ to be estimated (linked to the covariance structure of the  $k$ -dimensional Gaussian kernel), increases strongly, often implying problems with identification and overparameterization.

Such problems are well known in standard interpolation and smoothing techniques based on  $k$ -dimensional kernel regressors. They imply that Gaussian emulators are only effective, *in practice*, for model structures having a small number of significant main effects and very mild interactions, for which such problems are made irrelevant by the very few highly identifiable elements of the  $f(\cdot)$  mapping.

In other words, in regression/smoothing techniques, metamodels are based on subsets of input factors and/or truncated HDMR expansions of order smaller than  $k$ , and their identification and estimation *incorporate* sensitivity analysis criteria, in that nonsignificant contributions to  $Y$  are identified and eliminated *within* the process of construction of the approximation to  $Y$ . In contrast to this, Gaussian emulators aim first to estimate a full  $k$ -order mapping on the basis that a sensitivity analysis applied afterwards to the emulator will automatically reveal the significant contributions to  $Y$ .

Once identified, estimated and parameterized, metamodels provide a direct, albeit approximated, analytic expression of the  $Y = f(X_1, \dots, X_k)$  mapping, which accounts for nonlinearities and interaction terms of increasing order. As such, they can be used for various purposes:

- sensitivity analysis, by helping to highlight the most important input factors of the mapping;
- model simplification, by finding a surrogate model containing a subset of the input factors that account for most of the variability of  $Y$ ;
- model calibration, in which the metamodel is used to find directly the optimal parameterization for the fulfilment of the given calibration criteria.

A detailed description of all the available metamodeling techniques is beyond the scope of this book: readers can refer to the cited works for further information. We will concentrate here on nonparametric methods and, in particular, we will demonstrate simple implementations of univariate nonparametric smoothing methods that give the ‘flavour’ of the more sophisticated multivariate, recursive procedure of Young (2001), as used for metamodeling in Ratto *et al.* (2004, 2007). In nonparametric methods, the function  $E(Y|X_i)$  is not approximated by a basis of functions that span

the entire domain of  $X_i$ ; rather many ‘local’ approximations are identified which move along the  $X_i$ -axis. Such ‘local’ functions are subsequently joined using ad hoc criteria, such as imposing some smoothness properties like continuity (piecewise linear interpolation is an example of this). This in practice gives a ‘look-up’ table of the function  $f_i = g^*(X_i)$  which can subsequently be parameterized using functional bases, such as polynomials, Fourier expansions, linear wavelets or Radial Basis functions (RBFs).

### 5.3.1.1 Smoothing scatterplots using the Haar wavelet

Wavelets, and in particular the Haar wavelet, provide a very simple approach to smoothing signals.

The  $2 \times 2$  Haar matrix is given by

$$H_2 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}.$$

Given an MC sample of  $f(\cdot)$  whose length  $N$  is a power of 2 ( $y_1, y_2, \dots, y_{2^n-1}, y_{2^n}$ ), i.e.  $N = 2^n$ , and where the sample is sorted with respect to the input factor  $X_i$  under analysis, we may group its elements as  $((y_1, y_2), \dots, (y_{2^n-1}, y_{2^n}))$  and we may right-multiply each term by the matrix  $H_2$ ,

$$H_2 \begin{pmatrix} y_{2j-1} \\ y_{2j} \end{pmatrix} = \begin{pmatrix} s_j \\ d_j \end{pmatrix} \quad \text{for } j = 1, \dots, 2^{n-1}$$

obtaining two new sequences  $(s_1, \dots, s_{2^{n-1}})$  and  $(d_1, \dots, d_{2^{n-1}})$ . The sequence  $s$  gives the sum between two consecutive points while the sequence  $d$  gives the difference. Since the original signal has a length equal to  $2^n$ , one can recursively apply the same procedure to  $s$ -sequences up to  $n$  times. For each  $\lambda = 1, \dots, n$  we call the associated sequence  $s^\lambda$  the  $\lambda$ th Haar approximation coefficients and  $d^\lambda$  the  $\lambda$ th Haar detail coefficients.

For each  $\lambda = 1, \dots, n$  we may use  $s^\lambda$  to create an approximation  $\hat{f}^\lambda$  of the original signal  $f$ . This is obtained first by rescaling each value of  $s^\lambda$  by  $\sqrt{2^\lambda}$  and then by replicating each of them  $2^\lambda$  times.

*Example* Consider a sample of length  $2^4 = 16$  from a function  $Y = f(X) = (X - 0.5)^2 + \varepsilon$ , where  $X \sim U[0, 1]$  and  $\varepsilon$  is a white noise normally distributed  $N(0, 0.03)$ :

$$\begin{aligned} f = & (0.21, 0.19, 0.14, 0.1, 0.05, 0.01, 0.03, -0.01, 0.01, \\ & -0.03, 0.01, 0.06, 0.04, 0.1, 0.13, 0.19). \end{aligned}$$

- First stage ( $\lambda = 1$ ). From the first pair of  $y$ -points we compute the first element of  $s^1$ :  $(0.21 + 0.19)/\sqrt{2} = 0.2828$ . Repeating this with all pairs of  $y$  we get

$$s^1 = (0.2828, 0.1697, 0.0424, 0.0141, -0.0141, 0.0495, 0.0990, 0.2263).$$

Scaling the first term of  $s^1$  by  $\sqrt{2}$  we get 0.2, which is replicated 2<sup>1</sup> times to construct the first two elements of  $\hat{f}^1$ . This is repeated to get

$$\hat{f}^1 = (0.2, 0.2, 0.12, 0.12, 0.03, 0.03, 0.01, 0.01, -0.01, -0.01, 0.035, 0.035, 0.07, 0.07, 0.07, 0.16, 0.16).$$

- Second stage ( $\lambda = 2$ ): Replicating the steps of the first stage to the  $s^1$  sequence, we get

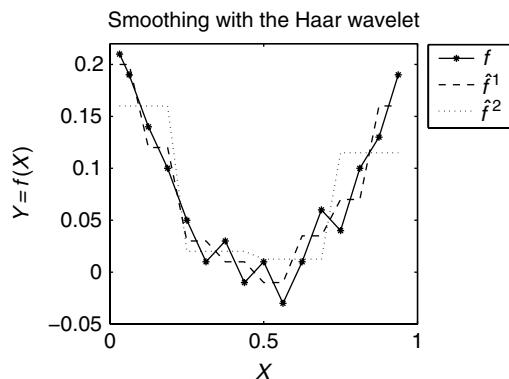
$$s^2 = (0.32, 0.04, 0.025, 0.23)$$

and

$$\hat{f}^2 = (0.16, 0.16, 0.16, 0.16, 0.02, 0.02, 0.02, 0.02, 0.02, 0.013, 0.013, 0.013, 0.013, 0.12, 0.12, 0.12, 0.12, 0.12)$$

- and so on

If we compare the graph of the original signal  $f$  and its first- and second-level approximations  $\hat{f}^1, \hat{f}^2$  we obtain the following picture:



The picture above shows that  $\hat{f}^\lambda$  may be used to infer the smoothed behaviour of the signal  $f$ , where  $\lambda$  plays the role of a smoothing parameter:

the higher  $\lambda$ , the smoother the signal extraction. At the highest level of smoothing  $\lambda = n$ , the Haar wavelet will simply provide the unconditional mean  $E(Y)$ . Note also that this smoothing approach can be implemented recursively, and does not require any matrix inversion.

*Exercise* Write a code for the Haar wavelet and reproduce the results shown in the previous example.

### 5.3.1.2 Spline smoothing

Smoothing splines are a nonparametric method which is very useful for understanding the more sophisticated methodology to be discussed later in this chapter. Given a Monte Carlo sample of size  $N$ , a cubic smoothing spline is a function  $\hat{g}$  that minimizes the penalized residuals' sum of squares:

$$\sum_{j=1}^N [y_j - \hat{g}(x_j)]^2 + \lambda \int_a^b \left[ \frac{d^2 \hat{g}(x)}{dx^2} \right]^2 dx \quad (5.19)$$

where  $a \leq \min(x_j)$ ,  $b \geq \max(x_j)$ ,  $j = 1, \dots, N$  and  $\lambda$  is the Lagrange multiplier, which plays the role of a smoothing parameter (i.e. the bigger  $\lambda$ , the smoother  $\hat{g}$ ). In (5.19), the first term is the sum of squared residuals, measuring fit to the data, while the second term penalizes too high a curvature in  $\hat{g}$ . This approach is also known in numerical analysis as *regularization* (or deterministic regularization, DR).

The unique, explicit solution to (5.19) is given by a natural cubic spline with knots at each observed value  $x_j$  (see Hastie and Tibshirani, 1990). A cubic polynomial spline is a function that is a cubic polynomial on any interval defined by adjacent knots, has two continuous derivatives and a third which is a step function that jumps at the knots.

Spline smoothing can easily be implemented by taking the discrete formulation of (5.19), where the long-term signal  $\hat{t}$  is given by the solution of the minimization problem:

$$\min \left( \sum_{s=1}^N [y_s - \hat{t}_s]^2 + \lambda \sum_{s=2}^{N-1} [(\hat{t}_{s+1} - \hat{t}_s) - (\hat{t}_s - \hat{t}_{s-1})]^2 \right), \quad (5.20)$$

where the index  $s$  scans the data in a *sorted* order with respect to the input factor under analysis. In econometrics this is called the Hodrick-Prescott (HP) filter (Hodrick and Prescott, 1980), and it is used for trend extraction in economic time-series analysis (in such cases  $s$  scans the data in temporal order). As Young and co-workers have shown (Jakeman and Young, 1984; Young and Pedregal, 1999), this same problem (5.20) can

be solved by a very simple recursive filtering and smoothing algorithm that yields identical results to that of HP but is more sophisticated in statistical terms<sup>2</sup>. This recursive solution also has the advantage that it involves no matrix inversion, while the HP *en-bloc* solution, as we see below, involves the inversion of a matrix with dimension equal to that of the data length.

For the present, tutorial purposes, let us consider only the HP *en-bloc* solution, which can be formulated by taking derivatives with respect to  $\hat{t}_s$ : i.e.,

$$\begin{aligned}
 10 \quad y_1 &= (1 + \lambda)\hat{t}_1 - 2\lambda\hat{t}_2 + \lambda\hat{t}_3 \\
 11 \quad y_2 &= -2\lambda\hat{t}_1 + (1 + 5\lambda)\hat{t}_2 - 4\lambda\hat{t}_3 + \lambda\hat{t}_4 \\
 13 \quad &\dots \\
 14 \quad y_s &= \lambda\hat{t}_{s-2} - 4\lambda\hat{t}_{s-1} + (1 + 6\lambda)\hat{t}_s - 4\lambda\hat{t}_{s+1} + \lambda\hat{t}_{s+2} \\
 15 \quad s &= 3, \dots, N-2 \\
 17 \quad &\dots \\
 19 \quad y_{N-1} &= \lambda\hat{t}_{N-3} - 4\lambda\hat{t}_{N-2} + (1 + 5\lambda)\hat{t}_{N-1} - 2\lambda\hat{t}_N \\
 20 \quad y_N &= \lambda\hat{t}_{N-2} - 2\lambda\hat{t}_{N-1} + (1 + \lambda)\hat{t}_N.
 \end{aligned}$$

This can easily be put into matrix form,

$$y = (\mathbf{I} + \lambda \mathbf{U}^T \mathbf{U}) \cdot \hat{\mathbf{t}}^\lambda, \quad (5.21)$$

where  $\mathbf{I}$  is the  $N \times N$  identity matrix,  $y$  is the  $1 \times N$  vector of model output data and  $\mathbf{U}$  is the following  $N \times N$  matrix:

$$\mathbf{U} = \begin{bmatrix} 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & \dots & 0 & 0 & 0 \\ 0 & 1 & -2 & 1 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \dots & 1 & -2 & 1 \end{bmatrix}.$$

The explicit solution is easily found to be

$$\hat{\mathbf{t}}^\lambda = (\mathbf{I} + \lambda \mathbf{U}^T \mathbf{U})^{-1} \cdot y = \mathbf{W}^{-1} \cdot y. \quad (5.22)$$

---

<sup>2</sup> This IRWSM algorithm is available in the CAPTAIN Toolbox for Matlab, which can be downloaded from <http://www.es.lancs.ac.uk/cres/captain/>

The ‘trend’  $\hat{t}^\lambda$  is a nonparametric estimate of the univariate ‘metamodel’  $f_i(X_i) = E(Y|X_i)$ , which approximates the function  $f(\cdot)$ . The dependence of such an estimate on the smoothing parameter is made explicit in (5.21) and (5.22) by the  $\lambda$  exponent in  $\hat{t}^\lambda$ . The appropriate value for  $\lambda$  is not immediately apparent: cross-validation, graphical methods and measures of degrees of freedom are used for this purpose (see Hastie and Tibshirani, 1990 and Storlie and Helton, 2008, for more details). Note that, as pointed out above, since the solution (5.21) involves the inversion of a  $N \times N$  matrix, it can be computationally intensive and require a large memory size for large MC samples. Note also that, in the *en-bloc* approach, it is also possible to obtain the standard errors of the estimated  $\hat{t}^\lambda$ . Readers can refer to Hastie and Tibshirani (1990) for a detailed discussion of *en-bloc* methods and estimation of standard error bands and to Young and Pedregal (1999) for a combined discussion of these topics in the case of recursive and *en-bloc* approaches.

*Example* Consider the same example used above for the Haar wavelet. Using the same data, we obtain the following estimates for  $\hat{t}^\lambda$ , at various smoothing levels:

- $\lambda = 1$ :

$$\begin{aligned}\hat{t}^1 = & (0.22, 0.18, 0.14, 0.096, 0.055, 0.026, 0.011, \\ & -0.0012, -0.0064, -0.0069, 0.01, 0.036, 0.059, 0.095, 0.14, 0.18).\end{aligned}$$

- $\lambda = 10$ :

$$\begin{aligned}\hat{t}^{10} = & (0.21, 0.17, 0.13, 0.095, 0.061, 0.033, 0.013, \\ & 0.00069, -0.0035, 0.00068, 0.014, 0.036, 0.063, 0.096, 0.13, 0.17).\end{aligned}$$

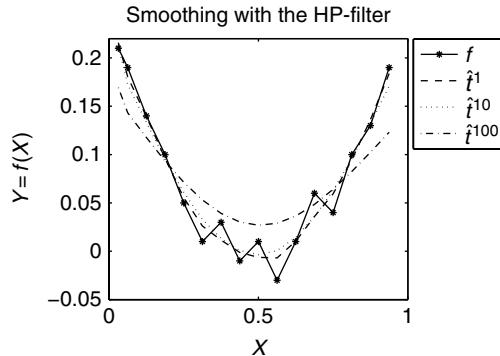
- $\lambda = 100$ :

$$\begin{aligned}\hat{t}^{100} = & (0.17, 0.14, 0.12, 0.093, 0.071, 0.053, 0.039, \\ & 0.03, 0.027, 0.029, 0.036, 0.048, 0.064, 0.082, 0.1, 0.12).\end{aligned}$$

Such smoothed estimates are shown in the plot at the top of next page.

This plot shows the smoothing effect of increasing  $\lambda$ . If  $\lambda$  tends to infinity, the HP-filter simply provides the unconditional mean  $E(Y)$ . Judging by eye, the best smoothing seems be obtained using  $\lambda$  values between 1 and 10.

*Exercise* Write a code for the spline smoothing (HP-filter) and reproduce the results shown in the previous example.



### 5.3.1.3 State-dependent regressions

Ratto *et al.* (2004, 2007) have recently presented a flexible and efficient approach to the estimation of  $g_I^*(\mathbf{X}_I) = E(Y|\mathbf{X}_I)$  and of truncated ANOVA-HDMR decompositions. This estimation procedure is based on considering the HDMR as a State-Dependent Parameter (SDP) relationship (Young, 2000; Young *et al.*, 2001) and, in particular, an example of the State-Dependent Regression (SDR) model estimation, as discussed in Young (2001). In this form, it is a non-parametric approach, based on recursive filtering and smoothing estimation procedures similar to those mentioned in the previous sub-section and available in the CAPTAIN Toolbox for Matlab (see earlier footnote).

In brief, the fundamental concept underlying the SDR approach is that any term like  $E(Y|X_I)$  can be viewed as an SDR model of the form

$$Y_s = p_{I_s}(\xi_I) + e_s \quad (5.23)$$

where the state-dependent parameter (SDP)  $p_{I,s}(\xi_I)$ ,  $I = i_1, \dots, i_l$ , depends on a state variable  $\xi_I$  that moves, according to a generalized sorting strategy, along the coordinates of the single factors or groups of factors indexed by  $I$ ; and  $e_s$  is the residual, i.e. the portion of variability of  $Y$  that cannot be explained by the group of factors indexed by  $I$ .

Extending this definition, the truncated ANOVA-HDMR expansion can also be expressed as an SDR model of the following form:

$$Y_s - f_0 = \sum_i p_{i,s}(\xi_i) + \sum_{j>i} p_{ij,s}(\xi_{ij}) + \sum_{l>j>i} p_{ijl,s}(\xi_{ijl}) + e_s \\ = \sum_i f_{i,s}(X_i) + \sum_{j>i} f_{ij,s}(X_i, X_j) + \sum_{l>j>i} f_{ijl,s}(X_i, X_j, X_l) + e_s \quad (5.24)$$

where  $e_s$  now represents the higher-order terms of the ANOVA-HDMR. Note also that, in the formulation (5.23), the SDP accounts for all cumulative effects within group  $I$ , be they first-order or interaction terms. As such,

it can be applied to any type of dependency structure amongst the input factors. On the other hand, in the HDMR formulation (5.24), each SDP accounts only for its associated first-order or interaction term of the HDMR.

According to the generalized sorting strategy adopted in (5.23) and (5.24), the group of input factors of interest  $I$  is characterized by a low-frequency spectrum (e.g. by some quasi-periodic pattern) while the remaining ones present a white spectrum. In this way, the estimation of the various HDMR terms is reduced to the extraction of the low-frequency component (i.e. of a ‘trend’) from the sorted output  $Y$ . To do so, the SDPs are modelled by one member of the Generalized Random Walk (GRW) class of nonstationary processes. For instance, the Integrated Random Walk (IRW) process turns out to produce good results, since it ensures that the estimated SDR relationship has the smooth properties of a cubic spline<sup>3</sup>.

Fixing ideas to the IRW characterization of each SDP, the model (5.24) can be put into the state-space form as

$$\begin{aligned} \text{Observation equation (HDMR): } & Y_s = \mathbf{z}_s^T \mathbf{p}_s + e_s \\ \text{State equations for each SDP: } & p_{I,s} = p_{I,s-1} + d_{I,s-1} \\ & d_{I,s} = d_{I,s-1} + \eta_{I,s} \end{aligned} \quad (5.25)$$

where  $\mathbf{z}_s^T$  is the transposed regression vector, composed entirely of unity elements;  $\mathbf{p}_s$  is the SDP vector; while  $e_s$  (observation noise) and  $\eta_{I,s}$  (system disturbances) are zero-mean white-noise inputs with variance  $\sigma^2$  and  $\sigma_{\eta(I)}^2$  respectively. Given this formulation, the SDPs are estimated using the recursive Kalman filter and associated recursive Fixed Interval Smoothing (FIS) algorithm (Kalman, 1960; Bryson and Ho, 1969; Young, 1999b). The recursive state estimation requires that each SDP be estimated in turn, each with a different ordering of the data, within a backfitting procedure (Young, 2000, 2001). At each backfitting iteration, the hyperparameters associated to (5.25), namely the white noise variances  $\sigma^2$  and  $\sigma_{\eta(I)}^2$ , are optimized by maximum likelihood (ML), using prediction error decomposition (Schweppe, 1965). In fact, by a simple reformulation of the KF and FIS algorithms, each SDP and its stochastic IRW process model can be entirely characterized by one Noise Variance Ratio (NVR) hyperparameter, where  $NVR_I = \sigma_{\eta(I)}^2 / \sigma^2$ . Hence, only NVRs need to be optimized.

One very useful implication of the KF/FIS algorithms underlying SDR estimation is that the standard error  $\sigma_{f,s}$  of the SDPs is recursively produced in a natural manner by reference to the covariance matrix of the state vector. This allows us to distinguish the significance of the estimated functions  $E(Y|\mathbf{X}_I)$ .

---

<sup>3</sup> Random Walk (RW) or Smoothed Random Walk (SRW) might be identified as being preferable in certain circumstances because they yield less smooth estimates.

01       The recursive formulation of the SDR model also implies a great flexibility  
 02       in the estimations, whenever this is required, for instance in the case of heteroscedastic behaviour in the observation noise or in the case of  
 03       discontinuities in the model output.<sup>4</sup> In practice, the basic SDR implementa-  
 04       tion used here can be easily extended to adapt to such situations, *typical*  
 05       in *non-linear systems*, where one single, constant smoothing parameter  $\lambda$   
 06       does not allow us to follow appropriately the observed patterns of the  $f(\cdot)$   
 07       mapping.

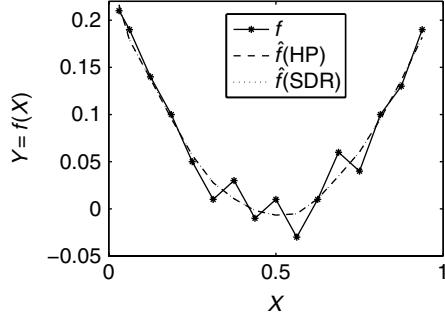
08       In its basic IRW formulation, the links between the SDR approach and  
 09       the HP-filter smoothing are clear: both of them have the properties of a  
 10       smoothing cubic spline. Moreover, it is also easy to verify the equivalence  
 11       between the NVR and  $\lambda$ , linked by the simple relationship:  $\lambda = 1/NVR$ :  
 12       see Young and Pedregal (1999). The NVR therefore plays the role of  
 13       the inverse of a smoothing parameter. SDR advantages, however, are in  
 14       terms of the ML estimation of the NVR, which makes the choice of the  
 15       smoothing parameter completely objective, and in its great flexibility, as  
 16       mentioned above. These properties provide optimal convergence properties  
 17       of the SDR estimates to the best least-squares predictor of  $Y$ , given by  
 18        $g^*(\mathbf{X}_I)$ .

19       The SDR smoothing techniques based on GRW processes can also be  
 20       seen as low-pass filters. In the case of IRW, the 50% cutoff frequency  $\omega^*$   
 21       is linked to the NVR by the relationship  $NVR = 4(1 - \cos(2\pi\omega^*))^2$  (see e.g.  
 22       Young and Pedregal, 1999). The period  $T^* = 2\pi/\omega^*$ , which is obtained via  
 23       the maximum likelihood estimation, can be compared to  $N$  to obtain an  
 24       idea of ‘typical’  $T^*/N$  ratios and to identify some rule-of-thumb criterion  
 25       for the smoothing parameter  $\lambda$  of the HP-filter. Our experience suggests  
 26       that a reasonable rule of thumb can be to set  $T^* = N/3 \rightarrow N/2$  and to  
 27       derive  $\lambda$  accordingly. In the last step of the SDR analysis, the smoothed  
 28       nonparametric ‘curves’ obtained from the SDR model estimation are param-  
 29       eterized by, for example, a linear wavelet functional approximation or a  
 30       summation of RBFs, allowing us to build a full metamodel to replace the  
 31       original one.

32  
 33  
 34       Example Consider again the simple example used before. Using the same  
 35       data, we obtain  $NVR = 0.59$  from ML estimation. This implies that the  
 36       equivalent optimal  $\lambda$  for the HP-filter would be about 1.7, matching  
 37       the values that ‘looked’ acceptable in the HP-filter analysis. The plots of  
 38       the SDR estimate and the equivalent HP-filter estimate using  $\lambda = 1/NVR$   
 39       are shown next:  
 40  
 41

---

42  
 43       <sup>4</sup> See Young and Ng (1989); Young and Pedregal (1996); Young (2002) and the discussion in  
 44       Ratto *et al.* (2007).



This clearly shows the identity between the HP-filter and IRW smoothing (the curves are the same), as well as the importance of the SDR estimation procedure linked to maximum likelihood, providing for optimal identification of the smoothing parameter rather than the *ad-hoc* tuning used in the HP-filter.

#### 5.3.1.4 Estimating sensitivity indices

Once the smoothed estimates  $\hat{g}_I$  of  $E(Y|\mathbf{X}_I)$  have been obtained, the estimation of sensitivity indices  $S_I = V[E(Y|\mathbf{X}_I)]/V(Y)$  is straightforward. As discussed in Doksum and Samarov (1995), three estimators can be applied for this purpose. The one we use is

$$\hat{S}_I = \frac{N^{-1} \sum_{s=1}^N (\hat{g}_I(\mathbf{x}_{I,s}) - \bar{g})^2}{\sigma_Y^2} \quad (5.26)$$

where  $\bar{g} = N^{-1} \sum \hat{g}_I(\mathbf{x}_{I,s})$  and  $\sigma_Y^2 = N^{-1} \sum (y_s - \bar{Y})^2$ . Doksum and Samarov (1995) also provide the error estimate for (5.26), by showing that  $N^{1/2}(\hat{S}_I - S_I)$  is asymptotically normal with mean zero and variance  $(1 - S_I)^2 V[y^*]^2 - u^2$ , where  $y^*$  and  $u$  are the standardized output and residual respectively, i.e.  $y_s^* = (y_s - \bar{Y})/\sigma_Y$  and  $u_s = [y_s - \hat{g}_I(\mathbf{x}_{I,s})]/(\sigma_Y(1 - S_I)^{1/2})$ . Hence, the standard error of the estimate of  $S_I$  is given by

$$SE(\hat{S}_I) = (1 - \hat{S}_I) \text{std}[y_s^*]^2 - u_s^2 / N^{1/2} \quad (5.27)$$

#### 5.3.2 A Simple Example

We give here an example of the smoothing estimation procedures. Let us consider the simple model

$$Y = X_1 + X_2^2 + X_1 \cdot X_2 \quad (5.28)$$

01 with input distributions  $X_i \sim N(0, 1)$ . This model has the simple ANOVA-  
 02 HDMR representation:

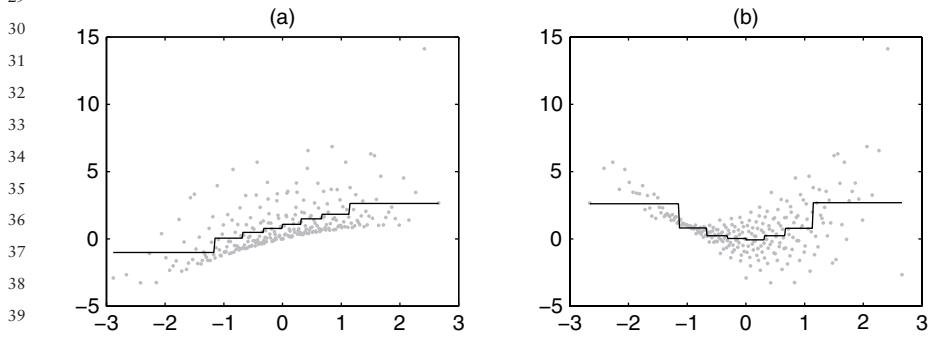
$$\begin{aligned} 04 \quad f_0 &= 1 \\ 05 \quad f_1(X_1) &= X_1 \\ 06 \quad f_2(X_2) &= X_2^2 - 1 \\ 07 \quad f_{1,2}(X_1, X_2) &= X_1 \cdot X_2 \\ 08 \end{aligned}$$

09  
 10 We apply the smoothing procedures described above, by using an  $LP_\tau$   
 11 sample of  $N = 256$  model evaluations.

12  
 13 *5.3.2.1 Haar wavelet smoothing*

14 Let us first perform the smoothing with the Haar wavelet. As a rule-of-  
 15 thumb criterion for the smoothing parameter of the Haar wavelet, we  
 16 dictate that the extracted signal be made of  $8 = 2^3$  values, i.e. we construct  
 17 the smoothing by taking eight local averages from the sample of  $Y$  divided  
 18 into eight bins. Given the sample of  $N = 256 = 2^8 = 2^n$ , this implies that  
 19  $\lambda = 8 - 3 = 5$ . The sample of the output  $Y$  has to be sorted according to  
 20 each input factor and the Haar smoothing procedure described above has  
 21 to be applied for each sorted sample.

22 The results of this procedure are shown in Figure 5.3. This shows that  
 23 the rule of thumb of eight local means is able to provide an illustrative idea  
 24 of the  $f_i$  patterns.



41 **Figure 5.3** Haar estimation of the first-order HDMR of the simple model (5.28).  
 42 (a, b) Scatterplots of  $Y$  versus  $X_1$  and  $X_2$  (grey dots), with the smoothed estimates  
 43 of the  $f_i + f_0$  functions (solid lines)

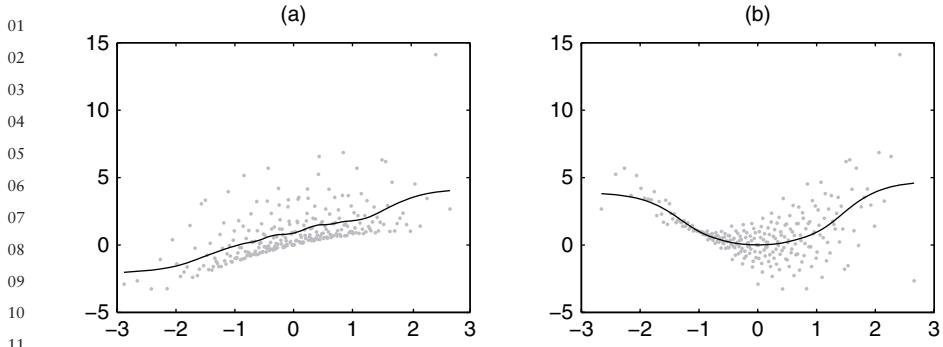


Figure 5.4 HP-filter estimation of the first-order HDMR of the simple model (5.28).  
 (a, b) Scatterplots of  $Y$  versus  $X_1$  and  $X_2$  (grey dots), with the smoothed estimates of the  $f_i + f_0$  functions (solid lines)

### 5.3.2.2 Spline smoothing (HP-filter)

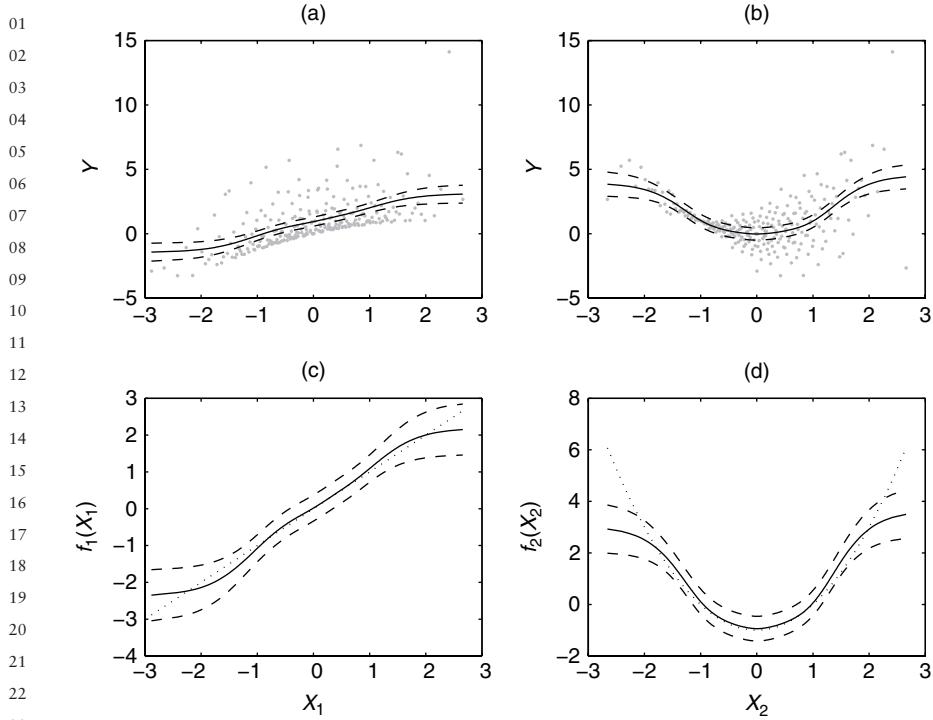
In this case we have to choose the value for the smoothing parameter of the HP-filter. Using  $\lambda = 50\,000$ , which is in the range of rule-of-thumb values for the cut-off frequency  $\omega^*$  described above, we get the results shown in Figure 5.4. We can observe the much nicer pattern provided by the cubic spline properties of the HP-filter with respect to the Haar wavelet. The problem, however, still lies in the approximate choice of  $\lambda$ .

### 5.3.2.3 SDR estimation

Here, the maximum likelihood optimization of the NVRs gives the following results for the two input factors:  $NVR_1 = 4.46e-6$ ,  $NVR_2 = 4.675e-5$ .

In Figure 5.5 (a, b) we show the scatterplots of the modified output  $Y_i^* = Y - f_0 - \sum_{j \neq i} f_j(X_j)$ , used in the backfitting procedure, versus the two model parameters together with the result of the SDR recursive filtering and smoothing estimation of the  $f_i$  terms. In Figure 5.5 (c, d) we show the detail of the SDR estimates, compared to the analytical values (5.29). Apart from expectable border phenomena, the SDR estimates are excellent. In Figure 5.5 (c, d) the dashed lines show the 95% error bands ( $= \pm 2 \cdot \sigma_{f,s}$ ) of the estimated patterns. This permits us to assess the significance of the estimated patterns by simply checking whether the zero-line is always included in the error band (implying insignificance) or not.

Naturally, given the equivalence of SDR and the HP-filter, using  $1/NVR_i$  as smoothing parameters for the HP-filter analysis produces the same results as for the SDR analysis, provided that the backfitting procedure is also applied – otherwise the results will be slightly different.



**Figure 5.5** SDR estimation of the first-order HDMR of the simple model (5.28). (a, b) Scatterplots of the modified output  $Y^* = Y - \sum_{j \neq i} f_j(X_j)$  used in the backfitting procedure versus  $X_1$  and  $X_2$  (grey dots), with the smoothed estimates of the  $f_i + f_0$  functions (solid lines) and their 95% error bands (dashed lines). (c, d) Detail of the estimated  $f_i$  functions (solid lines) with estimated 95% error bands (dashed lines) and analytic  $f_i$  functions (dotted lines)

### 5.3.3 Another Simple Example

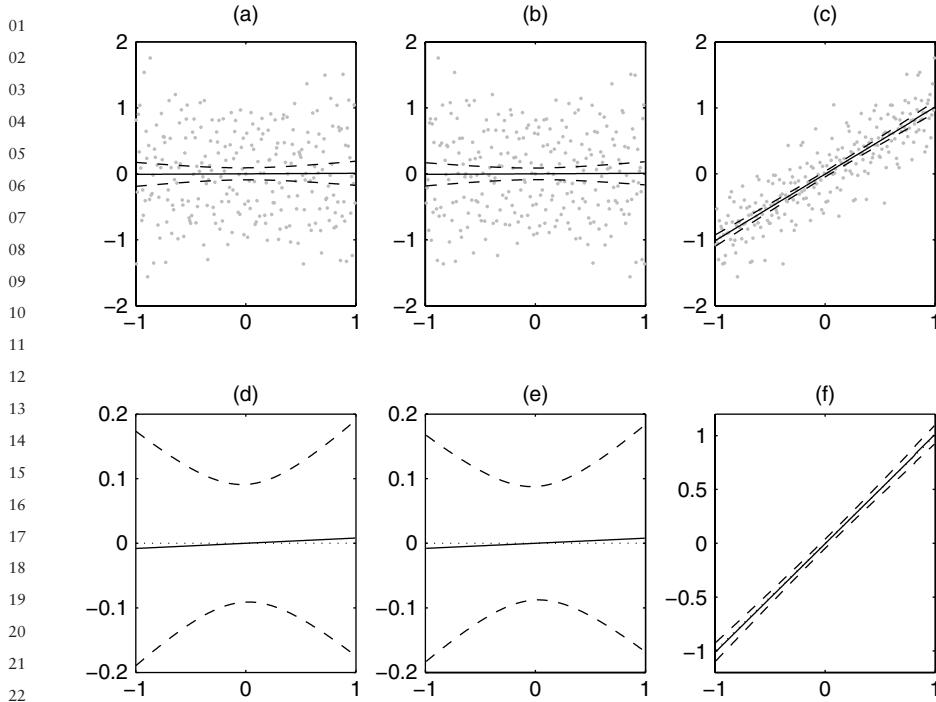
Let us consider the function

$$Y = X_1 \cdot X_2 + X_3 \quad (5.29)$$

with

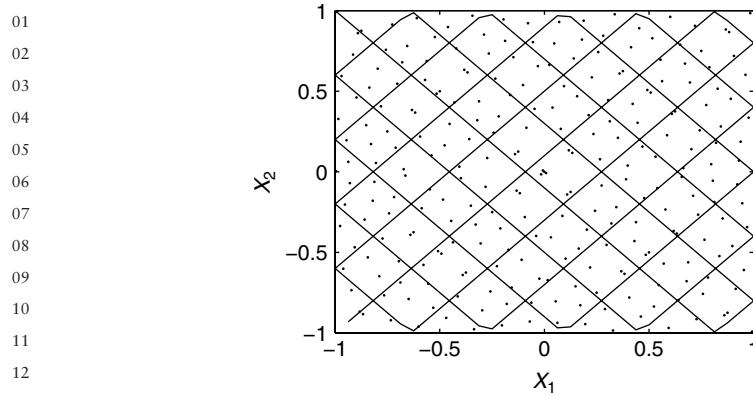
$$X_i \sim U(-1, 1).$$

We perform an analysis using a Sobol'  $LP_r$  sample of dimension 256. This model has only one non-zero main effect for  $X_3$  and one second-order interaction term for  $(X_1, X_2)$ . In Figure 5.6 we show the SDR estimation of the first-order HDMR terms  $f_1$ ,  $f_2$  and  $f_3$ . We also report the standard error band, showing that only  $f_3$  has a significant main effect.

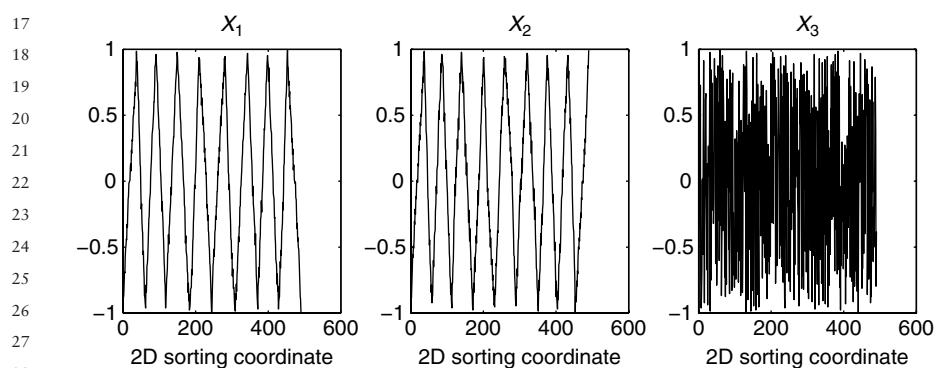


**Figure 5.6** SDR estimation of the first-order HDMR of the simple model (5.29). (a, b, c) Scatterplots of  $Y$  versus  $X_i$  (grey dots), with the smoothed estimates of the  $f_i + f_0$  functions (solid lines) and their 95% error bands (dashed lines). (d, e, f) Detail of the estimated  $f_i$  functions (solid lines) with estimated 95% error bands (dashed lines) and analytic  $f_i$  functions (dotted lines)

In order to give the flavour of the generalized sorting strategy used in the SDR methodology for interaction terms, let us perform the analysis of second-order interaction term ( $X_1, X_2$ ). Since we want to compute the  $f_{12}$  interaction effect, the 2D sorting requires exploration of the  $(X_1, X_2)$  plane along a closed trajectory, like the one shown in Figure 5.7, with the sorting of the sample points carried out as they fall within the band delimited by two adjacent lines. This allows for the identification of an ordering in which  $(X_1, X_2)$  has low-frequency characteristics while  $X_3$  maintains the white spectrum (Figure 5.8). The corresponding sorted output signal  $Y$  can then be analysed to identify the second-order interaction term. This is shown in Figure 5.9, where we compare the analytic values and the SDP estimates of the sorted  $f_{1,2}$  interaction term.



14      **Figure 5.7** Sorting trajectory in the  $(X_1, X_2)$  plane  
15



29      **Figure 5.8** Sorted sample used to compute the  $(X_1, X_2)$  interaction  
30  
31

### 32      5.3.4 Exercises 33

- 34      1. Compute the analytic HDMR expansion of the function  $Y = X_1 + X_2 +$   
35       $X_3$ , with  $X_i \sim N(\mu_i, \sigma_i)$ . Assign values to  $(\mu_i, \sigma_i)$  and perform the regres-  
36      sion/smoothing analysis with the Haar wavelet and spline smoothing.  
37      2. Compute the analytic HDMR expansion of the Ishigami function  
38      (Ishigami and Homma, 1990):  
39

40      
$$Y = \sin X_1 + A \sin^2 X_2 + BX_3^4 \sin X_1$$
  
41

42      where  $X_i \sim U(-\pi, \pi)$ . Perform the regression/smoothing analysis with  
43      the Haar wavelet and spline smoothing, when  $A = 7$  and  $B = 0.1$ .  
44

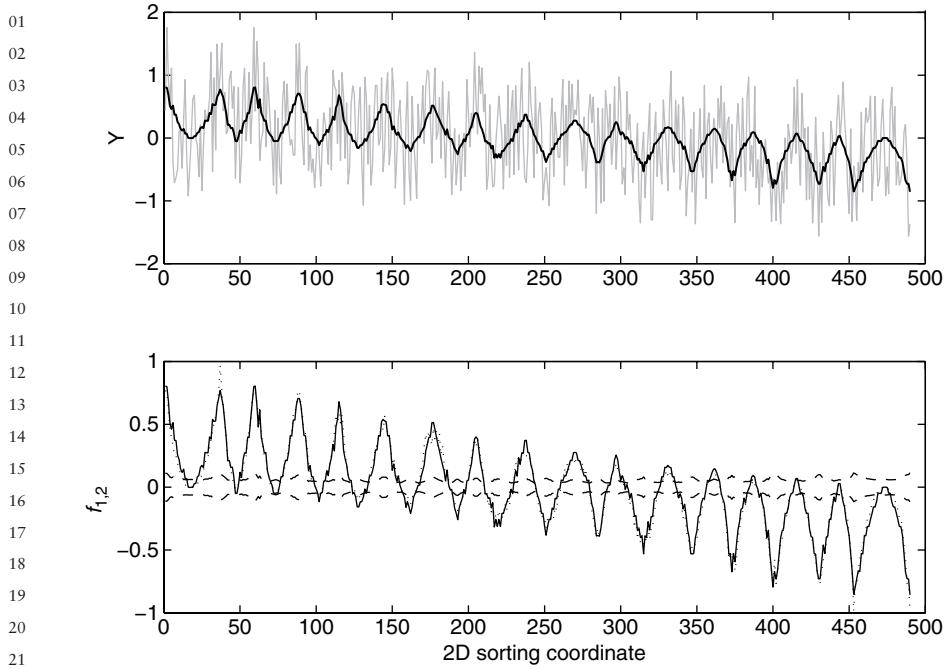


Figure 5.9 Upper panel: Sorted output signal (grey line) and smoothed low-frequency component (bold line) attributable to the  $(X_1, X_2)$  interaction. Lower panel: Smoothed low-frequency component (solid line) with standard error (dashed lines: shown around zero rather than estimate in order to simplify the plot) and sorted analytic  $(X_1, X_2)$  interaction (dotted line)

3. Compute the analytic HDMR expansion of the Sobol'  $g$ -function. Perform the regression/smoothing analysis with the Haar wavelet and spline smoothing, when:

- $\alpha = [0, 1, 4.5, 9, 99, 99, 99, 99]$ ;
  - $\alpha = [0, 0, 1, 1, 4.5, 4.5, 9, 9, 99, 99, 99, 99, 99, 99, 99]$ ;
  - $\alpha = [0, 0.01, 0, 0.2, 0.3, 0, 0.5, 1, 1.5, 1.8, 3, 4.5, 8, 9, 99]$ ;
4. Compute the HDMR expansion of the model  $Y = \prod_{i=1}^k X_i$ , with  $X_i \sim U(0, \text{MAX}_i)$ . Is there a clever way to map this function synthetically? Perform the regression/smoothing analysis with the Haar wavelet and spline smoothing for the output  $Y$  and for the ‘clever’ transformation of  $Y$ , for  $k = 3, 4$ , assigning values to  $\text{MAX}_i$ .
5. Compute the HDMR expansion of the model  $Y = \prod_{i=1}^k X_i$ , with  $X_i \sim N(0, \sigma_i)$ . Is there a clever mapping in this case as well?

01      Perform the regression/smoothing analysis with the Haar wavelet and  
 02      spline smoothing for the output  $Y$  and for the ‘clever’ transformation of  
 03       $Y$ , for  $k = 3, 4$ , assigning values to  $\sigma_i$ .

04  
 05      **5.3.5 Solutions to Exercises**

06      1. First we compute the unconditional mean

$$07 \quad f_0 = E(Y) = \mu_1 + \mu_2 + \mu_3.$$

08      Then the first-order terms  $f_i = E(Y|X_i) - f_0$ :

$$09 \quad f_1 = X_1 + \mu_2 + \mu_3 - f_0 = X_1 - \mu_1$$

$$10 \quad f_2 = X_2 + \mu_1 + \mu_3 - f_0 = X_2 - \mu_2$$

$$11 \quad f_3 = X_3 + \mu_1 + \mu_2 - f_0 = X_3 - \mu_3.$$

12      It is easy to verify that any other term of order higher than one is null.

13      2. Looking at the analytic form of the Ishigami function one can say that  
 14      the decomposition will have the following terms:

$$15 \quad Y = f_0 + f_1(X_1) + f_2(X_2) + f_3(X_3) + f_{13}(X_1, X_3).$$

16      Given the uniform probability density of  $X_i$ , we have that  $p(X_i) = 1/2\pi$   
 17      if  $-\pi < X_i < \pi$  and  $p(X_i) = 0$  elsewhere. The unconditional mean is  
 18      therefore

$$19 \quad f_0 = E(Y) = \iiint_{-\pi}^{\pi} Y dX_1 dX_2 dX_3 / 8\pi^3$$

$$20 \quad = \int_{-\pi}^{\pi} \sin X_1 dX_1 / 2\pi + \int_{-\pi}^{\pi} A \sin^2 X_2 dX_2 / 2\pi + \iint_{-\pi}^{\pi} BX_3^4 \sin X_1 dX_1 dX_3 / 4\pi^2$$

$$21 \quad = 0 + A/2 + 0.$$

22      The first-order terms are

$$23 \quad f_1 = E(Y|X_1) - f_0 = \iint_{-\pi}^{\pi} Y dX_2 dX_3 / 4\pi^2 - A/2$$

$$24 \quad = \sin X_1 + \int_{-\pi}^{\pi} A \sin^2 X_2 dX_2 / 2\pi + \sin X_1 \int_{-\pi}^{\pi} B \cdot X_3^4 dx_3 / 2\pi - A/2$$

$$25 \quad = \sin X_1 (1 + B \cdot 2\pi^5 / 5 / (2\pi)) + A/2 - A/2$$

$$26 \quad = \sin X_1 (1 + B\pi^4 / 5).$$

$$27 \quad f_2 = E(Y|X_2) - f_0 = \iint_{-\pi}^{\pi} Y dX_1 dX_3 / 4\pi^2 - A/2$$

$$\begin{aligned}
01 &= \int_{-\pi}^{\pi} \sin X_1 dX_1 / 2\pi + A \sin^2 X_2 + \iint_{-\pi}^{\pi} BX_3^4 \sin X_1 dX_1 dX_3 / 4\pi^2 - A/2 \\
02 &= 0 + A \sin^2 X_2 + 0 - A/2 \\
03 &= A(\sin^2 X_2 - 1/2). \\
04 \\
05 &f_3 = E(Y|X_3) - f_0 = \iint_{-\pi}^{\pi} Y dX_1 dX_2 / 4\pi^2 - A/2 \\
06 &= (1 + BX_3^4) \cdot \int_{-\pi}^{\pi} \sin X_1 dX_1 / 2\pi + \int_{-\pi}^{\pi} A \sin^2 X_2 dX_2 / 2\pi - A/2 \\
07 &= 0 + A/2 - A/2 = 0. \\
08 \\
09 \\
10 \\
11
\end{aligned}$$

12 It is easy to verify that all second-order terms are null except:

$$\begin{aligned}
14 &f_{13} = E(Y|X_1, X_3) - f_1 - f_3 - f_0 \\
15 &= \sin X_1 + BX_3^4 \sin X_1 + \int_{-\pi}^{\pi} A \sin^2 X_2 dX_2 / 2\pi \\
16 &\quad - \sin X_1 (1 + B\pi^4/5) - 0 - A/2 \\
17 &= \sin X_1 - \sin X_1 + BX_3^4 \sin X_1 - B\pi^4/5 \sin X_1 + A/2 - A/2 \\
18 &= B(X_3^4 - \pi^4/5) \sin X_1. \\
19 \\
20 \\
21 \\
22
\end{aligned}$$

23 In order to compute the HDMR expansion of the Sobol'  $g$ -function,

$$24 \quad f = \prod_{i=1}^k g_i(X_i) = \prod_{i=1}^k \frac{|4X_i - 2| + a_i}{1 + a_i}$$

25 with  $X_i \sim U(0, 1)$ , it is useful to recall the result from Chapter 4:

$$26 \quad \int_0^1 g_i(X_i) dX_i = \int_0^1 \frac{|4X_i - 2| + a_i}{1 + a_i} dX_i = 1$$

27 valid for any  $X_i$  and any  $a_i$ .

28 So the unconditional mean is

$$29 \quad f_0 = \prod_i \int_0^1 g_i(X_i) dX_i = 1.$$

30 The first-order terms are

$$\begin{aligned}
31 &f_i = E(Y|X_i) - f_0 \\
32 &= g_i(X_i) \prod_{j \neq i} \int_0^1 g_j(X_j) dX_j - f_0 \\
33 &= g_i(X_i) - 1. \\
34
\end{aligned}$$

01       The second-order terms are

$$\begin{aligned}
 02 \quad f_{ij} &= E(Y|X_i, X_j) - f_i - f_j - f_0 \\
 03 \quad &= g_i(X_i)g_j(X_j) \prod_{l \neq (i,j)} \int_0^1 g_l(X_l) dX_l - f_i - f_j - f_0 \\
 04 \quad &= g_i(X_i)g_j(X_j) - (g_i(X_i) - 1) - (g_j(X_j) - 1) - 1 \\
 05 \quad &= g_i(X_i)g_j(X_j) - g_i(X_i) - g_j(X_j) + 1.
 \end{aligned}$$

10       All higher-order HDMR terms are obtained recursively, considering that,  
 11       for any group of input factors indexed by  $I = (i_1, \dots, i_l)$ :

$$\begin{aligned}
 13 \quad E(Y|X_I) &= \prod_{i \in I} g_i(X_i). \\
 14
 \end{aligned}$$

15       The Sobol'  $g$ -function has nonzero interaction effects of any order.

16       4. The unconditional mean is

$$\begin{aligned}
 18 \quad f_0 &= E(Y) = \prod_{i=1}^k \int_0^{\text{MAX}_i} X_i dX_i / \text{MAX}_i \\
 19 \quad &= \prod_{i=1}^k \text{MAX}_i / 2.
 \end{aligned}$$

24       The first-order terms are

$$\begin{aligned}
 26 \quad f_i &= E(Y|X_i) - f_0 \\
 27 \quad &= X_i \prod_{j \neq i} \int_0^{\text{MAX}_j} X_j dX_j / \text{MAX}_j - f_0 \\
 28 \quad &= X_i \prod_{j \neq i} \text{MAX}_j / 2 - f_0 \\
 29 \quad &= (X_i - \text{MAX}_i / 2) \prod_{j \neq i} \text{MAX}_j / 2.
 \end{aligned}$$

35       The second-order terms are

$$\begin{aligned}
 37 \quad f_{ij} &= E(Y|X_i, X_j) - f_i - f_j - f_0 \\
 38 \quad &= X_i \cdot X_j \prod_{l \neq (i,j)} \int_0^{\text{MAX}_l} X_l dX_l / \text{MAX}_l - f_i - f_j - f_0 \\
 39 \quad &= X_i \cdot X_j \prod_{l \neq (i,j)} \text{MAX}_l / 2 - f_i - f_j - f_0 \\
 40 \quad &= (X_i X_j - X_i \text{MAX}_j / 2 - X_j \text{MAX}_i / 2 - \text{MAX}_i \cdot \text{MAX}_j / 4) \prod_{l \neq (i,j)} \text{MAX}_l / 2.
 \end{aligned}$$

01 All higher-order terms are obtained recursively, remembering that  
 02

$$03 E(Y|X_I) = \prod_{i \in I} X_i \prod_{j \notin I} \text{MAX}_j / 2.$$

04  
 05 As with the  $g$ -function, this example also has nonnull interaction effects  
 06 of any order.  
 07

08 A clever way to map the function  $Y$  is to consider its log-transformed  
 09 version. This is allowed, since  $X_i > 0$  for all  $X_i$ . This gives

$$10 \quad 11 \quad \log(Y) = \sum_{i=1}^k \log(X_i)$$

12  
 13 which has an easy HDMR expansion of only first-order terms that  
 14 describes 100% of  $Y$ !  
 15

16 In general, trying to analyse the log-transformed version of a func-  
 17 tion can produce interesting results. In particular, if the the log-  
 18 transformation of  $Y$  is described up to a large extent (e.g. > 90% of the  
 19 variance of  $\log(Y)$ ) by first-order HDMR terms, this suggests that the  
 20 mapping between  $X_i$  and  $Y$  can be factorized.

- 21 5. All the HDMR terms of this model are null except for the highest,  $k$ th  
 22 order term:

$$23 \quad 24 \quad f_{1,\dots,k} = \prod_{i=1}^k X_i = f.$$

25 This is a very unattractive model. Even if the input factors had different  
 26  $\sigma_i$  values (i.e. different uncertainties), neither variance-based sensitivity  
 27 indices nor HDMR analysis would be able to produce a ranking of the  
 28 importance of input factors.  
 29

30 One possible way of analysing sensitivity for this kind of model is to  
 31 apply MCF techniques and, similarly to Exercise 6 of Section 5.2.3, to  
 32 try to map quantiles of  $Y$ , e.g.  $Y > 1$  or  $Y < -1$  (we leave this as an  
 33 additional exercise for the reader).  
 34

35 In metamodeling terms, however, one can still identify a clever trans-  
 36 formation of  $Y$ , extracting useful hints about the effect of each input  
 37 factor on the outcome  $Y$ .  
 38

39 The conditional expectation  $E(Y|X_I)$  is null whatever the single input  
 40 factor or group of input factors. So,  $Y$  is a pure ‘noise’ process, without  
 41 any shift in the mean, and the effect of each input factor is simply to  
 42 modulate the noise amplitude, similarly to heteroscedastic processes.  
 43

44 One could therefore conceive of trying to build a metamodel for the  
 45 variance of  $Y$ . In order to do this, one could consider the transformation  
 46  $\log(Y^2)$ . By doing so, the function to be analysed becomes

$$\log(Y^2) = \sum_{i=1}^k \log(X_i^2)$$

which is a simple, additive mapping between the (log of the) squared input factors and the (log of the) squared output. Remembering that any expectation of  $Y$  (unconditional or not) is null, taking the square of  $Y$  is equivalent to taking its variance. Then, the main effect  $f_i = E(\log(Y^2)|\log(X_i^2))$  describes effect of  $X_i$  in modulating the variance of  $Y$ , and the further  $X_i$  is from zero, the greater the variance of  $Y$ . So, the greatest impact in modulating the variance of  $Y$  will come from the input factor with the highest variance  $\sigma_i^2$ . This allows for a nice ranking of the importance of input factors, which will be proportional to the magnitude of the  $\sigma_i$ 's.

This ‘extreme’ example shows that, in nasty cases where ‘standard’ global sensitivity analysis tools seem to fail in providing clear answers, functional transformations of  $Y$  can facilitate a better explanation of the model properties.

## 5.4 CONCLUSIONS

Chapter 4 demonstrated best available practices for computing sensitivity indices based on points thrown into a  $k$ -dimensional space. In this chapter we have discussed methods capable of greatly accelerating the computation of the indices (in terms of reduced number of model executions), based on metamodelling. All smoothing and metamodelling techniques are based on fitting a model approximation based on a single Monte Carlo (or, better, quasi-Monte Carlo) sample. This is a major advantage with respect to ‘classical’ variance-based techniques, which require some ad hoc sampling. Moreover, metamodelling techniques usually converge much more quickly, i.e. they are more efficient. This is possible since such techniques rely on assumptions of regularity and smoothness in  $Y$  that allow us to infer the value of  $Y$  at untried points, based on the information available from MC samples at nearby points. This also implies that, in contrast to ‘classic’ variance-based estimators which rely only on square-integrability of  $Y$ , smoothing methods are not robust in the face of heavily discontinuous mappings, e.g. piecewise continuous functions, in which the values of  $Y$  jump continuously in an apparently random fashion (i.e. presenting patterns similar to the one shown in Chapter 2, Figure 2.1(f)). In this regard, the recursive approach of Ratto *et al.* (2007) provides elements of meaningful flexibility to adjust the estimated model approximation to local jumps and spikes, provided that these are not as numerous as in Figure 2.1(f).

When to use what? The decision is evidently based on a trade-off between model execution cost and the analyst’s time.

- The method of Saltelli (2002) is straightforward to encode and comes at the cost of  $N(k+2)$  model executions, with  $N = 1000$  or higher, to compute both the  $S_i$ 's and the  $S_{Ti}$ 's.
- The method of Tarantola *et al.* (2006) described in Chapter 4 is also easy to encode and requires only a single set of  $N$  runs to compute the whole of set of  $S_i$ 's. However, any information about interaction terms or total effects is missed.
- The approach of Ratto *et al.* (2004, 2007) discussed in this chapter is, according to our experience, an excellent metamodeling practice in terms of model executions, robustness of estimation and flexibility of implementation. It can give a fairly precise estimate of all indices of the first order at the overall cost of 200–500 simulations, although to obtain reliable estimates of second- and third-order interaction terms, somewhat longer samples are needed: e.g. 1000–2000. In its full formulation, it is less simple to encode with respect to the previous ones. Other methods mentioned here based on parametric regressions using polynomial bases to estimate HDMR terms could be helpful at a preliminary stage of identification of the most relevant terms for explaining the variability of  $Y$ .
- The total effect estimation is a weak element of metamodeling. Such an estimate requires adding all the first-order and interaction terms associated with each input factor. However, the precision of the mapping of the function  $f(\cdot)$  is inversely proportional to the order of interactions, while the maximum order of interactions that can be reliably estimated with metamodeling techniques can hardly exceed the order of three, if one wants to reduce to the minimum the number of model evaluations. This implies that some relevant high-order interaction might always be missed in the metamodeling exercise. In this case, jointly performing an EE analysis, as discussed in Chapter 3, would allow for a cheap and quite comprehensive assessment in terms of low-order ANOVA-HDMR terms and EE, which replaces variance-based total effects.

Ideally a model-building environment should have software for both approaches at its disposal, unless the model is truly inexpensive to run.

Software developed for SDR modelling is available at <http://sensitivity-analysis.jrc.cec.eu.int/>.

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# 6

## Sensitivity Analysis: From Theory to Practice

SCOPE OF THE CHAPTER. EXAMPLES. A COMPOSITE INDICATOR. FINANCIAL OPTIONS MODELLING. A CHEMICAL REACTOR. A SIMPLE ANALYSIS. WHEN TO USE WHAT.

In this chapter a few examples are offered of how the different sensitivity analysis methods can be put to use. The aim is to offer suggestions rather than prescriptions, as we did in our discussion of possible ‘settings’ in Chapters 1 and 4. The setting up of a sensitivity analysis will in general depend upon:

- number of uncertain factors and computational cost of the model;
- characteristic of the output of interest (e.g. variance of the output, tails of its distribution, . . . );
- scope of the analysis;
- nature and dispositions of the recipients of the analysis (owners of the problem, stakeholders, . . . ).

The last bullet is a reminder that the audience to which the analysis is addressed may also influence its set-up, for example in the degree of sophistication allowed in the presentation of the results.

## 01           6.1 EXAMPLE 1: A COMPOSITE INDICATOR 02

### 03           6.1.1 Setting the Problem 04

05           Imagine that an international organization or academic institution tries to  
06           capture in a single number, usually termed a composite indicator or index,  
07           the relative performance of several countries or regions in a multidimensional  
08           field. The Consumer Price Index, for example, considers the costs of various  
09           items purchased by a typical household each month. When a basket of about  
10           60 goods and services is combined in the Consumer Price Index, it offers  
11           a more complete picture of the relative cost of living in different countries  
12           than would the price of bread or fuel alone.<sup>1</sup> A Handbook on Composite  
13           Indicators (Nardo *et al.*, 2005) offers a review and guidelines for composite  
14           indicator development which we aim to adhere to in the present example.

15           However appealing the idea of summarizing complex phenomena into  
16           single numbers may be, the development of a composite indicator is not  
17           straightforward. It involves both theoretical and methodological assump-  
18           tions which need to be assessed carefully to avoid producing results of  
19           dubious analytic rigour (Saisana *et al.*, 2005). Furthermore, a composite  
20           indicator is likely to be received by a polarized audience, a fact which calls  
21           for stringent standards of rigour and robustness (Saltelli, 2006).

22           Composite indicators tend to sit between advocacy (when they are used  
23           to draw attention to an issue) and analysis (when they are used to capture  
24           complex multidimensional phenomena), and for this reason both their  
25           production and their use in the policy discourse are on the increase. This is  
26           also due to the media hunger for the apparently simple ‘facts’ purveyed by  
27           these measures.

28           To maximize their utility and minimize their misuse, therefore, developers  
29           must base these indices on the best available evidence, document clearly their  
30           structures, and validate them using appropriate uncertainty and sensitivity  
31           analyses. In the example that follows, we address two main questions that  
32           a developer of a composite indicator may be asked to respond to regarding  
33           the reliability of the results: Given the uncertainties during the development  
34           of an index, which of them are the most influential in determining the  
35           variance of:

- 36
- 37           • the difference between the composite scores of two countries with similar  
38            performance? This question could be used to address stakeholders’  
39            concern about a suspected bias in the score of a given country.

40

41

42           <sup>1</sup> An extensive list of such indices from various fields, such as the economy, environment,  
43           society and globalization, is presented on an information server on composite indicators  
44           <http://composite-indicators.jrc.ec.europa.eu/>

- 01     • the countries' ranking? This question pertains to the overall 'plausibility'  
 02           or robustness of the index.

03  
 04     This example will show the potential of using the Elementary Effects (EE)  
 05       method and variance-based methods in tandem for conducting sensitivity  
 06       analysis of nonlinear models that have numerous uncertain factors. In brief,  
 07       if the model is both expensive to run and/or has numerous input factors, one  
 08       can use the EE method to reduce the number of factors first, and can then  
 09       run a variance-based analysis on a reduced set of factors. A Monte Carlo  
 10       filtering application complements the case study. For didactic purposes, we  
 11       have chosen to work with an example that can be easily reproduced and  
 12       with negligible model execution time.

13  
 14  
 15     **6.1.2 A Composite Indicator Measuring Countries'**  
 16       **Performance in Environmental Sustainability**

17  
 18     In general, an index is a function of underlying indicators. Weights are  
 19       assigned to each indicator to express the relevance of the indicators in the  
 20       context of the phenomenon to be measured. Assume that there are  $m$  coun-  
 21       tries, whose composite score is to be constructed based on  $q$  indicators.  
 22       Let  $X_{ij}$  and  $w_i$  respectively denote the value for a country  $j$  with respect to  
 23       indicator  $i$  and the weight assigned to indicator  $i$ . All indicators have been  
 24       converted into benefit-type ones, so that higher values indicate better perfor-  
 25       mance. The problem is to aggregate  $X_{ij}(i = 1, 2, \dots, q, j = 1, 2, \dots, m)$   
 26       into a composite index  $CI_j(j = 1, 2, \dots, m)$  for each country  $j$ . The most  
 27       commonly used aggregation method is the weighted arithmetic mean:

28  
 29  
 30       
$$CI_j = \sum_{i=1}^q w_i X_{ij}. \quad (6.1)$$

31  
 32     The popularity of this type of aggregation is due to its transparency and  
 33       ease of interpretation. An alternative aggregation method is the weighted  
 34       geometric mean:

35  
 36       
$$CI_j = \prod_{i=1}^q X_i^{w_i}. \quad (6.2)$$

37  
 38     One argument in favour of a geometric approach instead of arithmetic  
 39       could be the feature of compensability among indicators. A sometimes  
 40       undesirable feature of additive aggregation (e.g. weighted arithmetic mean)  
 41       is the full compensability they imply, whereby poor performance in some  
 42       indicators can be compensated by sufficiently high values of other indica-  
 43       tors. To give an example, assume that a composite indicator is formed by

01 four indicators: inequality, environmental degradation, GDP per capita and  
 02 unemployment. Two countries, one with values [21, 1, 1, 1] and the other  
 03 with [6, 6, 6, 6], would have equal arithmetic mean (= 6), but different  
 04 geometric mean (2.14 and 6, respectively). In this case, the geometric  
 05 approach properly reflects the different social conditions in the two coun-  
 06 tries, which are, however, masked by the arithmetic aggregation.<sup>2</sup>

07 We will base our example on the Pilot 2006 Environmental Performance  
 08 Index developed by the Yale and Columbia universities and described in Esty  
 09 *et al.* (2006). The index focuses on a core set of environmental outcomes  
 10 linked to 16 policy-related indicators for which governments in more than  
 11 130 nations should be held accountable. However, for didactic purposes  
 12 and with a view to provide an easy to reproduce case study, we will restrict  
 13 ourselves to a set of five indicators and six countries. The full, real-life  
 14 example of sensitivity analysis for the Environmental Performance Index  
 15 can be found in Esty *et al.* (2006). Table 6.1 lists the indicators that are  
 16 included in our simplified composite indicator. There are two basic indica-  
 17 tors related to air quality (regional ozone concentrations and urban partic-  
 18 iculate matter concentrations), two indicators related to sustainable energy  
 19 (energy efficiency and CO<sub>2</sub> emissions per GDP) and finally the percentage  
 20 of the population with access to drinking water.

21 The values for all five indicators and six countries are assumed to be  
 22 uncertain in this exercise. For example, it could be that the set of countries  
 23 we are studying was lacking these indicator values, which were therefore  
 24 estimated by means of multiple imputation (Little and Rubin, 2002), or  
 25 the data were provided by a statistical agency with an estimate of their  
 26 sampling error. Data imputation could help to minimize bias and the need  
 27 for ‘expensive-to-collect’ data that would otherwise be avoided only by  
 28 omitting the relevant countries from the analysis. However, imputation may  
 29 also influence the index. The uncertainty in the imputed data is reflected

32 **Table 6.1** List of indicators in the simplified  
 33 Environmental Performance Index

<i>Abbreviation</i>	<i>Description</i>
OZONE	Regional ozone
PM10	Urban particulate matter
ENEFF	Energy efficiency
CO2GDP	CO <sub>2</sub> emissions per GDP
WATSUP	Drinking water

41  
 42  
 43 <sup>2</sup> For a proper discussion of compensability and other theoretical aspect of composite indica-  
 44 tors building see Nardo *et al.* (2005).

01                   **Table 6.2** Distributions (normal:  $\mu, \sigma$ ) for the inputs of the simplified index and  
 02                   the trigger to decide the aggregation method (discrete distribution)

<i>Country</i>	<i>OZONE</i>	<i>PM10</i>	<i>ENEFF</i>	<i>CO2GDP</i>	<i>WATSUP</i>
A	(25.3, 10.1)	(53.3, 6.4)	(78.5, 3.9)	(56.3, 7.7)	(76.5, 10.5)
B	(29.0, 10.0)	(37.4, 6.6)	(58.9, 4.3)	(58.8, 7.6)	(56.7, 9.9)
C	(35.0, 9.9)	(26.8, 6.7)	(69.2, 4.1)	(43.8, 7.9)	(20.6, 8.9)
D	(78.7, 9.2)	(33.2, 6.6)	(77.9, 3.9)	(73.3, 7.4)	(27.8, 9.1)
E	(24.1, 10.1)	(32.2, 6.6)	(61.3, 4.3)	(66.9, 7.5)	(62.1, 10.1)
F	(30.5, 10.0)	(54.6, 6.4)	(67.3, 4.1)	(37.2, 8.1)	(22.4, 8.9)
Weight	(0.21, 0.05)	(0.25, 0.05)	(0.15, 0.05)	(0.23, 0.05)	(0.16, 0.05)
Aggregation: Discrete. 0: linear, 1: geometric, selected with equal probability					

14 by variance estimates. This allows us to take into account the impact of  
 15 imputation in the course of the analysis. The weights that are attached to  
 16 these indicators are also considered uncertain for the sake of the example.  
 17 Weights could derive either from statistical approaches (e.g. factor analysis,  
 18 data envelopment analysis) or by consulting experts. In any case, different  
 19 approaches will result in different values for the weights. In our example,  
 20 all indicators values and weights follow a normal distribution. Mean and  
 21 standard deviation values are reported in Table 6.2. Additionally, a trigger  
 22 decides on the aggregation method for the basic indicators. The trigger  
 23 is sampled from a discrete distribution, where 0: linear aggregation, 1:  
 24 geometric aggregation.

### 28                   6.1.3 Selecting the Sensitivity Analysis Method

30                   In a general case, the validity and robustness of a composite indicator could  
 31                   depend on a number of factors, including:

- 33                   • the model chosen for estimating the measurement error in the data;
- 34                   • the mechanism for including or excluding indicators in the index;
- 35                   • the indicators' preliminary treatment (e.g. cutting the tails of a skewed  
                      distribution, or removing outliers);
- 36                   • the type of normalization scheme applied to the indicators to remove  
                      scale effects;
- 37                   • the amount of missing data and the imputation algorithm;
- 38                   • the choice of weights attached to the indicators;
- 39                   • the choice of the aggregation method.

42                   All these assumptions can heavily influence countries' scores and ranks in  
 43                   a composite indicator, and should be taken into account before attempting

an interpretation of the results. In this example, we will examine three of the sources of uncertainty listed above: the indicators' values, the weights, and the aggregation method (weighted arithmetic mean versus weighted geometric mean). The questions we will address are:

- which are the most influential input factors in the difference between the composite scores of two countries with similar performance?
- which are the most influential input factors in the countries' ranking?

The latter question can be more closely focused on our problem by asking: if we could invite experts to reach consensus on some of the weights, which ones should they focus on with a view to reducing the output variance the most? Which indicators' values need to be re-examined given that they affect the output variance the most?

#### 6.1.4 The Sensitivity Analysis Experiment and Results

The baseline scenario for the composite indicator model is the weighted arithmetic mean, where all indicators' values and weights are at their nominal value. In this scenario (see Table 6.3), country D would rank on top with a score of  $57.8 (= 78.7 \times 0.21 + 33.2 \times 0.25 + 77.9 \times 0.15 + 73.3 \times 0.23 + 27.8 \times 0.16)$ , while country C has the lowest performance of the six countries (score of 37.8).

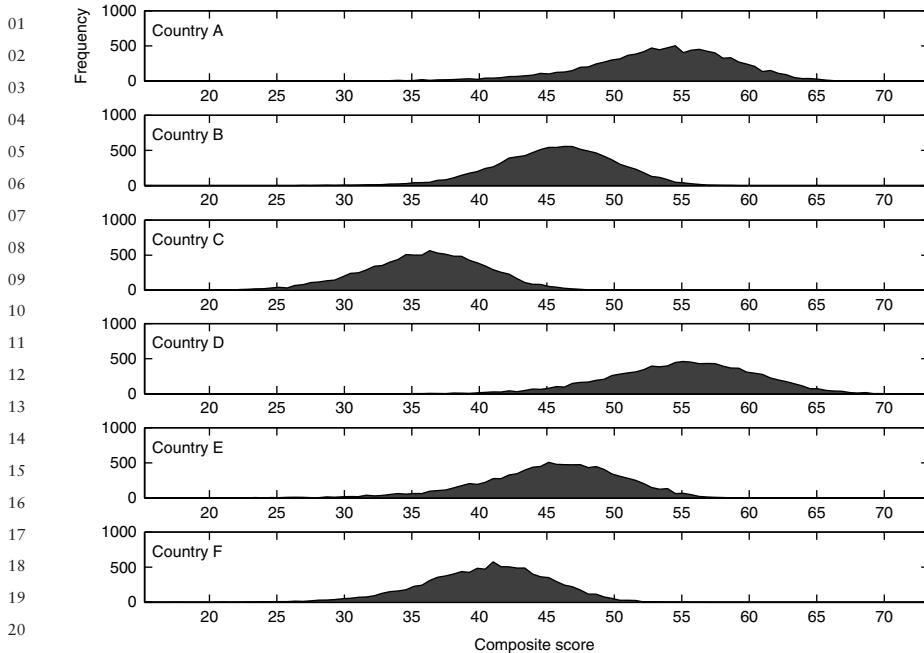
When the three sources of uncertainty are acknowledged, then each country score is no longer a single number, but a random variable. In total, there are 36 input factors in our sensitivity analysis (56 indicators values, 5 weights, 1 trigger to decide the aggregation method).

To get an idea of how the distributions of the countries' scores look when uncertainties are acknowledged, we present in Figure 6.1 the relevant histograms produced by 10 000 random combinations of the input factors. The countries' scores look roughly Gaussian, and the standard deviations among them are very similar, ranging from 4.4 for country B to 5.5 for country A.

We can easily observe that the histograms for several countries display significant overlap, e.g. countries A and D, B and E, and C and F. In

**Table 6.3** Composite indicator scores for six countries, baseline scenario (weighted arithmetic mean). Numbers in parentheses represent ranks

A	B	C	D	E	F
55.6 (2)	46.9 (4)	37.8 (6)	57.8 (1)	47.6 (3)	42.3 (5)

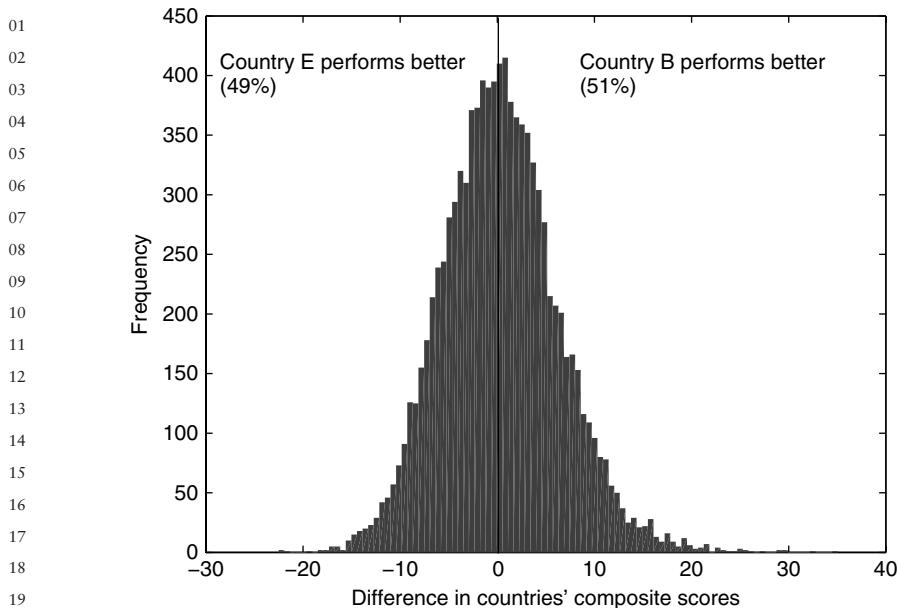


**Figure 6.1** Uncertainty analysis: Composite indicator scores for six countries when accounting for uncertainties in the indicators' values, weights, aggregation method

all those cases, the message about the countries' relative performance, or the reasons for a good or bad performance, are not explicit. At the same time, the country rankings produced by the Monte Carlo simulations are different from the baseline ranking. This casts doubt on the belief that the composite indicator gives a fair representation of all scenarios regarding the countries' environmental performance. Yet, we could already conclude that the performance of the countries is of the order of:  $(A, D) > (B, E) > (C, F)$ . We will next study both issues, i.e. the reasons behind the overlap of two countries' scores, and the cumulative shift from the baseline ranking.

Figure 6.2 presents the histogram of the differences between the composite scores of countries B and E, which correspond to 10 000 Monte Carlo runs. Country B performs better than country E in 51% of the cases. It would be interesting to find out which uncertainties are driving this result. Since we are looking for important factors and we do not know a priori if the model is additive or not, we will use a variance-based method because of its model independence (appropriate for nonlinear and nonadditive models). However, from the exercises in Chapter 1, the reader will suspect that geometric aggregation will result in a nonadditive model.

The 16 input factors (2 countries  $\times$  5 indicator values, plus 5 weight values, and 1 trigger to decide the type of aggregation) are sampled using a



**Figure 6.2** Uncertainty analysis: difference in the composite indicator scores between countries B and E. Input factors: 10 indicator values, 5 weight values, 1 trigger (weighted arithmetic mean versus weighted geometric mean)

quasi-random scheme (Sobol', 1967) of size  $N = 1024$  and the composite scores per country are calculated performing 18 432 simulations (recall that based on the computational recipes in Chapter 4, for a model of  $k$  factors, only  $N(k + 2)$  model runs are needed). The sensitivity indices  $S_i$  and  $S_{T_i}$  are calculated for the score of countries B and E, and for their difference, and reported in Table 6.4. The first-order sensitivity indices,  $S_i$ , show that the interactions between input factors do not have an impact on the score for either country B or E, since the output variance explained by the single factors is 92.5% for country B and 90.6% for country E. The composite score for country B is mainly influenced by the uncertainty in the values of OZONE, PM10 and CO2GDP. Similarly, the variance of the composite score for country E is mostly attributed to OZONE and PM10 and the choice of the aggregation method. None of the weights has a significant impact on the composite scores of the two countries.<sup>3</sup> Regarding the difference between the two countries' composite scores, this is mostly attributed to the values for OZONE for both countries. It is interesting to

<sup>3</sup> In a real-life application the noninfluence of weights could be of crucial importance in the discussion among stakeholders and could facilitate acceptance of the index.

01                   **Table 6.4** Sensitivity indices for the composite scores of two countries (B  
 02                   and E) and their scores' difference

<i>Input factors</i>	$S_{i,Bscore}$	$S_{i,Escore}$	$S_{i,(B-E)score}$	$S_{Ti,(B-E)score}$
OZONE(B)	0.369	-	0.192	0.210
PM10(B)	0.155	—	0.079	0.079
ENEFF(B)	0.013	-	0.007	0.009
CO2GDP(B)	0.112	-	0.059	0.061
WATSUP(B)	0.090	-	0.047	0.053
OZONE(E)	-	0.343	0.274	0.332
PM10(E)	-	0.117	0.087	0.091
ENEFF(E)	-	0.009	0.007	0.008
CO2GDP(E)	-	0.062	0.046	0.051
WATSUP(E)	-	0.049	0.036	0.042
w(OZONE)	0.043	0.051	0.000	0.017
w(PM10)	0.011	0.017	0.004	0.005
w(ENEFF)	0.017	0.019	0.000	0.001
w(CO2GDP)	0.019	0.026	0.002	0.005
w(WATSUP)	0.010	0.019	0.001	0.006
Aggregation	0.086	0.194	0.023	0.096
Sum	0.925	0.906	0.864	1.064

21 note that PM10, despite its influence on both countries' scores, does not  
 22 have an impact on their difference. The 16 input factors taken individually  
 23 account for 86.4% of the variance of the difference of the two countries  
 24 scores, while the remaining 13.6% is due to interactions.

25 The next issue we come to is: which factors have the strongest impact  
 26 on differences in the country ranking with respect to the baseline ranking?  
 27 To express this mathematically, we calculate the cumulative shift from the  
 28 baseline ranking, so as to capture in a single number the relative shift in  
 29 the position of the entire system of countries. This shift can be quantified  
 30 as the sum over  $m$  countries of the absolute differences in countries' ranks  
 31 with respect to the baseline ranking:

$$33 \quad R_S = \sum_{j=1}^m |Rank_{baseline}(CI_j) - Rank(CI_j)| \quad (6.3)$$

36 Figure 6.3 provides the histogram of 10 000 random Monte Carlo calcu-  
 37 lations of the cumulative shift from the baseline ranking. In most cases  
 38 the shift with respect to the baseline ranking is of 2, 4 or 6 positions  
 39 in total.  
 40

41 Our aim is to identify which of the 36 input factors ( $5 \times 6$  indicators'  
 42 values, 5 weights, 1 trigger) are highly influential in our output, namely the  
 43 cumulative shift in countries' ranks. Although, the computational cost of  
 44 running the model is not high for this simple model we will assume that

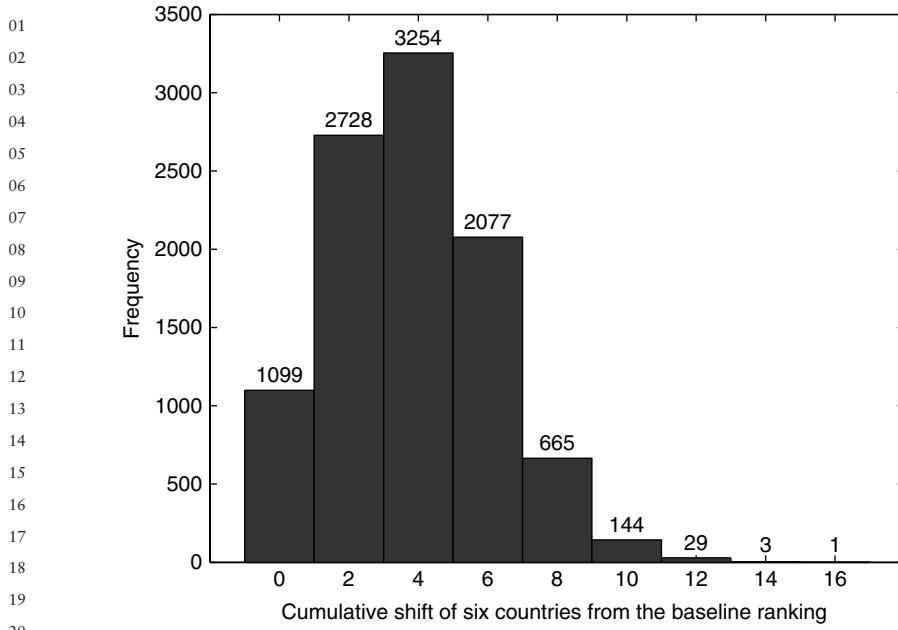


Figure 6.3 Uncertainty analysis. Output: cumulative shift from the baseline ranking for six countries. Uncertain input factors: 30 indicator values, 5 weight values, 1 trigger to decide the aggregation method (arithmetic vs geometric mean)

it is to illustrate an application of factor screening. We therefore resort to a screening method to help us reduce the number of input factors. We use the EE method described in Chapter 3 employing the recommended configuration of four levels for each input factor and ten trajectories. The total number of model executions performed to estimate the EET is 370 (=number of trajectories × (number of factors +1)).

Figure 6.4 shows the EET value for the 36 input factors. The most influential factors are the aggregation scheme, the weights for OZONE, WATSUP and PM10, and the indicators' values of OZONE(E), CO2GDP(B) and WATSUP(F). At the lower end, 13 factors are screened as nonimportant ( $EET < 0.5$ ). By fixing these noninfluential input factors to their nominal values, we can study the impact of the remaining 23 factors more thoroughly using a variance-based approach. Recall that our aim is to identify the indicator values and weights that need to be re-estimated, so that the country ranking is not strongly affected by the remaining uncertainties. The total number of model executions to estimate the first-order and total effect sensitivity indices  $\{S_i, S_{T_i}, i = 1, \dots, 23\}$  is 25 600 ( $1024 \times (23 + 2)$  where 1024 is the base sample), using the recipe in Chapter 4. Results are reported in Table 6.5. The impact on the cumulative shift in countries' ranks on the

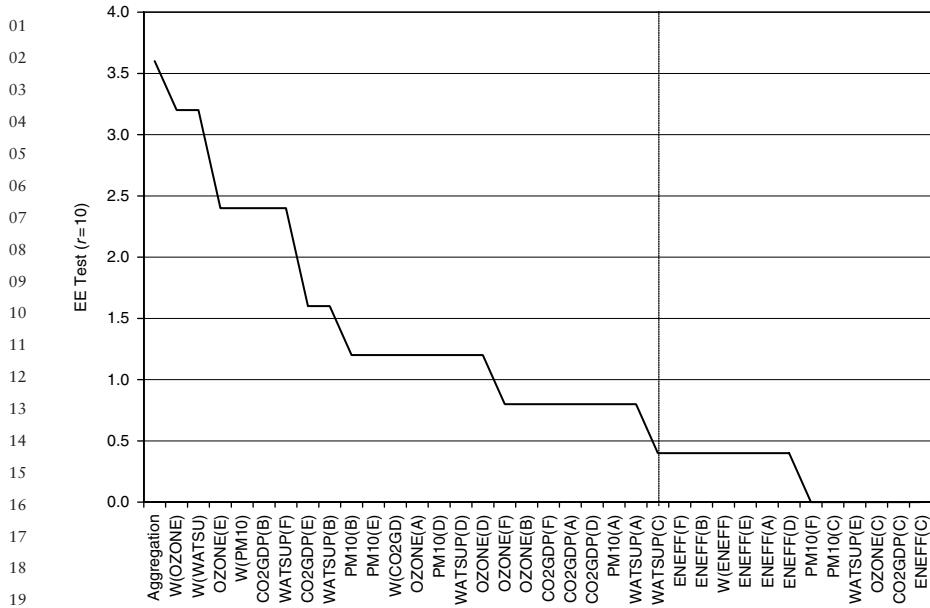


Figure 6.4 Results of the Elementary Effect screening exercise for 36 input factors

input factors is highly nonlinear. Only 56% of the output variance can be explained by the single factors, a great part of which is attributable to the aggregation method and the value of OZONE for country E. The aggregation method is the most influential both in single terms (highest  $S_i$ ) and through interactions (highest  $S_{T_i}$ ). The greatest  $S_{T_i}$ 's among the indicator values are found for OZONE in most countries, followed by PM10 for country E and WATSUP for country D. It is interesting to note that the estimated value for PM10 for country E has a relatively low standard deviation compared to other indicators' values (for example those of CO2GDP), yet the analysis showed that this factor is very influential due to interactions. Regarding the weights, although they have low values, they become very influential due to interactions – in particular w(OZONE), w(PM10) and w(WATSUP). Overall, the interactions and the nonlinearity account for 44% ( $= 100 - 56\%$ ) of the variance in the cumulative shift in countries' ranks. This result could guide the developers of the composite indicator to optimal resource allocation in terms of time and money spent to improve the reliability of just the few indicators' values that are most crucial to the policy message conveyed by the composite score or rank.

As a final consideration in our example, we will assume that a developer of a composite indicator is interested in a particular form of mapping. The objective of the analysis is to measure what fraction of the model realizations

01                   **Table 6.5** Sensitivity indices for the cumulative shift from the baseline  
02                   ranking

<i>Input factor</i>	<i>First order</i> ( $S_i$ )	<i>Total effect</i> ( $S_{T_i}$ )	$S_{T_i} - S_i$
Aggregation	0.182	0.357	0.175
OZONE(E)	0.072	0.224	0.152
W(WATSUP)	0.022	0.178	0.157
W(OZONE)	0.001	0.158	0.158
OZONE(A)	0.023	0.149	0.126
OZONE(B)	0.020	0.147	0.127
W(PM10)	0.004	0.134	0.130
WATSUP(D)	0.038	0.128	0.091
OZONE(F)	0.019	0.122	0.104
PM10(B)	0.007	0.109	0.103
PM10(E)	0.035	0.106	0.072
WATSUP(F)	0.017	0.105	0.088
CO2GDP(F)	0.011	0.105	0.094
PM10(D)	0.033	0.100	0.067
W(CO2GDP)	0.008	0.090	0.081
WATSUP(B)	0.000	0.082	0.082
CO2GDP(B)	0.014	0.082	0.068
OZONE(D)	0.011	0.072	0.061
CO2GDP(E)	0.027	0.070	0.043
PM10(A)	0.001	0.066	0.065
CO2GDP(D)	0.008	0.060	0.053
WATSUP(A)	0.003	0.053	0.050
Sum	0.558	2.745	2.187

25  
26 fall within established bounds or regions. This objective can be pursued  
27 using Monte Carlo filtering (MCF) that we discussed in detail in Chapter 5.  
28 Recall that in MCF one samples the space of the input factors as in ordinary  
29 MC, and then categorizes the corresponding model output as either within  
30 or without the target region (the terms behaviour,  $B$ , or nonbehaviour,  $\bar{B}$ , are  
31 used). This categorization is then mapped back onto the input factors, each  
32 of which is thus also partitioned into a behavioural and nonbehavioural  
33 subset. When the two subsets  $B$ ,  $\bar{B}$  for a given factor are proven to be statis-  
34 tically different (by employing a Smirnov test for example), then the factor  
35 is an influential one. In our example we set the model's target behaviour  
36 as  $R_s \leq 2$  (see Equation 6.3), that is we accept as behavioural an overall  
37 shift in rank of a maximum of two positions. Then, an MCF procedure  
38 can identify a significant correlation ( $> 0.2$ ) between three pairs of input  
39 factors, OZONE(B)-WATSUP(B), OZONE(E)-CO2GDP(E), OZONE(F)-  
40 CO2GDP(F). The corresponding patterns are shown in Figure 6.5. The  
41 correlation coefficients are negative and slightly over 0.2. This implies that  
42 in order to have practically no shift in the countries' ranks with respect to  
43 the baseline scenario, then high values of OZONE have to be combined with  
44

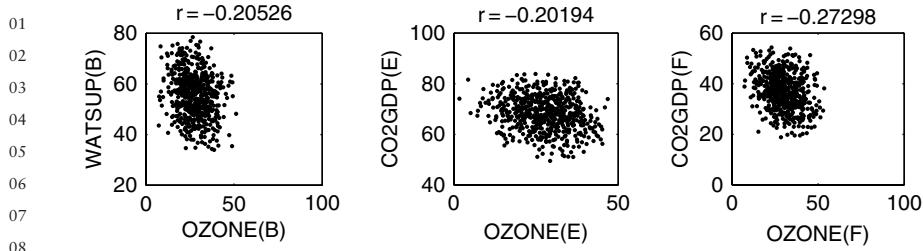


Figure 6.5 Bidimensional projection of the B subset for the three pairs of input factors that have significant correlation coefficients ( $> 0.2$  in the MC sample). Target behaviour  $R_s \leq 2$  (see Equation (6.3))

low values of WATSUP for country B, and vice versa. The same high–low combination of values should be observed for country E and country F, but in these cases the variables that play a role are OZONE and CO2GDP.

In order to gain further insight into the combinations of input factors that lead to high values of the cumulative shift in ranking (e.g.  $R_s > 8$  in the  $\bar{B}$  subset), we apply a similar approach. The MCF identifies the pair OZONE(E)–WATSUP(D) as the one having the highest correlation coefficient ( $-0.24$ ) in the  $\bar{B}$  subset. Figure 6.6 presents the bidimensional

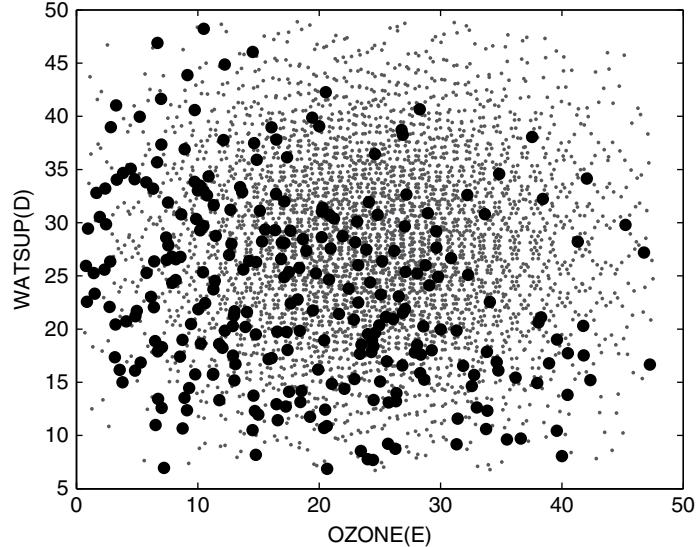


Figure 6.6 Bidimensional projection of the B (small points) and  $\bar{B}$  (larger dots) subsets for OZONE(E) and WATSUP(D). This pair of input factors had the highest correlation ( $-0.24$ ) in the  $\bar{B}$  subset. Target behaviour  $R_s \leq 8$

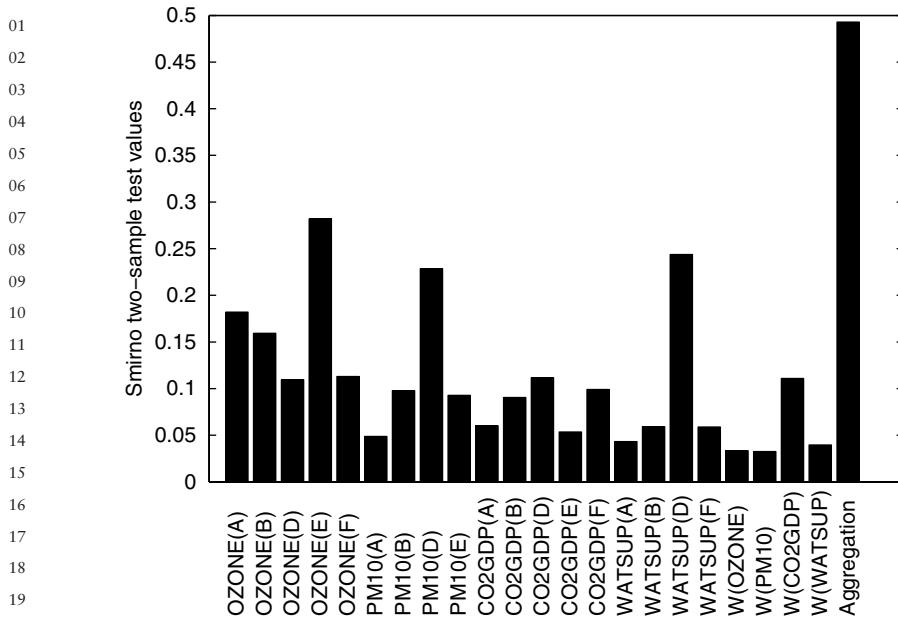


Figure 6.7 Smirnov two-sample test values (two-sided version) for all 23 input factors in the model. Target behaviour  $R_s \leq 8$

projection of the  $B$  (small points) and  $\bar{B}$  (larger dots) subsets for the OZONE(E) and WATSUP(D). It is apparent that the  $\bar{B}$  subset is characterized by a lack of points in the top right part. For example, WATSUP(D) values at about 45 or higher will result in a cumulative shift of more than eight positions in ranking if the OZONE (E) value is less than 15, while greater OZONE(E) values will result in much smaller shifts in ranking.

Figure 6.7 shows the values of the Smirnov statistics for all 23 input factors in our model, and considering the target behaviour  $R_s \leq 8$ . Four input factors are highly influential in the target values in the  $B$  or  $\bar{B}$  subset. These are, in order of importance, the trigger on the aggregation method, OZONE(E), WATSUP(D) and PM10(D). It is notable that not all of these factors have a high impact on the total variance of  $R_s$ . In fact, WATSUP(D) and PM10(D) have a total effect sensitivity index of less than 0.13, as opposed to 0.224 for OZONE(E) and 0.357 for the trigger on aggregation. This result indicates that the sensitivity analysis conclusions depend on the question we want to answer and not on the model output per se. This is why the settings and the objectives of sensitivity analysis must be clearly stated at the outset. Figure 6.8 is a graphical representation of the Smirnov test for the most important parameters that decide model realizations  $R_s > 8$  (dotted curves). Only parameters with Smirnov statistics

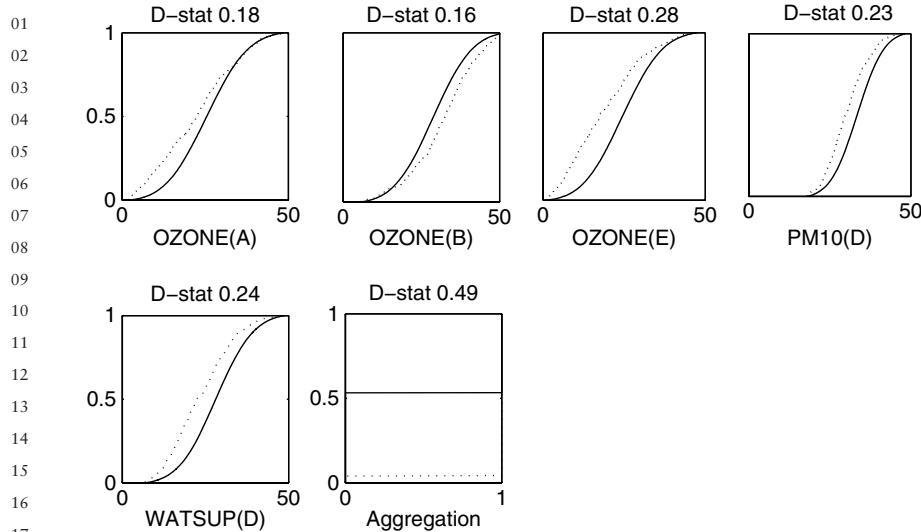


Figure 6.8 Smirnov test for the most important parameters (with Smirnov statistic  $> 0.15$ ) that drive the partition into  $B$  ( $R_s \leq 8$ , continuous lines) and  $\bar{B}$  (dotted lines) model realizations

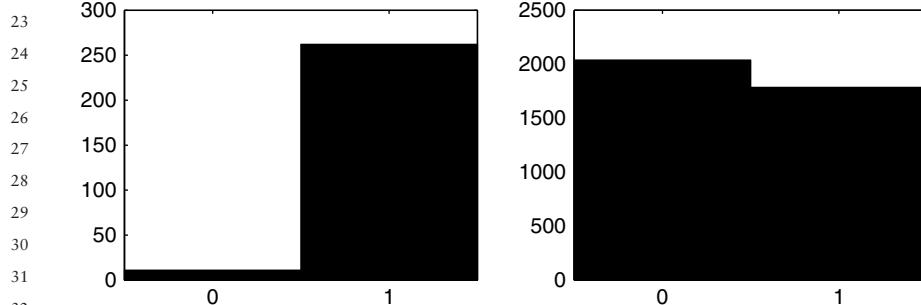


Figure 6.9 Histograms of the  $\bar{B}$  subset ( $R_s > 8$ , left graph) and  $B$  ( $R_s \leq 8$ , right graph) for the trigger

greater than 0.15 are shown. Model realizations in the  $R_s > 8$  subset are more likely when OZONE(A), OZONE(E), PM10(D) and WATSUP(D) fall on the left part of their predefined range, or when OZONE(B) falls on the right part of its predefined range. It is also interesting to note that the cumulative distribution for aggregation in the  $R_s > 8$  subset is almost entirely concentrated in 1, i.e. for geometric aggregation.

The impact of the aggregation trigger is better depicted in Figure 6.9. The figure evidences the high impact of the aggregation trigger on the partitioning

of the model realizations. Very high shifts in the ranking ( $> 8$ ) are almost entirely due to the use of geometric aggregation, while lower shifts are produced by either aggregation method. This outcome was expected since the geometric aggregation tends to penalize countries that compensate for very bad performance in few indicators with very good performance in others.

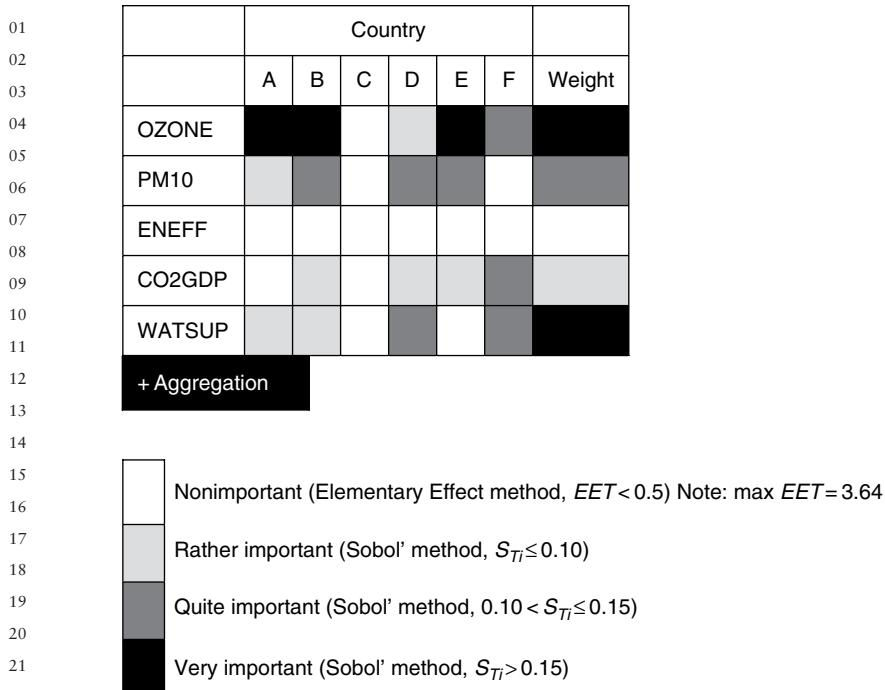
### 6.1.5 Conclusions

We have illustrated, using a simple composite indicator on environmental sustainability, how uncertainty analysis and sensitivity analysis can be applied to gain useful insights during the process of composite indicator building and to assess the reliability of country ranking. During the sensitivity analysis process, we first used the more qualitative approach based on the EE method to screen important from nonimportant factors in a numerous set (i.e. 36 factors). After fixing the non-important factors to their nominal value, we then followed a more quantitative approach using a variance-based method to identify those few factors that have the greatest impact on the variance of the cumulative shift from the baseline ranking. Finally, we applied Monte Carlo filtering to identify which input factors result in very high values of the cumulative shift from the baseline ranking.

We summarize in Figure 6.10 the conclusions from the in-tandem application of the EE method and the variance-based method. Country A presents the most extreme picture, having four indicators' values classified as nonimportant or of low importance, while the value for OZONE for country A is considered to be highly influential in the variance of the entire ranking (all six countries). All indicators' values for country C are nonimportant. The pattern for the remaining countries varies. The Monte Carlo filtering approach identified a few more input factors, PM10(D) and WATSUP(D), whose uncertainty can result in high values for the cumulative shift in countries' ranks. These results could guide a subsequent revision of the composite indicator in the following way:

- If the experts who assigned weights to the indicators can be engaged in a Delphi process to reach consensus on a few of the weights, then this should be done for the weights assigned to OZONE and WATSUP.
- If the amount of resources (in time/money) is sufficient for improving the quality of just a few indicators' values, then those should be the values of OZONE for countries A, B and E and of the PM10 and WATSUP for country D.

Of course even more stable results would be obtained if the experts could reach consensus on the aggregation method to be used, rather than using a combination of linear and geometric as in the present example.



**Figure 6.10** Classification of the 36 input factors regarding their impact on the cumulative shift from the baseline ranking. Methods used: first EE method, then variance-based

We have applied almost all methods described in this book to the composite indicator example. Clearly this is not to imply that all methods should always be used in combination on any given model. To compare abstraction with real life, the reader can study the sensitivity analysis performed on the actual Environmental Performance Index in Esty *et al.* (2006).

## 6.2 EXAMPLE 2: IMPORTANCE OF JUMPS IN PRICING OPTIONS

### 6.2.1 Setting the Problem

Imagine that an investor enters into a European call option contract that gives the holder the right (not the obligation) to buy an asset at a certain date  $T$  (e.g. two months) for a certain price. The price in the contract is

known as the exercise price or strike price  $K$ ; the date in the contract is known as the expiration date or maturity. To enter into an option contract there is a cost corresponding to the right purchased. This cost, referred to as premium  $C(K, T)$ , is the price of the option at present day and it is established according to the theory of arbitrage-free pricing (Hull, 1997).

Classic deterministic arbitrage involves buying an asset at a low price in one market and immediately selling it at a higher price in another market to make a risk-free profit. Instead, in the present exercise we will assume a market where arbitrage is not allowed, i.e. an arbitrage-free market or risk-neutral world. The theory of arbitrage-free prices stipulates that the prices of different instruments be related to one another in such a way that they offer no arbitrage opportunities. In practice, to price the option we make use of a model describing the evolution in time of the underlying asset price and then impose no arbitrage arguments.

Let us give an illustration of how the profit an investor makes depends on the underlying asset price  $P = \{P_t, t \geq 0\}$ . Figure 6.11 shows how much profit can be gained from buying this option. The plot refers to the date of maturity of the option. The premium paid at time  $t = 0$  is assumed to be 5 euros, and the strike price is 100 euros. The profit depends on the price of the underlying asset at time  $t = T$ , which is uncertain at the time the option is bought by the investor.

The risk associated with an option contract derives from the unknown evolution of the price of the underlying asset on the market. This risk can

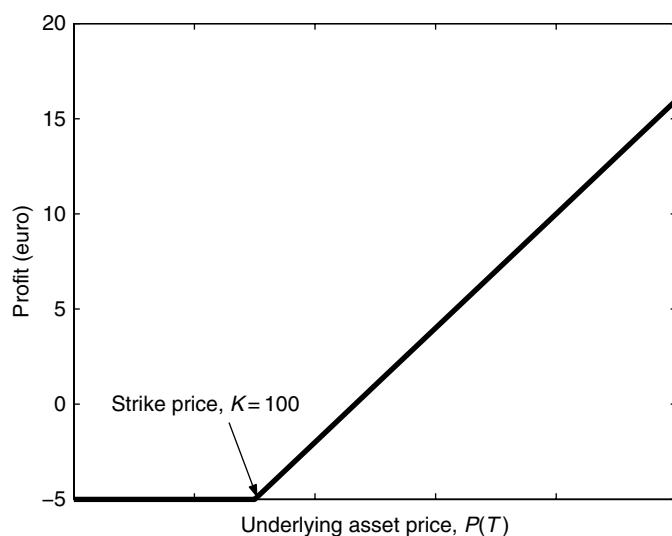


Figure 6.11 Profit (euro) gained from buying an European call option with strike price of 100 euros and premium of 5 euros

neither be controlled, nor avoided, and is an intrinsic feature of the contract itself (it is represented by the stochastic parts of the model). Besides this type of risk, another element of risk is due to the fact that the current option price is a quantity estimated via a mathematical model of a number of input variables whose values are affected by uncertainty. This uncertainty propagates through the model and produces uncertainty in the current option price. The questions we come to answer in this example are:

- How much is the uncertainty associated with a current option price?
- Which are the main sources of this uncertainty?
- Is it important to consider the effects of jumps in modelling the underlying dynamics?

The model chosen for describing the evolution of  $P = \{P_t, t \geq 0\}$  over time is the Heston stochastic volatility model (Heston, 1993) with jumps (Bakshi *et al.*, 1997). Volatility behaves stochastically over time and jumps are included in the dynamics of the asset. In the analysis, we will study how uncertainties in the input factors propagate through to the output using different scenarios that correspond to combinations of different strike prices and times to maturity.

### 6.2.2 The Heston Stochastic Volatility Model with Jumps

Heston (1993) proposes a stock price model which introduces stochastic volatility in the famous Black–Scholes model (Black and Scholes, 1973). In the Heston model the price paths of a stock (and the volatility) are continuous. Later, extensions of the Heston model were formulated that allowed for jumps in the stock price paths (Bakshi *et al.*, 1997). We investigate these extensions and ask ourselves whether the introduced jumps play a significant role in explaining the variance of the prices of derivatives under this model.

In the following we will assume that the underlying asset is a stock with price process denoted by  $P = \{P_t, t \geq 0\}$  and assume that the stock pays out a continuous compound dividend yield of  $q \geq 0$ . Moreover, we assume that in our market we have a risk-free bank account at our disposal, paying out a continuous risk-free interest rate  $r$ . In the Heston stochastic volatility model with jumps the stock price process is modelled by a stochastic differential equation given by

$$\frac{dP_t}{P_t} = (r - q - \lambda\mu_j)dt + \sigma_t dW_t + J_t dN_t, \quad P_0 \geq 0 \quad (6.4)$$

where  $P_0$  is price at time zero and  $N = \{N_t, t \geq 0\}$  is a Poisson process with intensity parameter  $\lambda > 0$ , i.e.  $E[N_t] = \lambda t$ .  $J_t$  is the percentage jump size

(conditional on a jump occurring) that is assumed to be log-normally, identically and independently distributed over time, with unconditional mean  $\mu_J$ . The standard deviation of  $\log(1 + J_t)$  is  $\sigma_J$ :

$$\log(1 + J_t) \sim N\left(\log(1 + \mu_J) - \frac{\sigma_J^2}{2}, \sigma_J^2\right) \quad (6.5)$$

The (squared) volatility follows the classical Cox–Ingersoll–Ross (CIR) process:

$$d\sigma_t^2 = k(\eta - \sigma_t^2)dt + \theta\sigma_t d\tilde{W}_t, \sigma_0 \geq 0 \quad (6.6)$$

where  $W = \{W_t, t \geq 0\}$  and  $\tilde{W} = \{\tilde{W}_t, t \geq 0\}$  are two correlated standard Brownian motions such that  $\text{Cov}[dW_t, d\tilde{W}_t] = \rho dt$ . Finally,  $J_t$  and  $N$  are independent, as well as  $W_t$  and  $\tilde{W}_t$ . The parameter  $\eta$  is interpreted as the long-run squared volatility;  $\kappa$  is the rate of mean reversion to the level  $\eta$  and  $\theta$  governs the volatility of volatility. The characteristic function  $\phi(u, t)$  of the logarithm of the stock price process for this model is given by

$$\begin{aligned} \phi(u, t) &= E\{\exp(iu \log(P_t)) | P_0, \sigma_0^2\} \\ &= \exp(iu(\log P_0 + (r - q)t)) \\ &\quad \times \exp(\eta\kappa\theta^{-2}((\kappa - \rho\theta ui - d)t - 2\log((1 - ge^{-dt})/(1 - g)))) \\ &\quad \times \exp(\sigma_0^2\theta^{-2}((\kappa - \rho\theta ui - d)(1 - e^{-dt})/(1 - ge^{-dt}))) \\ &\quad \times \exp(-\lambda\mu_J tui + \lambda t((1 + \mu_J)^{ui} \exp(\sigma_J^2(ui/2)(ui - 1)) - 1)) \end{aligned} \quad (6.7)$$

where

$$d = ((\rho\theta ui - \kappa)^2 - \theta^2(-ui - u^2))^{1/2},$$

$$g = (\kappa - \rho\theta ui - d)/(\kappa - \rho\theta ui + d).$$

Pricing of European call options under this model can be done by the Carr and Madan (1998) pricing method which is applicable when the characteristic function of the logarithm of the risk-neutral stock price process is known. Let  $\alpha$  be a positive constant such that the  $\alpha^{\text{th}}$  moment of the stock price exists. Carr and Madan (1998) showed that the price  $C(K, T)$  at time  $t = 0$  of a European call option with strike  $K$  and time to maturity  $T$  is given by

$$C(K, T) = \frac{\exp(-\alpha \log(K))}{\pi} \int_0^{+\infty} \exp(-iv \log(K)) \rho(v) dv$$

01 where

$$\begin{aligned}
 02 \quad \rho(v) &= \frac{\exp(-rT)E[\exp(i(v - (\alpha + 1)i)\log(P_T))]}{\alpha^2 + \alpha - v^2 + i(2\alpha + 1)v} \\
 03 \quad &= \frac{\exp(-rT)\phi(v - (\alpha + 1)i, T)}{\alpha^2 + \alpha - v^2 + i(2\alpha + 1)v}. \tag{6.8}
 \end{aligned}$$

08 Using fast Fourier transforms, one can compute rapidly the complete option  
09 surface with an ordinary computer.

10 The input factors selected for sensitivity analysis purposes are listed in  
11 Table 6.6. They can be differentiated into two groups: those whose value  
12 can be estimated with a certain degree of confidence using market data,  
13 and therefore represent a source of uncertainty that can be defined as  
14 ‘controllable’; and those that cannot be checked with market data and are  
15 therefore regarded as completely ‘uncontrollable’. The first group consists  
16 of the initial condition for the dynamics of the volatility  $\sigma_0$ , the dividend  
17 yield  $q$ , and the interest rate  $r$ . The remaining inputs, among which are the  
18 jump parameters, belong to the second group.

21 **Table 6.6** List of input factors of the Heston model with jumps. The last two  
22 columns report the lower and upper bounds of the uniform distributions for each  
23 input

	<i>Input</i>	<i>Description</i>	<i>Minimum</i>	<i>Maximum</i>
27 Controllable	$\sigma_0$	Initial condition for the dynamics		
	$q$	of the volatility	0.04	0.09
30 Uncontrollable	$r$	Dividend yield	0.00	0.05
	$\kappa$	Interest rate	0.00	0.05
32	$\eta$	Rate of mean revision	0.00	1.00
	$\theta$	Long-run squared volatility	0.04	0.09
34	$\rho$	Parameter governing the volatility of volatility	0.20	0.50
		Correlation between Brownian motions		
36		in Equations ((6.4)) and ((6.6))	-1.00	0.00
	$\lambda$	Jumps parameter (intensity parameter of the Poisson process that models the stock price)	0.00	2.00
41	$\mu_j$	Jump parameter in Equation ((6.5))	-0.10	0.10
	$\sigma_j$	Jump parameter in Equation ((6.5))	0.00	0.20

### 01            6.2.3 Selecting a Suitable Sensitivity Analysis Method

02  
 03        In total there are 10 input factors in our model that could affect the pricing  
 04        of European call options. The model takes a few seconds to run and the  
 05        specific answers we try to get by the application of sensitivity analysis are:

- 07        • What is the relative importance of the 10 input factors affecting the  
 08        uncertainty in the current option pricing in difference scenarios, i.e.  
 09        combinations of the option strike price  $K$  and of the time to maturity  $T$ ?
- 10        • Does the impact of the uncertainties change from scenario to scenario?
- 11        • Is it the controllable or the uncontrollable input factors that drive most  
 12        of the output variance?

13  
 14        Given the low number of input factors, the low computational cost of the  
 15        model and the fact that we want to assess both first-order and total-effect  
 16        sensitivity indices  $\{S_i, S_{T_i}\}$ , the most appropriate sensitivity analysis method  
 17        to use is a variance-based method (see Chapter 4), as these methods do not  
 18        rely on assumptions about the model being additive, or monotonic in the  
 19        input–output relationship.

### 21            6.2.4 The Sensitivity Analysis Experiment and Results

22  
 23        The first-order  $S_i$  and total-effect  $S_{T_i}$  sensitivity indices are computed for  
 24        each input factor in different scenarios. These scenarios represent different  
 25        combinations of the option strike price  $K$  and the time to maturity  $T$ . The  
 26        initial condition for the stock is fixed at  $P_0 = 100$ , while seven values of the  
 27        strike price are considered ( $K = 70, 80, \dots, 130$ ) to represent situations in  
 28        which the option is in the money ( $K \leq P_0$ ), at the money ( $K = P_0$ ) or out of  
 29        the money ( $K \geq P_0$ ). Six different time horizons are examined from  $T = 0.5$   
 30        years up to  $T = 3$  years. Therefore, we study 42 scenarios in total. The total  
 31        number of model executions to estimate the entire set of the variance-based  
 32        indices  $\{S_i, S_{T_i}, i = 1, 2, \dots, 10\}$  is  $N = 24.576 (= 2048(10 + 2))$ .

33  
 34        Figure 6.12 shows the importance of the input factors in each of the 42  
 35        scenarios according to the  $S_{T_i}$  scaled in  $[0, 1]$  for presentational purposes.  
 36        Results reveal that, across all scenarios, the most influential parameters are:  
 37        the dividend yield  $q$ , the interest rate  $r$ , and the jump parameters  $\lambda$  and  $\sigma_J$ .  
 38        In particular,  $q$  and  $r$  are very important for low strike prices at all times  
 39        to maturity, while  $\lambda$  and  $\sigma_J$  become more relevant at higher strike prices.  
 40        As expected,  $\sigma_0$  is important only for low times to maturity, especially  
 41        when the option is not in the money. Note that among these four most  
 42        important factors,  $q$  and  $r$  belong to the group of ‘controllable’ factors.  
 43        More interesting are the roles of the jump parameters  $\lambda$  and  $\sigma_J$ , which are  
 44        the most relevant among the ‘uncontrollable’ factors. In general, if we limit  
 our attention to the ‘uncontrollable’ factors, the analysis proves that the

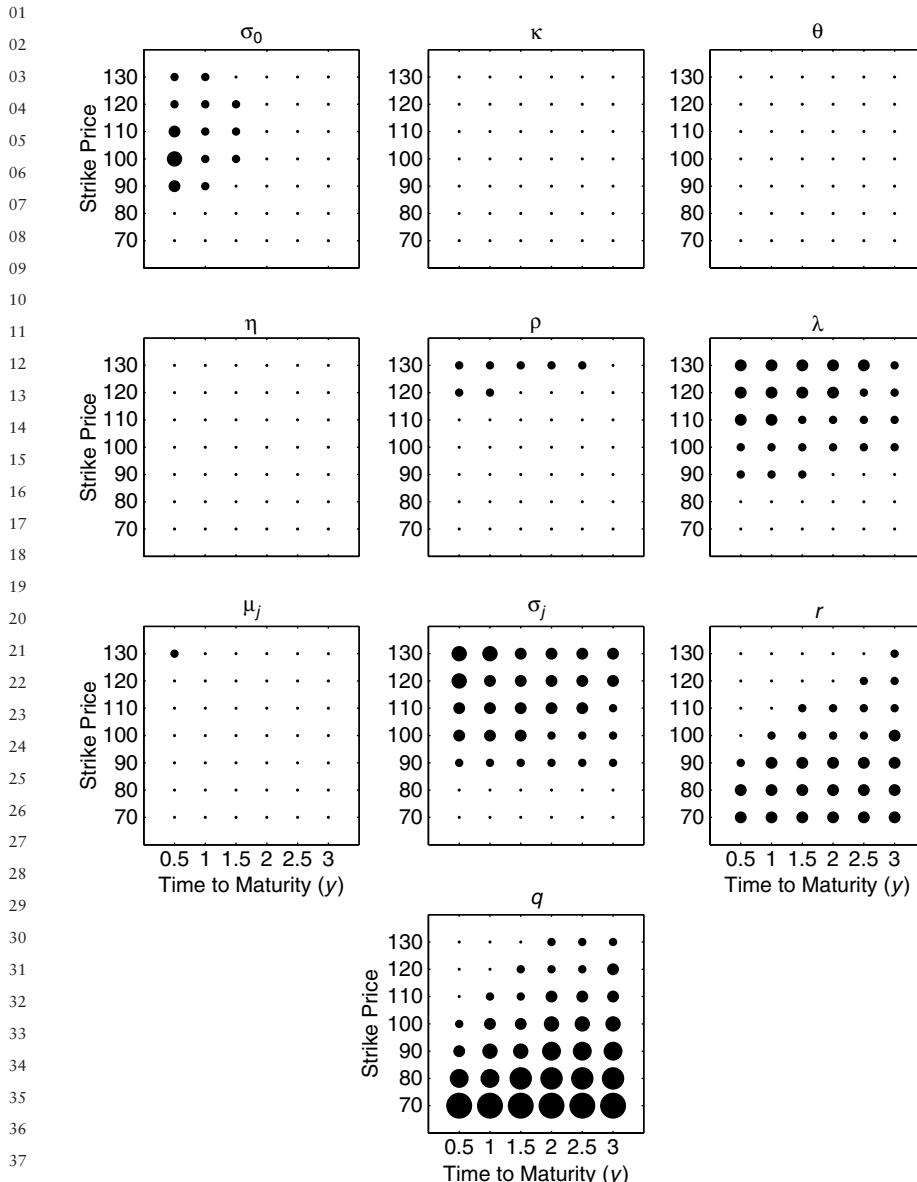


Figure 6.12 Importance of the factors in each of the 42 ( $6 \times 7$ ) scenarios according to  $S_{T_i}$  scaled in  $[0, 1]$ . Each graph refers to a selected input factor. Within a graph, each dot illustrates the input importance in a specific scenario. Ten different dots' sizes are considered, corresponding to 10 different classes of importance, ranging from values of  $S_{T_i}$  in  $[0, 0.1]$  to values of  $S_{T_i}$  in  $[0.9, 1]$

jumps group, i.e.  $\lambda$ ,  $\sigma_j$  and  $\mu_j$ , drives the greater amount of the total output variance in all scenarios.

If we compare the relative importance of the various factors in different scenarios, it emerges that factors' importance is less sensitive to shifts in the time horizon, than it is to the strike price value.

Finally, the influence of the input factors  $\kappa$ ,  $\eta$  and  $\theta$  is almost negligible in all scenarios and hence they could be fixed at any point in their domains without risk of losing any information about the output of interest. Similar conclusions are drawn by Campolongo *et al.* (2007), who analyse this problem by using, for comparative purposes, both the EE method and the variance-based method presented herewith.

In Figure 6.13 we show three scenarios that correspond to a fixed time to maturity ( $T = 1.5$  years) and to three different strike prices: an option in the

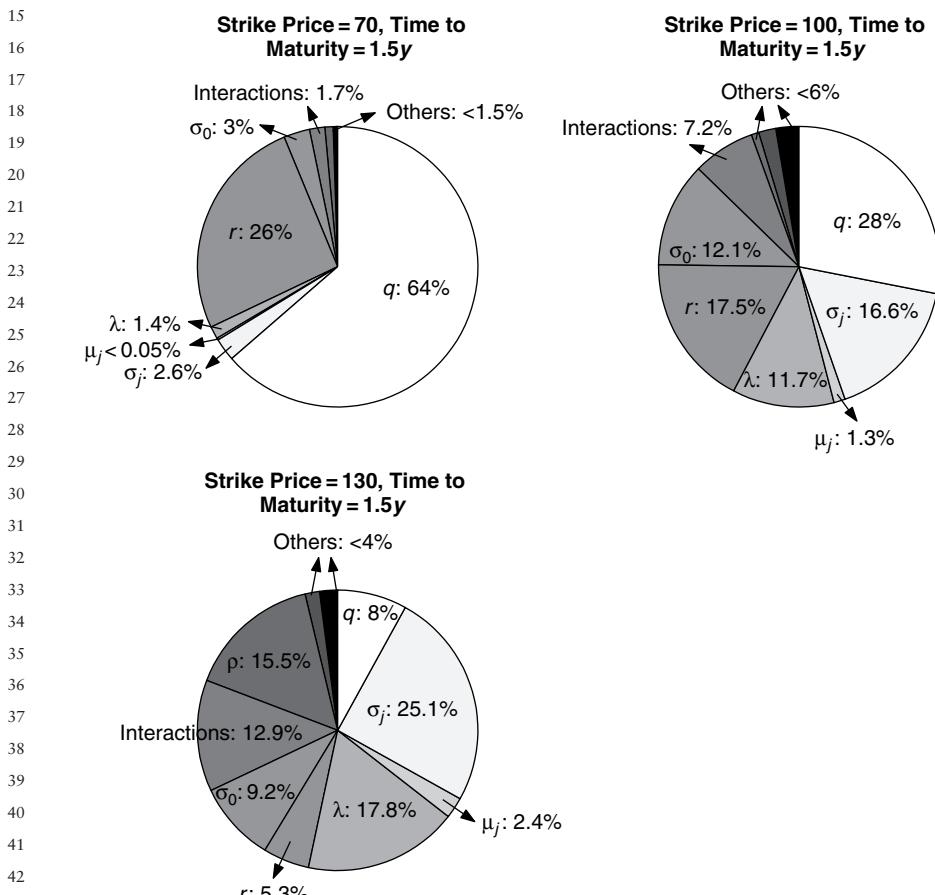


Figure 6.13 Decomposition of the total variance of the option price in three scenarios. Interactions of all orders are grouped in a single term

01 money ( $K = 70$ ), at the money ( $K = 100$ ) and out of the money ( $K = 130$ ).  
02 The variance of the option price is apportioned to the contributions due to  
03 the first-order effects of each input (i.e. the Sobol'  $S_i$ ) and to the interactions  
04 of all orders. Since we are not interested in quantifying interactions of  
05 different orders due to certain input factors, all interactions are summed up  
06 in a single term. The figure reveals that the importance of jumps (factors  $\lambda$   
07 and  $\sigma_j$ ) increases considerably with the strike price. The sum of their main  
08 effects goes from approximately 4%, when the option is in the money, to  
09 nearly 30% when the option is at the money, up to 45.3% when the option  
10 reaches 130 (out of the money). When the option is in the money, more than  
11 90% of the total variance is due to the controllable factors  $q$  and  $r$ , thus  
12 leaving little opportunity to reduce the uncertainty in the option price by  
13 increasing the modelling effort. As the strike price increases, the importance  
14 of jumps increases considerably, which stresses that their role in modelling  
15 the option price cannot be overlooked: jumps need to be included in the  
16 model and their representation should be as accurate as possible. We could  
17 summarize in two main points the impact of these findings on the investor's  
18 actions:

- 19
- 20 • Among the important factors,  $q$  and  $r$  are controllable. Therefore, the  
21 investor might reduce the uncertainty in  $C(K, T)$  by prioritizing his efforts  
22 to get good estimates of  $q$  and  $r$  from market data.
  - 23 • Among the uncontrollable factors, it is the jumps that drive most of the  
24 variance. However, this type of uncertainty remains in the model and  
25 there is no possibility for the investor to reduce it. But, from a modelling  
26 point of view, the analysis presented above has shown that the inclusion  
27 of jumps is of paramount importance in the estimation of the underlying  
28 asset price.

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### 30 6.2.5 Conclusions

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32 In this example we have analysed the uncertainty in the price of a European  
33 option estimated by the Heston model in its version with jumps. The uncer-  
34 tainty in the option price has been apportioned to its different sources via  
35 sensitivity analysis. In particular we have assessed the relative importance  
36 of jumps with respect to other model input factors.

37 The sensitivity analysis using variance-based sensitivity indices  $S_i$ ,  $S_{T_i}$  has  
38 shown that, among the 'uncontrollable' factors (i.e. those that cannot be  
39 estimated from market data), jumps play a major role in determining the  
40 option price, thereby emphasizing the need to include them in the model  
41 formulation. At low strike prices, most of the uncertainty in the option price  
42 is due to 'controllable' factors such as the dividend yield  $q$  and the interest  
43 rate  $r$ . As the option strike price increases, the importance of jumps increases  
44

01 considerably: for instance, for options with strike prices of 120 or 130 (the  
02 starting price being 100), the importance of jumps is superior to that of  $q$   
03 and  $r$  for all times to maturity. This underlines that an accurate assessment  
04 of the jump process becomes more urgent for out-of-the-money options. It  
05 also emerges that three of the inputs, namely the rate of mean reversion  $\kappa$ ,  
06 the long-run squared volatility  $\eta$  and the parameter governing the volatility  
07 of volatility  $\theta$ , do not affect the output in any of the studied scenarios. This  
08 result is useful, as it may allow a simplification of the model. Finally, as  
09 expected, at low time to maturity the initial condition for volatility needs  
10 to be accurately determined, while it becomes less important as the time to  
11 maturity increases.

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### 6.3 EXAMPLE 3: A CHEMICAL REACTOR

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#### 6.3.1 Setting the Problem

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Imagine that a chemist, in a routine procedure, attempts to create a model  
of reaction systems to understand reaction mechanisms, kinetic properties,  
process yields under various operating conditions, or the impact of chemicals  
on humans and the environment. These models are attempts to mimic  
the system by hypothesizing, extracting and encoding system features (e.g.  
a potentially relevant reaction pathway versus another plausible one). A  
model will hopefully help to corroborate or falsify a given description of  
reality, e.g. by validating a reaction scheme for a photochemical process in  
the atmosphere, and may also help to influence it, e.g. by facilitating the  
identification of optimal operating conditions for an industrial process or  
by suggesting mitigating strategies for an undesired environmental impact.

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These models are customarily built in the presence of uncertainties of  
various levels, in the pathway, in the order of the kinetics associated with  
the pathway, in the numerical value of the kinetic and thermodynamic  
constants for that pathway and so on. The job of the uncertainty analysis is  
to propagate all these uncertainties, via the model, onto the model output  
of interest, e.g. the yield of a process. The work of sensitivity analysis is to  
determine the strength of the relation between a given uncertain input and  
the output.

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The issues a chemist may want to deal with during this modelling process  
could include:

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- understanding the reaction path, mechanism, or rate-determining steps  
in a detailed kinetic model with a large number of elementary reactions  
(Turanyi, 1990; Saltelli and Hjorth, 1995);

- 01 • extracting important elementary reactions from a complex kinetic model  
02 to obtain a reduced model (e.g. a minimal reaction scheme) with equiv-  
03 alent predictive power;
- 04 • selecting important reactions for further analysis (Pandis and Seinfeld,  
05 1989; Vuilleumier *et al.*, 1997);
- 06 • estimating the output of a computer program in the neighbourhood  
07 of a given set of boundary conditions without rerunning the program  
08 (Grievank, 2000; Kioutsoukis *et al.*, 2005);
- 09 • reconciling model parameters with observations (Rabitz, 1989; Le Dimet  
10 *et al.*, 2002; Mallet and Sportisse, 2004).

### 13 6.3.2 Thermal Runaway Analysis of a Batch Reactor

15 The thermal runaway analysis of a batch reactor, where an exothermic  
16 reaction  $A \rightarrow B$  takes place, is performed considering the following mass  
17 and heat balance equations:

$$20 \quad \frac{d[A]}{dt} = -k(T) \cdot [A]^n \quad (6.9)$$

$$24 \quad \rho c_v \frac{dT}{dt} = (-\Delta H) \cdot k(T) \cdot [A]^n - s_v \cdot u \cdot (T - T_a) \quad (6.10)$$

26 where  $n$  is the order of the reaction,  $\rho$  the density of the fluid mixture  
27 [ $\text{kg}/\text{m}^3$ ],  $c_v$  the mean specific heat capacity of the reaction mixture  
28 [ $\text{J}/(\text{Kmol})$ ],  $\Delta H$  the reaction enthalpy [ $\text{J}/\text{mol}$ ],  $s_v$  the surface area per unit  
29 volume [ $\text{m}^2/\text{m}^3$ ],  $u$  the overall heat transfer coefficient [ $\text{J}/(\text{m}^2 \cdot \text{s} \cdot \text{K})$ ] and  $T_a$   
30 the ambient temperature [K]. The initial conditions are  $[A] = [A]_0$ ,  $T = T_0$ ,  
31  $t = 0$ . This is customarily rewritten in dimensionless form:

$$34 \quad \frac{dx}{d\tau} = \exp\left(\frac{\theta}{1 + \theta/\gamma}\right) \cdot (1 - x)^n = F_1(x, \theta)$$

$$37 \quad \frac{d\theta}{d\tau} = B \cdot \exp\left(\frac{\theta}{1 + \theta/\gamma}\right) \cdot (1 - x)^n - \frac{B}{\psi} \cdot (\theta - \theta_a) = F_2(x, \theta)$$

39 with initial conditions  $x = 0$ ,  $\theta = 0$  at  $\tau = 0$ , and the dimensionless variables:

$$42 \quad x = \frac{[A]_0 - [A]}{[A]_0} \quad \theta = \frac{T_0 - T}{T_0} \cdot \gamma \quad \tau = t \cdot k(T_0) \cdot ([A]_0)^{n-1}$$

and dimensionless parameters:

$$B = \frac{(-\Delta H) \cdot [A]_0}{\rho \cdot c_v \cdot T_0} \gamma \quad (\text{heat of reaction})$$

$$\gamma = \frac{E}{R_g T_0} \quad (\text{activation energy})$$

$$\psi = \frac{(-\Delta H) \cdot k(T_0) \cdot ([A]_0)^n}{s_v \cdot u \cdot T_0} \cdot \gamma \quad (\text{Semenov number expressed as heat release potential)/(heat removal potential)})$$

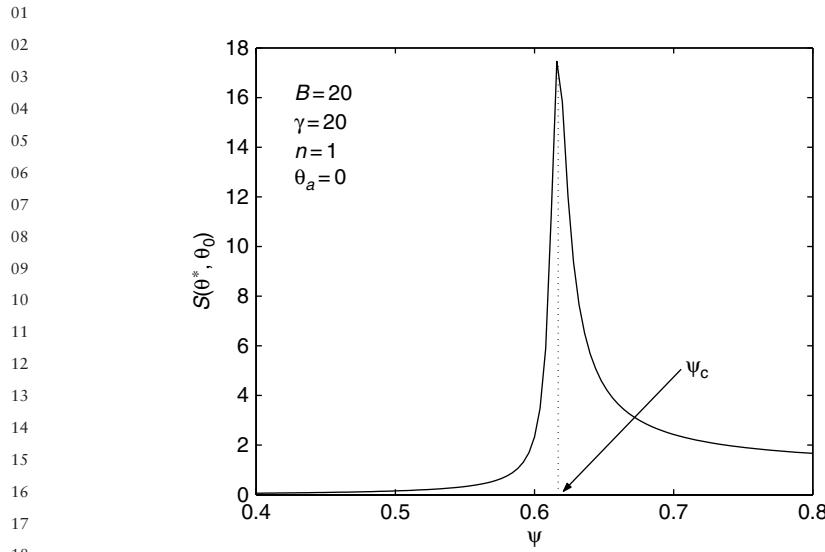
This system was widely analysed in the last century to characterize thermal runaway under varying operating conditions (Varma *et al.*, 1999). At a given constant rate and ambient temperature, the system is completely determined by the parameters  $B$  and  $\psi$ , and critical conditions are usually illustrated in the  $B$ - $\psi$  plane.

A reactor under explosive conditions is sensitive to small variations in, for example, the initial temperature, while under nonexplosive conditions, the system remains insensitive to such variations. The boundaries between runaway (explosive) and nonrunaway (nonexplosive) conditions can thus be identified based on the system's sensitivity to small changes in the operating parameters. The system can also be characterized by the derivative of the maximum temperature reached in the reactor versus the initial temperature, i.e.  $S(\theta^*, \theta_0) = d\theta^*/d\theta_0$  (Morbidelli and Varma, 1988).

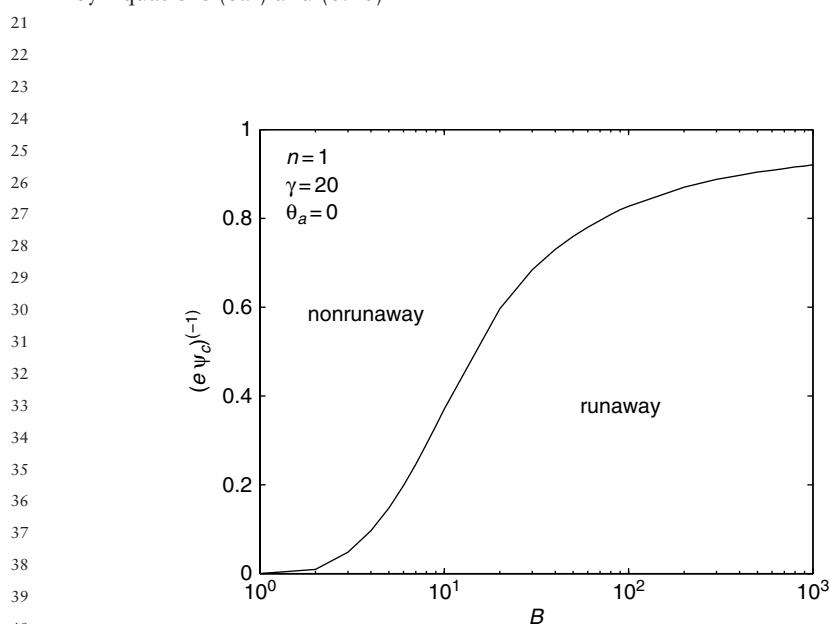
The runaway boundary is defined as the critical value of each parameter for which the sensitivity to the initial condition is at a maximum, e.g. for the Semenov number  $\psi$  we have the results in Figure 6.14.

For  $\psi$  values smaller than  $\psi_c$  the system is in nonrunaway conditions, i.e. the maximum temperature reached in the reactor is not very high and this maximum is insensitive to small variations in the inlet temperature. Increasing  $\psi$ , both the maximum temperature and its sensitivity to  $T_0$  increase smoothly until, in proximity to  $\psi_c$ , there is a sharp rise for both of them that rapidly brings the reactor to a strong temperature increase. For  $\psi$  values higher than  $\psi_c$ , the sensitivity decreases again, leaving unchanged the extreme temperature rise reached at  $\psi_c$ . By fixing the reaction kinetics ( $n, \gamma$ ) and the ambient temperature ( $\theta_a$ ), the curve in the  $B$ - $\psi$  plane can be obtained (Figure 6.15).

Consider the case of a system with nominal parameter design  $B = 20$ ,  $\gamma = 20$ ,  $n = 1$  and  $\psi = 0.5$ . Under these conditions the system should be in the nonrunaway region. The system, however, is characterized by uncertainties. Let us therefore assume the following uncertainty distributions for the model parameters:



19      **Figure 6.14**  $S(\theta^*, \theta_i) = d\theta^*/d\theta_i$  versus Semenov number  $\psi$  for the model expressed  
20      by Equations (6.9) and (6.10)



41      **Figure 6.15** Runaway versus nonrunaway in the plane  $B, 1/e\psi$  for fixed  $n, \gamma$  and  
42       $\theta_a$  ( $e$  is the number of Neper)

$$\begin{aligned}
 01 & B \sim N(20, 4) \\
 02 & \gamma \sim N(20, 2) \\
 03 & \theta_a \sim N(0, 0.2) \\
 04 & \theta_0 \sim N(0, 0.2) \\
 05 & \psi \sim U(0.4, 0.6)
 \end{aligned} \tag{6.11}$$

Under the chosen operating conditions ( $\gamma = 20$ ), a standard deviation of 0.02 for the ambient and initial dimensionless temperatures correspond to a standard deviation of about 3 K in the absolute temperature scale.

### 6.3.3 Selecting the Sensitivity Analysis Method

Since this example involves few input factors and the computational cost of the analysis is small, we employ several of the sensitivity analysis methods we discussed in the previous chapters, such as the standardized regression coefficients (SRC), the Sobol' variance-based method and the SDP smoothing metamodelling technique. As discussed in Chapter 5, metamodelling techniques produce extremely efficient sensitivity estimates and will be considered as the 'reference' values in the following example.

### 6.3.4 The Sensitivity Analysis Experiment and Results

We perform a Monte Carlo simulation and estimate the first-order and total-effect Sobol' indices following Saltelli (2002) as well as the standardized regression coefficients. We also perform the SDP metamodelling. The total cost for the Sobol' estimates is of 6144 model evaluations (i.e.  $N = 512$ ,  $k = 5$  and  $N(2k+2) = 6144$ ),<sup>4</sup> while for the SRC and SDP estimates it is of 512 model evaluations (simply using the base sample matrix of the Sobol' design). Our aim is to analyse the behaviour of the maximum temperature rise occurring in the batch reactor. From Figure 6.16 we can see that, even if the nominal conditions of the reactor are stable, there are threshold values of  $B$ ,  $\theta_a$  and  $\psi$  for which the maximum temperature in the reactor can undergo a sharp rise (the absolute temperature can double with a rise of about 300 K).

The relationship between the maximum temperature and the parameters is clearly nonlinear with interactions. To show this, let us consider the different sensitivity measures for the maximum temperature shown in

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<sup>4</sup> This is not the recipe given in Chapter 4, which would require  $N(k+2) = 3584$  model evaluations, but corresponds to the original design of Sobol'. This larger sample design has been used because, as discussed in Saltelli (2002), it allows us also to obtain estimates of second-order sensitivity indices, which are discussed later in this example.

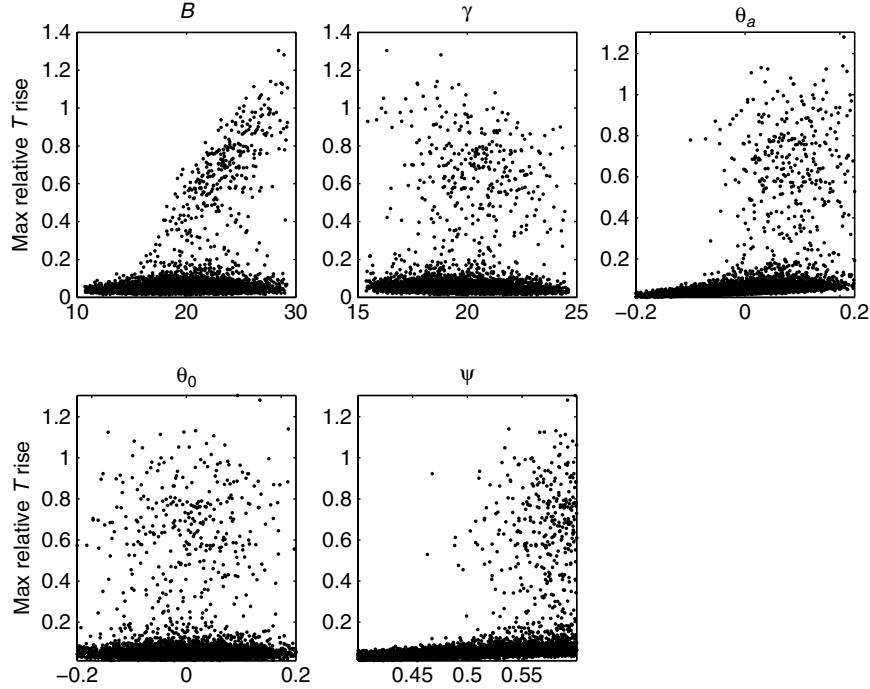


Figure 6.16 Relative temperature rise at the maximum  $[(T_{\max} - T_0)/T_0]$  versus the uncertain model parameters. The extreme values of about 1.2 for  $[(T_{\max} - T_0)/T_0]$  correspond to a temperature rise of about 300 K

Table 6.7 Sensitivity measures for model ((6.9))–((6.11))

	$\beta_i^2$	$S_i$ (Sobol')	$S_i$ (SDP)	$S_{T_i}$
$\psi$	0.17	0.1781	0.205	0.6738
$\theta_a$	0.14	0.1641	0.148	0.556
$B$	0.087	0.08	0.092	0.4692
$\gamma$	0.0012	0.0019	0.001	0.0322
$\theta_0$	0.0006	0.0015	0.0004	0.0128
Sum	0.40	0.43	0.45	

Table 6.7. Consider the  $\beta_i^2, S_i$  columns first. The sensitivity based on the  $\beta_i^2$ 's can only capture 40% of the variation of the maximum temperature. Taking the SDP estimate of the main effects into account, we get 45% (43% using the Sobol' method). This leaves 55% to interactions between the model parameters. Results in Table 6.7 also show that Sobol' estimates are reasonably close to the 'reference' SDP estimates.

We could terminate the analysis at this point or we could pursue our investigation to achieve a full mapping of the input–output relationship. Stopping here would mean that we are happy with having learned that the parameter which offers a better chance of reducing the variance in the maximum temperature is  $\psi$ . Yet this factor only accounts for about 20% of the variance, and the many unknown interactions suggest that a much larger reduction in variance might be achieved if one could identify the interacting factors and try to learn more about them.

One avenue would be to compute individual interaction terms. We can do this applying both the SDP smoothing and the Sobol' method (Saltelli, 2002). The analysis of second-order interaction effects tells us that the most significant terms involve the group of factors ( $B, \theta_a, \psi$ ). Estimated values are shown in Table 6.8, where these three interaction terms are shown to explain another 38.7% of the model output variance, i.e. the SDP meta-modelling of first- and second-order explains 83.7% of the model output. We can also see that interaction term  $S_{B\theta_a}$  is significantly overestimated using the Sobol' method.

This example points to the importance of identifying interactions in sensitivity analysis. The descriptive power of the total sensitivity indices  $S_{T_i}$  is evident by looking at the last column of Table 6.7. Even without computing second- and third-order interaction effects, it is evident from the difference between the  $S_i$  and  $S_{T_i}$  values for each factor that  $B, \theta_a$  and  $\psi$  are involved in significant interactions. From the total indices we can also see that all the interaction terms of factor  $\gamma$  with  $(B, \theta_a, \psi)$  cover about 3% of the total variance, while  $\theta_0$  has a negligible total effect, implying its irrelevance.

In Figure 6.17 we show the SDP estimates of first-order ANOVA-HDMR terms of the maximum relative temperature rise  $(T^{\max} - T_0)/T_0$  for the three most important parameters. These show that the first-order relationships are monotonic, which explains why the  $\beta_i^2$  give an acceptable estimate of the sensitivities in Table 6.7, with an overall error of about 0.05.

In Figure 6.18 we also show the SDP estimates of the second-order ANOVA-HDMR terms for the group of factors  $(B, \theta_a, \psi)$ . It can be clearly seen that extreme values of the temperature rise are associated with high–high combinations of each couple of factors. In particular, the highest peaks are obtained combining high values for  $B$  and  $\psi$ .

**Table 6.8** Second-order sensitivity indices for model ((6.9))–((6.11))

	$S_{ij}$ (Sobol')	$S_{ij}$ (SDP)
$S_{B\psi}$	0.17	0.169
$S_{\theta_a\psi}$	0.17	0.144
$S_{B\theta_a}$	0.166	0.074

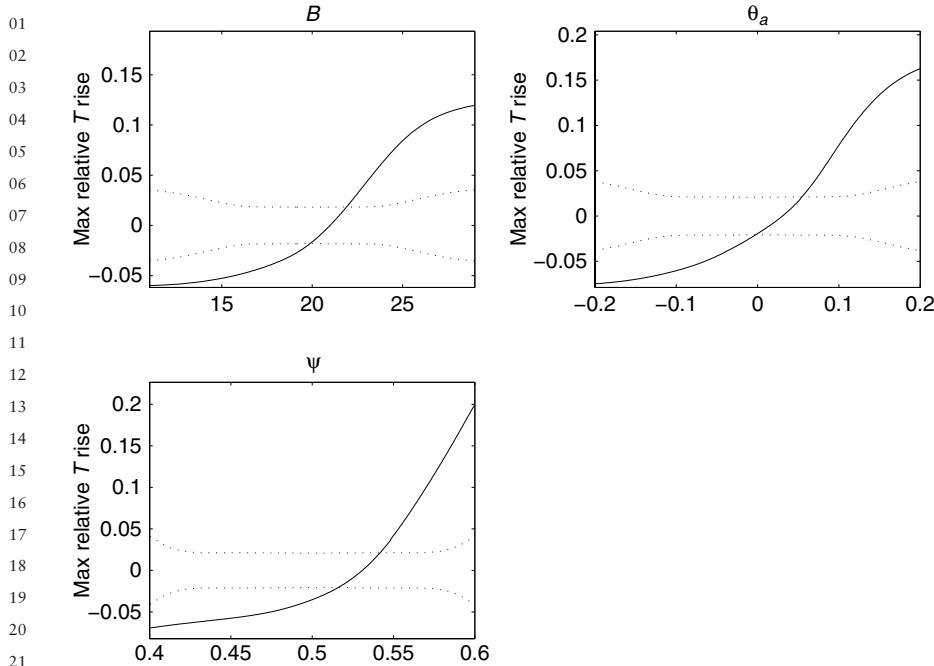


Figure 6.17 First-order ANOVA-HDMR terms (solid lines) of the subset of factors ( $B$ ,  $\theta_a$ ,  $\psi$ ) for the maximum relative temperature rise, estimated using the SDP procedure described in Chapter 5 (note: the mean value of the maximum temperature rise ( $T_{\max} - T_0$ ) /  $T_0$  is 0.1). Dotted lines show the 95% standard error band

### 6.3.5 Conclusions

In the analysis of thermal runaway of a batch reactor, the sensitivity analysis results can be summarized as follows:

- The parameter which offers better chances of reducing the variance in the maximum temperature is  $\psi$  (about 20% of the variance). The sensitivity based on the  $\beta'_i$ 's can capture only 40% of the variation of the maximum temperature. Considering the SDP estimate of the main effects, we can arrive at 45%. This implies that 55% is caused by interactions between the five model parameters.
- The most significant second-order interaction terms are:  $S_{B\psi} = 0.169$ ,  $S_{\theta_a\psi} = 0.14$ ,  $S_{B\theta_a} = 0.074$ . The SDP estimates also suggest that high-high combinations of such input factors are most responsible for extreme temperature rises. Joining these results with first-order terms, covers about 84% of the total output variance. The remaining part can be

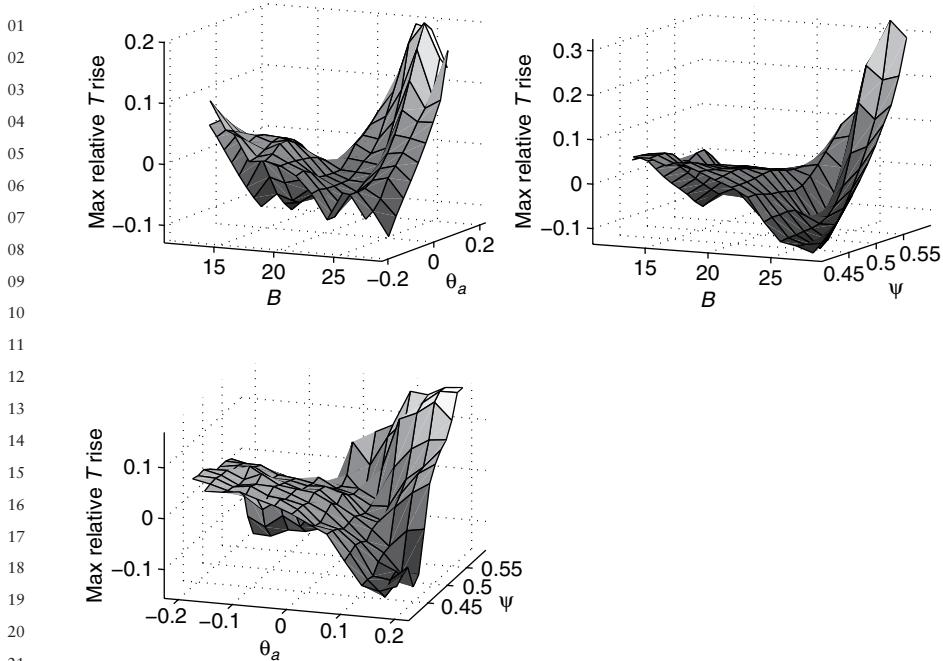


Figure 6.18 Second-order ANOVA-HDMR terms of the maximum relative temperature rise, estimated with the SDP procedure described in Chapter 5

attributed to higher interactions involving the most relevant group of factors ( $B, \theta_a, \psi$ ) as well as  $\gamma$  which has a nonnegligible total effect.

- The first-order ANOVA-HDMR terms of the ‘maximum relative temperature rise’ for the three most important parameters show that the first-order relationships are monotonic, which explains why  $\beta_i^2$  give an acceptable estimate of the sensitivities.

## 6.4 EXAMPLE 4: A MIXED UNCERTAINTY-SENSITIVITY PLOT

### 6.4.1 In Brief

As a last example, we treat a mixed uncertainty–sensitivity plot that might be meaningful to particular audiences and which could be used to convey information on the impact of changes in an influential factor on an output of interest. This resembles the one-at-a-time (OAT) type of sensitivity analysis discussed in Chapter 3.

The example is taken from a study on clearing and settlement (Schulze and Baur, 2006, p. 18), published on the European Commission Directorate General Internal Market website. Without entering into the details of the model, we focus on the impact of a single input factor (i.e. the trading costs) on an output of interest (i.e. GDP in the European Union). To demonstrate that trading costs are highly influential on GDP, the authors calculated the changes in GDP due to changes in trading costs, considering different mean values for the trading costs in the range 0–30% (in steps of 2.5%). A coefficient of variation of 30% is assumed for each mean value. Their plot, presented in Figure 6.19, showed that GDP increases strongly with higher reductions in trading costs, but so do the confidence bounds. For example, the average change in the level of GDP in the case of a 7% reduction in trading costs is 23 billion (with a 95% confidence interval: [8 billion, 47 billion]). Higher reductions in trading costs, e.g. of about 18%, could lead to a change in the level of GDP of 63 billion (95% confidence interval: [20 billion, 124 billion]).

This type of graph can serve a dual purpose. On one hand, it can be used to present the results of an uncertainty analysis, in which confidence bounds are estimated for an output of interest, such as GDP. On the other hand, it can show the results of a sensitivity analysis, revealing how a crucial uncertain factor (the percentage reduction in trading cost) can clearly

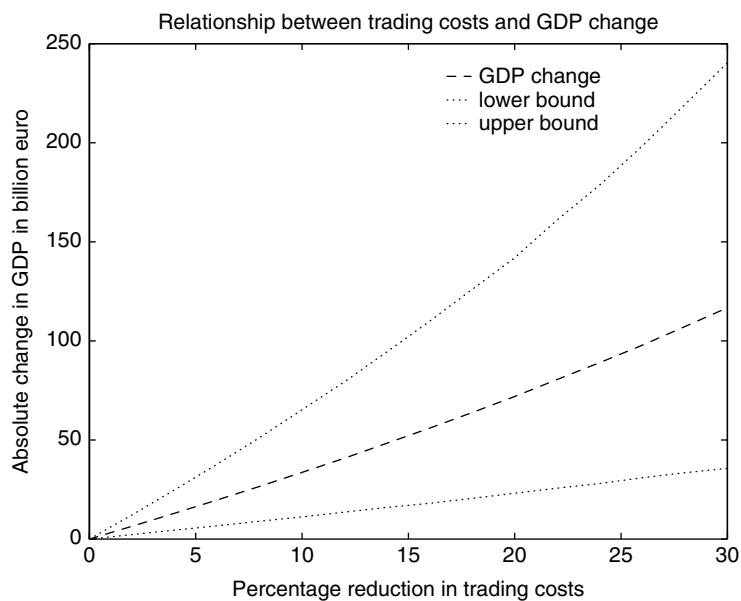


Figure 6.19 A mixed uncertainty-sensitivity analysis plot

influence the output of interest (GDP), taking account of the uncertainty in the other factors. Though very simple, this analysis helped the stakeholders to hold a well-structured negotiation on the estimated benefit of a possible reduction in trading cost.

## 6.5 WHEN TO USE WHAT?

The choice of the proper sensitivity analysis technique depends on such considerations as:

- the computational cost of running the model;
- the number of input factors;
- features of the model (e.g. linearity);
- the consideration of interactions among the input parameters in the model;
- the setting for the analysis and its audience.

Table 6.9 summarizes the explanations using these characteristics as discriminating criteria. These indications are not to be taken as a prescription. More than one method might be applicable to the same context. In choosing among the various methods based upon the cost of a single simulation (row: ‘CPU time (per run)’) we have assumed a single computing unit (no parallel computing) and a maximum computing time between two and three days (having in mind a typical weekend-long simulation).

For models that require a modest amount of CPU time (i.e. up to the order of one minute per run), and with a number of input factors which does not exceed, for example, 20, the class of variance-based techniques (Sobol’ method) yields, convergence aside, the most complete and general pattern of sensitivity. The implementation of Saltelli (2002) (very easy to code and with numerical recipes given in Chapter 4) provides all the pairs of first-order and total indices at a cost of  $(k+2)N$  model runs, where  $k$  is the number of factors and  $N$  is the number of rows of the matrices  $\mathbf{A}$  and  $\mathbf{B}$ . Typically  $N \approx 500 \div 1000$ . To give an idea of the order of magnitude of the computational requirement: for a model with 10 factors and half a minute of CPU per run, a good characterization of the system via  $S_i$  and  $S_{T_i}$  can be obtained at a cost of about 50 h of CPU. Moreover, any single interaction term can be easily computed at the additional cost of  $N$  model evaluations per sensitivity index, if desired. The Sobol’ method does not rely on any assumption about smoothness of the input–output mapping; it only relies on square-integrability of  $Y$ . This is both a strength and a weakness, since it implies a quite slow convergence rate of the estimator. The main drawback of this method is therefore in the computational cost, which depends on

**Table 6.9** When to use what. Note that these indications are not to be taken as a prescription. More than one method might be applicable to the same context. In choosing among the various methods based upon the cost of a single simulation (row: CPU per run) we have assumed a single computing unit (no parallel computing) and a maximum computing time between two and three days (having in mind a typical weekend-long simulation)

	<i>Chapter 1</i>	<i>Chapter 1</i>	<i>Chapter 2</i>	<i>Chapter 3</i>	<i>Chapter 4</i>	<i>Chapter 5</i>	<i>Chapter 5</i>
Characteristic	$\beta_i^2$	Scatterplots	Fractional factorial	Elementary effects	Variance based	Metamodelling	Monte Carlo filtering
Coping with nonlinearity	No <sup>a</sup>	Yes	Yes	Yes	Yes	Yes	Yes
Coping with interactions	No	Yes	Yes	Yes	Yes	Yes	Yes
Samples taken from	Distributions	Distributions	Levels	Levels	Distributions	Distributions	Distributions
Number of input factors	< 100	< 10	> 100 <sup>(b)</sup>	20–100 <sup>b</sup>	< 20 <sup>(b)</sup>	20–100	< 20
CPU time per run	1 min–1 h	< 1 h	< 10 h	< 1 h	< 1 min	< 1 h	< 1 h
Cost of analysis	500–1000	1000	$k \div 2k$ (FF)	$r(k+1)$	$N(k+2)$ (Saltelli, 2002)	100–1000	500–2000
(number of runs)			$N < k$ (supersat. FF)		$N$ (RBD)		
Setting for SA	FP	FM	FF	FF	FP, FF, VC	FP, FM	FM

*k*: number of factors.

*N*: typically  $N \approx 500 \div 1000$ .

*r* is generally set to  $r \approx (4 \div 10)$  and corresponds to the number of the trajectories.

FP: Factor prioritization; FF: Factor fixing; VC: Variance cutting; FM: Factor mapping.

Notes:

<sup>a</sup> Recommended when  $R^2 \geq 0.7$ . In its ranked transformed version it can be quite effective for *monotonic* models, irrespective of their degree of nonlinearity.

<sup>b</sup> Treating *groups* of factors would allow to treat problems of higher dimensionality.

01 the dimension  $k$  of the problem and in the relatively large  $N$  required for a  
02 reasonable accuracy of the sensitivity estimates.

03 When using Saltelli's recipe, we make use of quasi-random numbers to  
04 generate the sample matrices  $A$  and  $B$  (see Chapter 4) for the analysis. These  
05 are sequences of multidimensional points characterized by the property of  
06 'optimal' space filling (see Chapter 2). When the input factors are correlated  
07 an ad hoc computational scheme must be adopted (see the brief discussion  
08 in Chapter 1).

09 The method based on random balance design (RBD) provides only first-  
10 order indices. However, the method has the advantage of running a full  
11 analysis at a cost of  $N$  model runs, i.e. independent on the number of input  
12 factors  $k$ . At a given computational cost, RBD yields first-order estimates  
13 at higher accuracy than Saltelli (2002) (see comparison tests in Tarantola  
14 et al., 2006). In addition, RBD is very easy to code (see the few-line Matlab  
15 script in Chapter 4).

16 A cheaper alternative to the variance-based methods are the standardized  
17 regression coefficients,  $\beta_i$ . With a single batch of  $N$  sampled points (e.g.  
18  $N \approx 500 \div 1000$  points or fewer depending on the cost of the model) the  
19  $\beta_i$  and their rank transformed version can be estimated for all the input  
20 factors. The  $\beta_i$  are only effective for linear or quasi-linear models, i.e. for  
21  $R^2 \geq 0.7$ . Regression methods, also implemented in SIMLAB, are always  
22 useful to look at when investigating the degree of linearity of the model.

23 As discussed in Chapter 5, metamodelling techniques, like the SDP  
24 approach, can be applied successfully to produce both truncated ANOVA-  
25 HDMR decompositions up to third order as well as the relative sensitivity  
26 indices at the same cost of  $\beta_i$ . This strongly reduces the cost of the sensitivity  
27 analysis with respect to Saltelli (2002), with extremely reliable estimates  
28 of the full set of main effects at very small sample sizes ( $N = 250 \div 500$ ).  
29 The strongly improved convergence rate of metamodelling techniques with  
30 respect to the classic Sobol' method is due to their reliance of smoothness  
31 assumptions about  $Y$ . However, accurate estimates of the total effect are  
32 problematic in the metamodelling approach, unless the model has a small  
33 number of interaction terms of very small order, i.e. when the truncated  
34 ANOVA-HDMR covers 100% of the model output  $Y$ .

35 When the CPU time increases (up to, for example, 10 minutes per run),  
36 or the number of factors increases (e.g. up to 100), the EE method offers  
37 the best result. The number of sampled points required is  $r(k+1)$  where  $r$   
38 is generally set to  $r \approx (4 \div 10)$  and  $k$  the number of input factors. To give  
39 an example, with 80 factors and 5 minutes CPU time per run, all the model  
40 outputs can be ready in 27 hours if  $r = 4$  is taken. The EE method produces  
41 good proxies to variance-based total effects, thus allowing us to efficiently  
42 complement a metamodelling exercise.

43 When the number of input factors and/or the CPU time is even so large  
44 as to preclude the use of a screening method, then supersaturated fractional

01 factorial designs, where factors are iteratively perturbed in batches, can be  
02 used (see the discussion in Chapter 2). However, these methods preclude  
03 an effective exploration of the space of the inputs, as they mostly operate  
04 at very few factor levels and require strong assumptions of the model's  
05 behaviour.

06 Sensitivity analysis is also driven by the setting. When the purpose of the  
07 analysis is to prioritize factors, the first-order sensitivity indices  $S_i$  (or the  
08 standardized regression coefficients) have a good argument. If the objective  
09 is to fix noninfluential factors, then the total sensitivity indices  $S_{T_i}$ , or  
10 equivalently the EE method, come into use. If a particular region in the  
11 space of the output (e.g. above or below a given threshold) is of interest,  
12 then Monte Carlo filtering and associated methods can be tried alternatively  
13 or complementarily to the measures just mentioned. If the purpose of the  
14 analysis is a detailed mapping of the input–output relationship, then various  
15 types of metamodeling techniques can be successfully applied.

16 The reader of the present textbook may expect new developments in the  
17 computation of the important measure and screening texts described here.  
18 Ongoing research both on sampling strategies (thereby using true model  
19 points to map the space of the input) as well as metamodel/emulators  
20 (producing estimates of model output at untried points) is being intensively  
21 carried out by practitioners.

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## Afterword

12 The authors of the book hope that readers will find the tools of global  
13 sensitivity analysis presented here useful. As discussed in the introduction,  
14 these methods have been conceived to help avoid type II errors resulting  
15 from a poor (or wholly omitted) exploration of the space of the input factors  
16 or from neglecting the interaction between different system factors and/or  
17 compartments.

18 We have also stressed the need to consider more than just the uncertain  
19 factors or the measurement errors in the input data included in the model.  
20 Although the tools discussed in the book are capable of handling what we  
21 could call ‘technical’ uncertainty, they can also be used to tackle additional  
22 layers of epistemic uncertainty.

23 A model, being a human representation of a given problem, necessarily  
24 reflects the perceptions, values and interests of those concerned with struc-  
25 turing the issue being modelled. Whenever relevant, a sensitivity anal-  
26 ysis should incorporate these social and cultural dimensions. Post-Normal  
27 Science (PNS), as discussed in the introduction, offers some guidance as to  
28 when ‘extended peer community’ methods are advisable.

29 Clearly, modelling is subject to an unprecedented level of critique at  
30 present, not only from postmodern philosophers but also from intellectuals  
31 and scientists of diverse political tendencies. In his novel *State of Fear*,  
32 Michael Crichton writes:

33 If you read some author who says ‘We find that anthropogenic greenhouse gases  
34 and sulphates have had a detectable influence on sea-level pressure’ it sounds  
35 like they went into the world and measured something. Actually, they just run a  
36 simulation. They talk as if simulations were real-world data. They’re not. That’s a  
37 problem that has to be fixed. I favor a stamp: **WARNING: COMPUTER SIMU-**  
38 **LATION – MAY BE ERRONEOUS AND UNVERIFIABLE.** Like on cigarettes  
39 [⋯⋯⋯]. (Crichton, 2004, p. 556)

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

01 It is indeed a sign of the times that statements about the veracity of  
02 computational models can now be found on books belonging more on our  
03 bedside tables than on our desks.

04 A common fallacy in the use of computation models is – in the opinion  
05 of the authors – the idea that increasing the level of detail of a model must  
06 in general improve its pedigree.

07 An example discussed in Pilkey and Pilkey-Jarvis (2007) concerns  
08 the Yucca Mountain repository for radioactive waste disposal, where a  
09 very large model called TSPA (Total System Performance Assessment) is  
10 employed to guarantee the safe containment of waste. Composed of 286  
11 submodels, TSPA (as with any other model) is based on assumptions – a  
12 crucial one being the low permeability of the geological foundation and  
13 hence the extensive period of time needed for the water to percolate from  
14 the desert surface to the level of the underground disposal. However, the  
15 confidence of stakeholders in TSPA was not strengthened by the recent  
16 production of evidence to suggest that an upward revision of the value of  
17 this parameter by four orders of magnitude might be necessary.

18 Many people will take exception to the works just cited. Yet it cannot  
19 be denied that a paradigm shift has taken place. As discussed in Chapter 1,  
20 stakeholders and media alike will increasingly tend to suspect, or even  
21 expect, the instrumental use of computational models and the amplification  
22 or suppression of uncertainty for the sake of expedience (Michaels, 2005).

23 A global sensitivity analysis might serve variously the friends *and* the foes  
24 of a given model as applied to a particular issue, that is, both the modellers  
25 and the critics of the model. Yet there is no magic formula – a sensitivity  
26 analysis may reveal to which assumptions a model is more sensitive but say  
27 nothing about the defensibility of these assumptions. In the case of TSPA a  
28 range of 0.02–1 mm per year was used for percolation of flux rate. Applying  
29 the methods of this book to TSPA might or might not identify this as a  
30 crucial factor, but this information would be of scant use if the value of the  
31 percolation flux were later found to be of the order of 3000 mm per year.  
32 In other words, sensitivity analysis may not guard against type III errors,  
33 that is, a wrong framing of the analysis.

34 Have models fallen from grace, and is modelling – when applied to major  
35 environmental issues of the PNS type – just ‘useless arithmetic’, as claimed  
36 by Pilkey and Pilkey-Jarvis (2007)?

37 The crux of the matter is that, 15 years after Konikof and Bredehoeft  
38 proclaimed that ‘groundwater models cannot be validated’ (Konikov and  
39 Bredehoeft, 1992) and Naomi Oreskes wrote her sober reminder of the  
40 limits to validation of computational models in environmental systems  
41 (Oreskes *et al.*, 1994), the modelling community still lacks accepted quality  
42 criteria for assessing model’s adequacy (Van der Sluijs, 2002).

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