Sensitivity Analysis

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What is Sensitivity Analysis?

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1.1 INTRODUCTION

Sensitivity analysis (SA) is the study of how the variation in the output of a model (numerical or otherwise) can be apportioned, qualitatively or quantitatively, to different sources of variation, and of how the given model depends upon the information fed into it. On this basis, we contend that SA is a prerequisite for model building in any setting, be it diagnostic or prognostic, and in any field where models are used.

Models are developed to approximate or mimic systems and processes of different natures (e.g. physical, environmental, social, or economic), and of varying complexity. Many processes are so complex that physical experimentation is too time-consuming, too expensive, or even impossible. As a result, to explore systems and processes, investigators often turn to mathematical or computational models.

A mathematical model is defined by a series of equations, input factors, parameters, and variables aimed to characterize the process being investigated. Input is subject to many sources of uncertainty including errors of measurement, absence of information and poor or partial understanding of the driving forces and mechanisms. This imposes a limit on our confidence in the response or output of the model. Further, models may have to cope with the natural intrinsic variability of the system, such as the occurrence of stochastic events.

Good modelling practice requires that the modeller provide an evaluation of the confidence in the model, possibly assessing the uncertainties associated with the modelling process and with the outcome of the model itself.

Originally, SA was created to deal simply with uncertainties in the input variables and model parameters. Over the course of time, the ideas have been extended to incorporate model conceptual uncertainty, i.e. uncertainty in model structures, assumptions, and specifications. As a whole, SA is used to increase the confidence in the model and its predictions, by providing an understanding of how the model response variables respond to changes in the inputs, be they data used to calibrate it, model structures, or factors, i.e. the model-independent variables. SA is thus closely linked to uncertainty analysis (UA),

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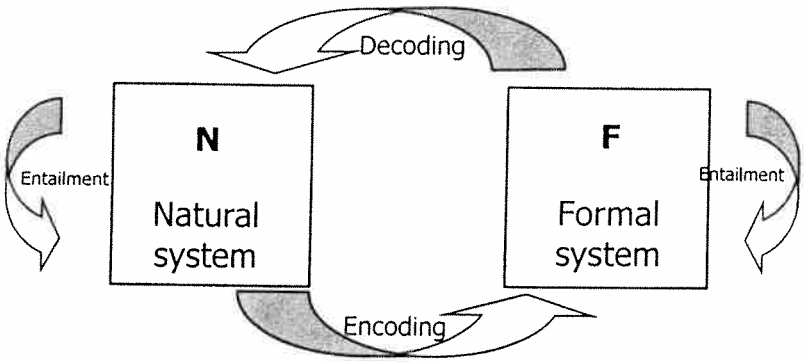

Figure 1.1 Formalization of the modelling process taken from Rosen (1991).

which aims to quantify the overall uncertainty associated with the response as a result of uncertainties in the model input. In this book, we shall, however, focus on SA.

All of the above might be summarized by the following loose definition of SA:

Definition *Sensitivity analysis studies the relationships between information flowing in and out of the model*

For the definition we have taken inspiration from Rosen's (1991) formalisation of the modelling activity (Figure 1.1), where the link between a model (driven by a formal entailment structure) and the world (driven by different classes of causality) is the process of 'encoding' (from world to model) and 'decoding' (from model to world). Encoding and decoding are not themselves 'entailed' by anything, i.e. they are the object of the modeller's craftsmanship. Yet those two activities are the essence and the purpose of the modelling process, i.e. one writes a model in the hope that the decoding operation will provide insight into the world. This is only possible, in our view, if the uncertainty in the information provided by the model (the substance of use for the decoding exercise) is carefully apportioned to the uncertainty associated with the encoding process.

In the remaining part of this introductory chapter, we shall briefly describe why, how and when to perform SA.

1.2 AN EXAMPLE

Having compromised ourselves with a definition of SA, we may now proceed to offer an example that illustrates different ways of measuring sensitivity. We start by highlighting the importance of what one uses to *measure* sensitivity.

Consider a model for a dry-cleaning bill,

$$C = \sum_i C_i, \tag{1.1}$$

where the total cost on the bill, C, equalling the sum of the individual costs of the items laundered, C_i, may be strongly influenced by an individual item (the cost of a fur present in the selection of items, say). One measure of sensitivity may tell us that the *variation* in the total cost C is equally sensitive to all items in the sample. This would be the case if the

sensitivity of an item were taken to be the derivative of the total bill with respect to the cost of a single item in the bill, i.e.

$$S_i = \frac{\partial C}{\partial C_i}. \tag{1.2}$$

Here the derivative is computed at a point $C^0 = (C_1^0, C_2^0, \ldots)$, i.e. a point where all the C_i are fixed to some reference value C_i^0 (the term 'nominal value' is often used). In other words, the quantity S_i is the local sensitivity index measuring the effect on C of perturbing C_i around a reference or central value C^0. In this case, S_i is equal to one for all items.

Another choice of sensitivity measure would explore what happens to the total cost if all the items in the sample are allowed a finite variation in cost. The derivative above could be normalized by the mean of output (the total cost) and input (the cost of the item). The sensitivity index would then measure the effect on C of perturbing C_i by a fixed fraction of C_i's reference value (C_i's mean value, in this case), i.e.

$$S_i = \frac{\partial C}{\partial C_i}\frac{C_i^0}{C^0}, \tag{1.3}$$

and the cost of the most expensive item, i.e. the fur, would be *measured* as the most influential factor. Alternatively, the sensitivity index could measure the effect on C of perturbing C_i by a fixed fraction of C_i's standard deviation, i.e.

$$S_i = \frac{\partial C}{\partial C_i}\frac{\mathrm{std}(C_i)}{\mathrm{std}(C)}. \tag{1.4}$$

If the standard deviations were equal, all items would again be judged to be equally important in determining the variation of the bill. If, more realistically, the standard deviations were different, e.g. higher standard deviations were associated with higher mean values, the cost of the fur would again be identified as the most influential factor.

SA is not concerned with what causes the output of the model to be what it is, but what the sources of variation in that output are. Using the measures defined by (1.4), the cost of the fur is found to be the predominant factor only if it drives most of the variation in the total cost. If we use the sensitivity measures defined by (1.2) then the cost of the fur is as important as all other factors, even if it contributes predominantly to the total cost. The purpose of this discussion on the measure is to highlight that the type of measure employed, selected on the basis of the context or use one desires to make of SA, has a direct consequence on the outcome of the analysis. Different measures have different uses and applications, and a universal recipe for measuring sensitivity does not exists. Good practice should instead be our goal, and this is the subject of the present volume.

1.3 WHY CARRY OUT A SENSITIVITY ANALYSIS?

In the context of numerical modelling, SA means very different things to different people (compare the reviews by Turanyi (1990a), Janssen *et al.* (1990), Helton (1993), and Goldsmith (1998)). For a reliability engineer, SA could be the process of moving or changing components in the design of a plant to investigate how a fault tree analysis for that plant would change. For a chemist, SA could be the analysis of the strength of the relation between kinetic or thermodynamic inputs and measurable outputs of a reaction system. For a

software engineer, SA could be related to the robustness and reliability of the software with respect to different assumptions. For an economist, the task of SA could be to appraise how stable the estimated parameters of a model (customarily derived via regression) are with respect to all factors that were excluded from the regression, thus ascertaining whether parameter estimation is robust or fragile. For a developer of expert systems, it is important to measure sensitivity with respect to the quantiles of the 'prior' distributions. For a statistician, involved in statistical modelling, sensitivity analysis is mostly known and practised under the heading of 'robustness analysis'. Statisticians are mostly interested in 'distributional robustness', intended as insensitivity with respect to small deviations from the assumptions about the underlying distribution assumed for the data (Huber, 1981a).

These different types of analyses have in common the aim to investigate how a given computational model responds to variations in its inputs. Modellers conduct SA to determine:

(a) if a model resembles the system or processes under study;
(b) the factors that mostly contribute to the output variability and that require additional research to strengthen the knowledge base;
(c) the model parameters (or parts of the model itself) that are insignificant, and that can be eliminated from the final model;
(d) if there is some region in the space of input factors for which the model variation is maximum;
(e) the optimal regions within the space of the factors for use in a subsequent calibration study;
(f) if and which (group of) factors interact with each other.

Under (a), the model does not properly reflect the processes involved if it exhibits strong dependence on supposedly non-influential factors or if the range of model predictions is not a sound one. In this case, SA highlights the need to revise the model structure. It often happens that the model turns out to be highly tuned to a specific value of a factor, up to the point that necessary changes, e.g. resulting from new evidence, lead to unacceptable variation in the model predictions. When this happens, it is likely that in order to optimize the simulation, some parameter values have been chosen incorrectly. This reflects lack of conceptual understanding of the role of the parameters in the system.

Under (b), SA can assist the modeller in deciding whether the parameter estimates are sufficiently precise for the model to give reliable predictions. If not, further work can be directed towards improved estimation of those parameters that give rise to the greatest uncertainty in model predictions. If the model sensitivity seems congruent with (i.e. does not contradict) our understanding of the system being modelled, SA will open up the possibility of improving the model by prioritizing measurement of the most influential factors. In this way, the impacts of measurement errors on computational results can be minimized.

Under (c), we mean insignificant in the sense of 'not affecting the variation of the output'; this concept is taken up at the end of the book, where we discuss the 'relevance' of models. According to some investigators, when the model is used in a case of conflicting stakes (e.g. siting a facility or licensing a practice), the model should not be more complex than needed, and factors/processes that are insignificant should be removed.

As far as (e) is concerned, we stress the need for 'global' optimization. One should investigate the space of the factors in its entirety, and not just around some nominal point (see also the Monte Carlo filtering approach mentioned in **Chapters 2** and **21**).

Point (f) is an important technicality: often factors have combined effects that cannot be reduced to the sum of the individual ones. This is relevant, since the presence of an

interaction has implications for all of the above points (calibration, determination of critical points, etc.).

1.4 HOW TO PERFORM SENSITIVITY ANALYSIS?

Anticipating here a notion offered in **Chapter 2**, i.e. that of a sampling-based sensitivity analysis, we try to draft a flow chart for the SA process. A sampling-based SA is one in which the model is executed repeatedly for combinations of values sampled from the distribution (assumed known) of the input factors. The following steps can be identified:

1. Design the experiment (identify what question the model should answer) and determine which of its input factors should concern the analysis.
2. Assign probability density functions or ranges of variation to each input factor.
3. Generate an input vector/matrix through an appropriate design.
4. Evaluate the model, thus creating an output distribution for the response of interest.
5. Assess the influences or relative importance of each input factor on the output variable(s).

The basic steps in a SA are illustrated in Figure 1.2, the process starting in the upper left corner of the diagram.

One starts by defining one or a series of candidate models to answer the question considered, and selecting factors for the analysis (Which factors shall I include? Do I vary all factors?). The output variable(s) are also selected at this time. Distributions must be defined for each uncertain input factor, where 'constant' is just a particular case. When using derivatives as a sensitivity measure (Equation (1.2) above), one apparently does not need this

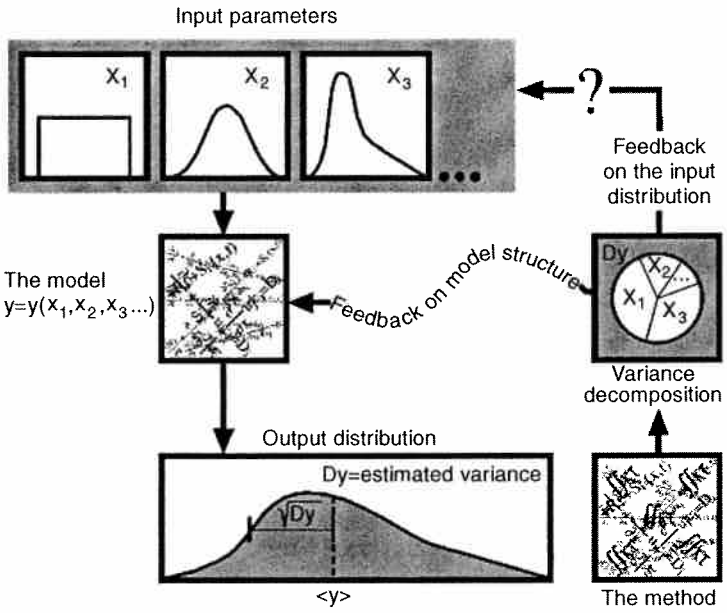

Figure 1.2 A schematic view of sampling-based sensitivity analysis.

step. Nevertheless, when derivatives are evaluated via incremental ratios, a uniform distribution is *de facto* assumed over the small interval selected for the evaluation.

As a rule, SA is performed on a set of factors. A factor could be:

- an input datum (e.g. an uncertain exchange rate);
- the distribution parameter describing some aleatory process (e.g. an unknown frequency rate for earthquakes in a given area);
- a trigger factor, whose value drives the selection of alternative mechanisms (e.g. a linear versus a nonlinear process) or scenarios (different greenhouse gas emission policies).

Factors can be varied one-at-a-time (OAT), all the other factors being held constant. When using random sampling, or experimental designs, several factors can be varied at once. If a correlation structure is specified for the input factors, realizations can be generated from the multivariate input distribution using *ad hoc* sampling procedures.

The sample is fed through the model, i.e. the model is run repeatedly for each realization to obtain an output sample for the variable(s) of interest. This can be used to build an empirical probability distribution for the response variable(s). Means, standard deviations, confidence bounds, cumulative distribution functions, etc. can then be estimated.

So far we have implemented an uncertainty analysis, i.e. we have quantified the variation in the model response. The next step, sensitivity analysis, is the apportioning of the uncertainty according to source (i.e. to the factors).

A possible representation of the results (shown in Figure 1.2) would be a pie chart that partitions the variance of the output. This variance decomposition allows the identification of the influential factors, forming a basis for all the modelling investigations described in the previous section.

As far as the implementation of the analysis is concerned, different formal approaches can be followed, and a very large number of techniques are available in the literature (see the review articles quoted above). SA articles can be found in a large number of journals, and a number of special issues and proceedings are available (JSCS, 1997; RESS, 1997; SAMO, 1998; CPC, 1999). The present volume aims to cover a wide range of techniques, as well as to provide a reference handbook and guide to sensitivity analysis as a discipline. Thus, we attempt a classification of the existing methods (see **Chapter 2**). This has been somehow complicated by the wealth of applications that can be found for SA, and the consequent fact that SA has many different meanings to different people, as discussed.

1.5 GOALS OF SENSITIVITY ANALYSIS

We have mentioned above why one should perform a sensitivity analysis, including model development, verification, calibration, model identification, and mechanism reduction. Without pretension of being exhaustive, we now try to elaborate some of these concepts, and indicate briefly the role SA has to play.

SA can be employed prior to a *calibration* exercise to investigate the tuning importance of each parameter, i.e. to identify a candidate set of important factors for calibration, since the difficulty of calibrating models against field or laboratory data increases with the number of processes to be modelled (and hence the number of parameters to be estimated). This may allow a dimensionality reduction of the parameter space where the calibration/optimization is made. SA can also help to ensure that the problem is not an ill-conditioned one. Quantitative SA methods (i.e. those that tell how much more important

one factor is than another, see **Chapter 2**) can be appropriate when both the model inputs and the available data are affected by uncertainties. The question answered is what factors are allowed to be calibrated and at what confidence, given the data and their uncertainty.

While SA was originally created to deal with the uncertainties in the input factors, recent developments have seen some of the ideas being extended to incorporate structural uncertainty as mentioned above. In this way, SA also touches on the difficult problem of *model quality*[1] and is an important element of judgement for the corroboration, or falsification, of the scientific hypotheses embedded in a model. SA can be used to ensure that the response of the model to its input factors can be accounted for, that the model does not exhibit strong dependence on supposedly non-influential factors and that the range of model predictions is a sensible one.

SA can be an effective tool for *model identification*. By pinpointing experimental conditions in which the ability to discriminate among the various models is a maximum, SA can identify the most appropriate model structures and specifications competing to describe available evidence.

This is closely related to *mechanism reduction*, determining a subset of input factors accounting for (most of) the output variance. This enables the insignificant factors to be identified and eliminated from the final model. In this way, irrelevant parts of the model can be dropped, or a simpler model can be built or extracted from a more complex one (*model lumping*).

The above points have some epistemological implications concerning the 'relevance' of a model (see also **Chapter 21**). It has been argued that often the complexity of models largely exceeds the actual 'requirements'. The view of Oreskes *et al.* (1994) is that models should be heuristic constructs built for a task. They should not be more complex than they need to be. Following this reasoning, a model would be 'relevant' when its input factors actually cause variation in the model response that is the object of the analysis. Model 'irrelevance' would flag a bad model, a model used out of context, or a model unable to provide the answer being sought.

Another possible goal for SA is to determine if there is some region in the space of input parameters for which the model variation is maximum or divergent. This is useful in control theory, where one might also be interested in the initiation of chaotic behavior for some combinations of model parameters.

In the field of risk analysis, the goal of SA is to identify risk-governing parameters. This may help the analyst, especially when he/she has knowledge on the factors that is not explicitly coded in the problem. For example, two factors are given the same uncertainty in input, but the analyst is more confident in (or scared of) one of them. If the dreaded factor turns out to be the risk-governing one, mitigating actions can be taken.

In general, SA can assist the modeller in deciding whether model performance is sufficient to the task, and when this is not the case, to provide guidance as to where to invest to solve the problem.

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[1] Judgements of merit on the quality of a model when applied to a given task are often made on the basis of processes known as verification and validation. Lately the meaning attached to these terms has been very much the subject of debate (see Sheng *et al.* (1993) for a classical system analysis approach, and Konikov and Bredehoeft (1992) and Oreskes *et al.* (1994) for a more radical criticism of these concepts). We shall often use the term 'corroboration', proposed by Oreskes *et al.*, to mean the reinforcement of an hypothesis by means of non-contradiction between the prediction of a model and the evidence, and the term 'falsification' of a hypotheses for the opposite occurrence. We shall try to avoid the terms 'verification' and 'validation' altogether.

1.6 PROPERTIES OF VARIOUS TYPES OF SENSITIVITY ANALYSIS TECHNIQUES

The choice of which SA method to adopt is difficult, since each technique has strengths and weaknesses. Such a choice depends on the problem the investigator is trying to address, on the characteristics of the model under study, and also on the computational cost that the investigator can afford.

One possible way of grouping sensitivity analysis methods is into three classes: *screening methods, local SA methods* and *global SA methods*. This distinction is somewhat arbitrary, since screening tests also can be viewed as either local or global. Further, the first class is characterized with respect to its use (screening), while the other two are characterized with respect to how they treat factors.

1.6.1 Screening

In dealing with models that are computationally expensive to evaluate and have a large number of input parameters, *screening experiments* can be used to identify the parameter subset that controls most of the output variability (with low computational effort). This is based on the experience that often only a few of the input parameters have a significant effect on the model output. As a drawback, these 'economical' methods tend to provide qualitative sensitivity measures, i.e. they rank the input factors in order of importance, but do not quantify how much more important a given factor is than another. In contrast, a quantitative method would give, for example, the exact percentage of the total output variance that each factor (or group of factors) is accounting for. There is clearly a trade-off between computational cost and information.

1.6.2 Local SA

Local SA concentrates on the local impact of the factors on the model. Local SA is usually carried out by computing partial derivatives of the output functions with respect to the input variables. In order to compute the derivatives numerically, the input parameters are allowed to vary within a small interval of fractional variation around a nominal value.[2] The interval is usually the same for all of the variables and is not related to our degree of knowledge of the variables. Present-day computational tools for local SA allow large numbers of sensitivity coefficients to be computed simultaneously. This is often used to solve a so-called 'inverse problem', e.g. how to back-calculate the value of kinetic constants for reactions whose output are not directly measurable, based on the concentration of end-products further down the reaction pathway (Rabitz, 1989). One can see local SA as a particular case of one-factor-at-a-time (OAT) approach, since when one factor is varied, all others are held constant.

Local methods are less helpful when SA is used to compare the effect of various factors on the output, as in this case the relative uncertainty of each input should be weighted. This can be achieved by some kind of differential analysis, where an incremental ratio is considered. As an example, in Capaldo and Pandis (1997), the target sensitivity measure is

$$S_i = \frac{x_i}{y}\frac{\partial y}{\partial x_i},$$

[2] This is not true if a 'direct' solution method is used, see Chapter 5, p. 83.

i.e. the effect on the relative variation of y of perturbing x_i by a fixed fraction of x_i's central value. S_i is estimated by

$$\hat{S}_i = \frac{\ln y - \ln y_b}{\ln x_i - \ln x_{ib}},$$

where the subscript b indicates a baseline value and x_i a generic input factor. Each of the x_i is then given a different variation between the baseline and a 'sensitivity test value'. This approach is practicable when the variation around a baseline of the input variables is small, since in general it allows the input–output relationship to be assumed linear. Sometimes, the range of variation is taken as identical for all the variables (e.g. $\pm 5\%$ of the nominal value in Falls *et al.*, 1989), and the relative importance of the input parameters is thus assessed. We should nevertheless advise against this practice unless the model is known in advance to be linear. It has been recognized in the literature for a number of years (Cukier *et al.*, 1973) that when the model is nonlinear and various input variables are affected by uncertainties of different orders of magnitude, a global SA method should be used.

1.6.3 Global SA

Global SA techniques have been discussed by Cukier *et al.* (1978), Iman and Helton (1988), Sobol' (1990b), Helton *et al.* (1991), and Saltelli and Homma (1992), among others. For a review of applications of global variance-based sensitivity analysis techniques, see Saltelli *et al.*, 2000. Global SA apportions the output uncertainty to the uncertainty in the input factors, described typically by probability distribution functions that cover the factors' ranges of existence. The ranges are valuable, since they represent our knowledge or lack of it with respect to the model and its parameterization. More specifically, we should define global methods by the following two properties:

First global property: The inclusion of influence of scale and shape *The sensitivity estimates of individual factors incorporate the effect of the range and the shape of their probability density functions.*

Second global property: Multidimensional averaging *The sensitivity estimates of individual factors are evaluated varying all other factors as well.*

A global SA technique thus incorporates the influence of the whole range of variation and the form of the probability density function of the input. A global method evaluates the effect of x_i while all other $x_j, j \neq i$, are varied as well. In contrast, the local perturbative approach is based on partial derivatives, the effect of the variation of the input factor x_i when all other $x_j, j \neq i$, are kept constant at their central (nominal) value.

1.7 CHOICE OF METHODS

An important property to consider when choosing which SA technique to employ, is the following:

Model independence property *The level of additivity or linearity of the model does not influence the accuracy of the method.*

Not all SA methods are model-independent. A Monte Carlo analysis coupled with a linear regression can provide useful insight into the relative influence of factors when these relate linearly to the output of interest. Differential analysis can be used with caution when the range of variation of the factors is small. Some methods for SA are fairly inexpensive but perform poorly for nonlinear, non-additive models. The choice of the method for a particular application is discussed in detail in **Chapter 2**.

Further important properties of SA methods will be introduced in **Chapter 8** when discussing the variance-based approaches. These touch on the capacity of a method to account for factor-to-factor interactions, the possibility to group factors into sets and to treat each set as a factor, and computational efficiency.

1.8 ABOUT THE CHAPTERS AHEAD

The book is divided into *Introduction, Methods, Applications,* and *Conclusions,* and is not meant to be read from start to finish. The reader should feel free to skip those sections not immediately relevant, and jump to the parts in which he/she is interested or which are relevant for the specific problem at hand. The hurried reader could simply read **Chapter 2** for the most appropriate tool to solve a problem, and jump to the chapter where the tool is described.

Part I: Introduction

Following this introductory chapter is **Chapter 2**: *Hitchhiker's Guide to Sensitivity Analysis,* where, as the title suggests, we offer a sort of simplified tourist guide to SA. It is composed of a summary description of the various methods with elements of evaluation and comparison, suggesting the most appropriate methods for different settings. This chapter is useful for the reader needing brief descriptions and a pointer to find the chapter most useful for his/her problem. It includes several different analytical functions used as test models throughout the book.

Part II: Methods

This section is devoted to more detailed descriptions of the SA methodologies. In **Chapter 3** we review briefly the theory of experimental design. In **Chapter 4**, we take a look at *Screening Methods,* including the methods of Morris, Cotter, and others. **Chapter 5** offers a description of *Local Methods,* including the adjoint method and the use of functional sensitivities. In **Chapter 6**: *Sampling-Based Methods,* a description is given of the various Monte Carlo-based sensitivity analyses. These include scatterplots, correlation, and regression analysis. Also described are the sampling techniques on which these are based. **Chapter 7**: *Reliability Algorithms: FORM and SORM* deals with sensitivity analysis for risk analysis, with a thorough description of the FORM and SORM methods. **Chapter 8** introduces *Variance-Based methods,* including Sobol' indices, FAST and extended FAST. **Chapter 9**: *Managing the Tyranny of Parameters in Mathematical Modelling of Physical Systems* presents a generalized model decomposition scheme (high-dimensional model replacement, HDMR) whose application to SA appears promising. **Chapter 10** gives a review of *Bayesian Sensitivity Analysis.* **Chapter 11** describes how *Graphical Methods,* such as cob-webs, can be employed.

Part III: Applications

The third section is more practically oriented. If the reader has a specific problem at hand, this section can give useful hints about what to use and how to implement the analysis. **Chapter 12** is an introduction to the Applications Section. It describes the modelling process from formulation of objectives, model building, development, and use. The following chapters give examples of specific uses. **Chapter 13** shows how to use SA to treats model and scenario uncertainty. **Chapter 14** is an *application of UA, SA to modelling time series*, and also includes a relevant application to model uncertainty. **Chapter 15** is an example of a dataless precalibration analysis in solid state physics (how SA can be used prior to calibration). **Chapter 16** is an application of the FORM method to a hydrogeological problem. **Chapter 17** offers one-at-a-time (OAT) and global analyses for interpreting air quality model predictions, with an interesting study of the interplay between system uncertainty and regulatory targets. **Chapter 18** is a comparison of *different SA methods on a chemical reaction model.* **Chapter 19** is an *application to logistic equations and population dynamics*; both **Chapters 18** and **19** show applications of SA in the model building process. **Chapter 20** deals with SA used to assess the quality of models used for environmental policy, and is interesting in its way of discriminating among uncertainties in the data versus uncertainty in the indicator building process.

Part IV: Conclusions

The final section rounds off the book by considering the epistemological aspects of SA. **Chapter 21**: *Assuring the Quality of Models Designed for Predictive Tasks* is a discussion of the scientific method in the context of model validation, including a description of generalized sensitivity analysis (GSA). The final **Chapter 22** is dedicated to the *Fortune and Future of SA*, and tries to probe some of the issues touched in the present introduction, such as model transparency and model relevance. It also offers an epistemic perspective of SA as an ingredient of the modelling process.

The Appendix

This aims to give an overview of some specialized SA software. It does not provide in-depth information about the software, but gives a brief description and a guide to where and how to obtain it.