The Propagation and Analysis of Uncertainty

8.1. Introduction

Suppose we have constructed a model to predict the consequences of various possible events and decisions. And suppose further we have identified various uncertainties in the inputs. How can we propagate these uncertainties through the model to discover the uncertainty in the predicted consequences? If the uncertainties are substantial, we may not immediately be able to make definitive recommendations about what decision is “best.” But we should be able to obtain useful insights about the relative importance to our conclusions of the various assumptions, decisions, uncertainties, and disagreements in the inputs. These can help us decide whether it is likely to be worthwhile gathering more information, making more careful uncertainty assessments, or refining the model, and which of these could most reduce the uncertainty in the conclusions. In this chapter, we examine various analytic and computational techniques for examining the effects of uncertain inputs within a model. These include:

- methods for computing the effect of changes in inputs on model predictions, i.e., sensitivity analysis,
- methods for calculating the uncertainty in the model outputs induced by the uncertainties in its inputs, i.e., uncertainty propagation, and
- methods for comparing the importance of the input uncertainties in terms of their relative contributions to uncertainty in the outputs, i.e., uncertainty analysis.

A considerable variety of such methods have been developed, with wide differences in conceptual approach, computational effort required, and the power of their results. When developing and analyzing a particular model, it can be difficult to decide which of these methods are most appropriate for the problem at hand. There have been a number of discussions and comparisons of these techniques in the literature (Cox, 1977; Ahmed, Metcalf, and Pegram, 1981; Cox and Baybut, 1981; Jackson, Hokenbury, and Yeater, 1981; Martz et al., 1983; Fiksel, Cox, and Ojha, 1984; Whitfield and Newsom, 1984; Iman and Helton, 1988). But they seem to have come to dismayingly divergent conclusions about the relative merits of these techniques. This can be at least partly explained by the differences among the kinds of models and problems each study was concerned with. Clearly no one method is always best; the choice should depend on both the nature of the problem and the resources available to the analyst. In this chapter, our objective is to provide an introduction and general review of the principal techniques, an assessment of their relative advantages and disadvantages, and some guidance on how to select techniques appropriate to particular situations.

8.2. Basic Concepts

Before turning to a more detailed review of these techniques, we introduce and illustrate some of the basic concepts using a simple example. Readers who are interested in only an introduction to the general arguments, without the details necessary for actual use, may wish to read this section, then skip to the final section on selecting a method. Students, practitioners, and users of analysis will find details about specific methods in the intervening sections.

Consider a model represented as a function, $f$, with two uncertain inputs, $x_1$ and $x_2$, and one output, $y$.

$$y = f(x_1, x_2)$$

We will assume both uncertain inputs are empirical quantities, that is, measurable, at least in principle, and so uncertainty about them can legitimately be represented by probability distributions.

Figure 8.1 shows a perspective drawing of such a function. The two inputs are represented by the two horizontal dimensions, and the output is represented by the vertical dimension. The surface displays directly how the value of $y$ changes with variations in the values of its inputs, and is sometimes termed a response surface.
A scenario is a particular situation, specified by a single value for each input variable. It defines a single point on the response surface. We can describe a scenario as a vector of values for the inputs, for example:

\[ X = (x_1, x_2) \]

Let us start by defining a nominal or "base-case" scenario, which consists of a single nominal value for each input. These are our initial "best guess" values for the inputs. Each might be the mean, median, or most likely (i.e., mode) values of the full probability distribution. But usually we will choose them before thinking much about the entire range or distribution. Indeed, we may never even get as far as assessing the full distribution.

Let us denote these nominal input values \( x_1^0 \) and \( x_2^0 \). Together these two input values specify the nominal scenario:

\[ X^0 = (x_1^0, x_2^0) \]

The corresponding nominal output value is defined as:

\[ y^0 = f(x_1^0, x_2^0) \]

The analysis of uncertainty involves measuring the degree to which each input \( x \) contributes to uncertainty in the output \( y \). A method to quantify this may be termed a measure of uncertainty importance, which we will denote by \( U(x, y) \). We will define a number of such measures, roughly in order of increasing sophistication. Perhaps the simplest measure of uncertainty importance is sensitivity, that is, the rate of change of the output \( y \) with respect to variation in an input \( x \). The two sensitivities in this case are the partial derivatives, of output \( y \) with respect to each input. These derivatives are evaluated at the values of the nominal scenario, as indicated by the subscript \( X^0 \) after each:

\[ \left[ \frac{\partial y}{\partial x_1} \right]_{X^0} \quad \left[ \frac{\partial y}{\partial x_2} \right]_{X^0} \]

These sensitivities, illustrated in Figure 8.2, are shown as the slopes of the two tangents to the response surface at the nominal scenario, along the two vertical planes parallel to each of the horizontal axes. Thus, we define simple sensitivity as our first measure of uncertainty importance:

\[ U_S(x, y) = \left[ \frac{\partial y}{\partial x} \right]_{X^0} \]

One problem with simple sensitivity for comparing the uncertainty importance of different inputs is that it depends on the scale, or units of measurement, of \( x \) and \( y \). Sensitivity to an input measured in millimeters will be a thousand times greater than sensitivity to the same input measured in meters. It seems desirable that importance measures should be unaffected by the units of measurement. A simple way to achieve this is to normalize the sensitivity, defining the changes in \( x \) and \( y \) in relative terms, as a fraction of their nominal values. The normalized sensitivity is defined as the ratio of the relative change in \( y \) induced by a unit relative change in \( x \) (e.g., the percent change in \( y \) induced by a 1 percent change in \( x \)). This measure of uncertainty importance is sometimes also known as elasticity:

\[ U_E(x, y) = \left[ \frac{\partial y}{\partial x} \right]_{X^0} \times \frac{y^0}{x^0} \]

A drawback of considering only the slopes of the response surface, as do simple sensitivity and elasticity, is that they ignore the degree of uncertainty in each input. An input that has a small sensitivity but a large uncertainty may be just as important as an input with a larger sensitivity but smaller uncertainty. The simplest approach to uncertainty analysis that considers both sensitivity and uncertainty is generally known as first order approximation or, Gaussian
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approximation, after Gauss, who is credited with developing this approach. Let us express the degree of uncertainty in each input \( x \) by its standard deviation, \( \sigma_x \). We can then measure its contribution to the output uncertainty, that is, its uncertainty importance, as the product of its sensitivity and uncertainty, more specifically as the product of the partial derivative and standard deviation:

\[
U_G(x, y) = \left( \frac{\partial y}{\partial x} \right)_{x=x} \sigma_x
\]

(Using subscript \( G \) for Gauss.)

This is appealing because we can use this measure directly for uncertainty propagation, that is, to estimate the uncertainty of the output. The variance of the output, \( \text{Var}[y] \equiv \sigma^2 \), is estimated as the sum of the squares of the contributions from each input. Denote the variance of each input by \( \text{Var}[x_1] \equiv \sigma_1^2 \) and \( \text{Var}[x_2] \equiv \sigma_2^2 \). Then the variance of the output is given by the Gaussian approximation as:

\[
\text{Var}[y] \approx \left( \left( \frac{\partial y}{\partial x_1} \right)_{x=x_1} \text{Var}[x_1] \right)^2 + \left( \left( \frac{\partial y}{\partial x_2} \right)_{x=x_2} \text{Var}[x_2] \right)^2
\]

Thus the total uncertainty in the output, expressed as variance, is explicitly decomposed as the sum of the contributions from each input. This is the basis for many techniques for error analysis widely used in the physical sciences and engineering.

Gaussian approximation is a local approach in that it considers the behavior of the function only in the vicinity of the nominal scenario. Effectively, it assumes that the response surface is a plane over the region of possible input values. This may be fairly accurate for smooth functions and small uncertainties, but it is likely to produce misleading results for complicated or discontinuous functions and for large uncertainties. In such cases we need to use a global approach that explicitly evaluates the function for scenarios distant from the nominal scenario.

Suppose we choose a low and high value for each input, selected to bound its range of plausible variation. They may or may not be symmetrically placed around each input’s nominal value. Let us denote these ranges for our two inputs as \([x_1, x_1']\) and \([x_2, x_2']\) respectively. The nominal range sensitivity method of sensitivity analysis is to compute the effect on the output of varying each input from its low to high value, while keeping the other inputs at their nominal values. For example,

\[
U_n(x_1, y) = f(x_1', y) - f(x_1, y)
\]

\[
U_n(x_2, y) = f(x_2', y) - f(x_2, y)
\]

Figure 8.3. An illustration of nominal range sensitivity, which is composed as the change in \( y \) caused by a change in each input, \( x_i \), from its low to high value, keeping the other inputs at their nominal values.

This is illustrated in Figure 8.3. These effects on the output of the changes in each input are sometimes known as swing weights.

The nominal range sensitivity is more than a local measure since it evaluates the model for extreme values of each input; but it is less than global because, when looking at the effect of each input, it holds all the others at their nominal values. For many functions, the effect of one input may depend on the values of other inputs, and so one may want to perform joint parametric analysis, graphing the effect of each parameter for several values of the other input(s). More detailed information about the effect of an input may be obtained by parametric analysis, that is, evaluating and plotting \( y \) for a sequence of different values for each input, holding the others constant. Figure 8.4 shows an example. It gives \( y \) as a function of \( x_1 \) for a range of different values of \( x_2 \). Of course, this is just a projection into two dimensions of some of the lines on the three-dimensional response surface depicted in Figure 8.1 and following figures. The perspective drawings used in these earlier figures are often a good way to display a parametric analysis for two inputs.

We have considered three particular values for each input, labeled low, nominal, and high. To investigate possible interactions between the effects of all the inputs at various levels, we might want to evaluate all possible combinations of each value of each input value with each value of each other input. We term
these the combinatorial scenarios, as in Figure 8.5. A useful way to represent a set of combinatorial scenarios is as a scenario tree, as in Figure 8.6. Each node represents an uncertain quantity or event, and each branch from that node, one of its possible outcome values. Each path through the tree from root to terminal represents a sequence of event outcomes determining a specific scenario. The combinatorial scenarios define a rectangular grid of points within the domain of the input space, in this case the two-dimensional rectangle defined by the lower and upper values of the two inputs.

It was easy to compute all combinatorial scenarios for our because function since it has only two inputs each with three levels. If we have, say, ten uncertain variables, each discretized to only three levels, a symmetric tree will have \(3^{10} = 59,049\) end branches. In other words, the number of scenarios increases exponentially with the number of uncertain inputs. So the computational burden is acceptable, the results of a parametric analysis with more than three or four dimensions are almost impossible to display in a comprehensible way, and so it is typically of little practical use.\(^1\)

In such situations, it generally makes sense to select only a few scenarios of special interest for examination. For example, in addition to the nominal or "base case" scenario, where every parameter is given its nominal value, we may define a "worst case" scenario, where every parameter is set to its "worst" value, and a "best case" scenario, where each is set to its "best" value. This will often give a very wide range of output values, and we may wonder what the

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1. In Chapter 9 we discuss graphical techniques for presenting multidimensional information.
calculating the probability and output value for each scenario (terminal node), we can obtain a discrete probability distribution for the output, sometimes known as the risk profile, an example of which is shown in Figure 8.7. This is the standard approach used in decision analysis (Raiffa, 1968; Watson and Buede, 1987).

Very often, as in our example, the uncertain quantities are actually continuous rather than discrete. Then it may be more natural to represent the probability distribution over each by a continuous distribution, as either a probability density function or as a cumulative distribution function. The task of uncertainty propagation is then to obtain the continuous probability distribution induced over the output quantity, as illustrated in Figure 8.8. Except in a few very simple cases, which we will mention in Section 8.3, it is hard to obtain analytically the probability distribution of a function of a set of continuous random variables. One approach is to approximate the continuous distributions by discrete ones.

Figure 8.7. Example of a probability tree (left), in which the uncertainty in each variable is quantified by attaching conditional probabilities to each branch of the scenario tree of Figure 8.6. The probability of each scenario is computed as the product of the probabilities of the branches that lead to it. The risk profile (right) is the cumulative probability distribution for output y, derived from the probabilities and y values for the nine scenarios.

and use the probability tree approach just described. However, if there are more than a few uncertain variables, even if each is approximated by only three discrete values, the combinatorial explosion in the number of terminal nodes is liable to cause severe computational problems.

An alternative approach to enumerating all the combinatorial scenarios, is to select a moderate-sized, random sample of scenarios for evaluation. In this approach, often called Monte Carlo simulation, each scenario is generated by selecting each branch at a node according to its assigned probability. Because the total effort depends on the sample size but not on the number of possible values for each quantity, the branch values may be generated directly from the underlying continuous distribution, without any need for discretization.

The resulting distribution for an output using a sampling approach is inevitably only an approximation to the exact distribution. But so is the result of any probability tree technique that involves discretizing continuous distributions. The accuracy of a Monte Carlo scheme can be increased simply by increasing the sample size. Unlike schemes involving discretization, the accuracy can easily be estimated using standard statistical techniques. The appropriate sample size
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8.3. Analytic Methods

we discuss a variety of related measures, employing correlation and regression coefficients.

We have just introduced a number of basic concepts for sensitivity analysis, uncertainty propagation, and uncertainty analysis. In the rest of the chapter we survey them in more detail, with special attention to the question of how to choose among them.

8.3. Analytic Methods

For all except the simplest cases, such as linear combinations of normal variables, exact analytic methods for propagation of uncertainty are intractable or require elaborate numerical integration (Springer, 1979). However, there are a variety of approximate analytic techniques based on Taylor series expansions of the function (Cheney, 1966). These are sometimes known as the method of moments, because they propagate and analyze uncertainty using the mean, variance, and sometimes higher order moments of the probability distributions. We already saw one simple approach, based on the first order or Gaussian approximation, in equation (10). We will now show how this first order approximation for the expectation and variance of a function is derived from the Taylor series, and we will examine its application to a range of important special cases, such as weighted sums and products of powers of uncertain variables. We will also touch on the use of more exact approximations using higher order terms from the Taylor series.

8.3.1. Approximation from the Taylor Series

Suppose, instead of just two inputs to function $f$, as in the example above, we have a vector of $n$ uncertain inputs:

$$X = (x_1, x_2, \ldots, x_n)$$

$$y = f(X)$$

We will assume that the nominal value for each input is equal to its expectation:

$$E[x_i]$$

So the nominal scenario is also the mean scenario, or the expectation of $X$:

$$X^0 = (x_1^0, x_2^0, \ldots, x_n^0) = E[X]$$

The Taylor series expansion provides a way to express deviations of output from its nominal value, $y - y^0$ in terms of deviations of its inputs from their nominal values, $x_i - x_i^0$. Successive terms contain higher order powers of
deviations and higher order derivatives of the function with respect to each input. Here is the expansion around the nominal scenario with the first three terms (e.g., see Korn and Korn, 1968):

\[ y - y^0 = \sum_{i=1}^{n} (x_i - x_i^0) \left[ \frac{\partial y}{\partial x_i} \right]_{x^0} + \]

\[ \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} (x_i - x_i^0) \quad (x_j - x_j^0) \left[ \frac{\partial^2 y}{\partial x_i \partial x_j} \right]_{x^0} + \]

(12)

\[ \frac{1}{3!} \sum_{i=1}^{n} \sum_{j=1}^{n} \sum_{k=1}^{n} (x_i - x_i^0) \quad (x_j - x_j^0) \quad (x_k - x_k^0) \left[ \frac{\partial^3 y}{\partial x_i \partial x_j \partial x_k} \right]_{x^0} + \cdots \]

Note that all derivatives are evaluated at the nominal (i.e., mean) scenario \( X^0 \). If the deviations \( x_i - x_i^0 \) are relatively small, the higher powers will become very small. And if the function is relatively smooth in the region of interest, the higher derivatives will be small. Under these conditions the Taylor series produces a good approximation when the higher order terms are ignored.

For example, let us derive an approximation for the mean of the deviation taking the expectation over equation (12) using terms up to the second order:

\[ E[y - y^0] \approx \sum_{i=1}^{n} E[(x_i - x_i^0)] \left[ \frac{\partial y}{\partial x_i} \right]_{x^0} + \]

\[ \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} E[(x_i - x_i^0) \quad (x_j - x_j^0)] \left[ \frac{\partial^2 y}{\partial x_i \partial x_j} \right]_{x^0} \]

(13)

Since the nominal values of each \( x_i \) is equal to its mean, we know \( E[x_i - x_i^0] = 0 \), so the first term disappears. The covariance between \( x_i \) and \( x_j \) is given by

\[ \text{Covar}(x_i, x_j) = \mathbb{E}[(x_i - x_i^0) \quad (x_j - x_j^0)] \]

Substituting this into (13) we obtain:

\[ E[y - y^0] \approx \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \text{Covar}(x_i, x_j) \left[ \frac{\partial^2 y}{\partial x_i \partial x_j} \right]_{x^0} \]

Note that so long as the second derivative terms are nonzero (i.e., the function is nonlinear) the mean output value \( E[y] \) is not equal to the nominal output \( y^0 \) but is a function of the variances and covariances of the inputs. But another way, the expected value of the output cannot be computed simply by evaluating the model with all inputs set to their expected values, unless the model is linear.
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8.3.3. Weighted Sums

If the function actually is linear, the Gaussian formulas are exact. The weighted sum is a very simple but useful example of such a model:

\[ y = \sum_{i=1}^{n} a_i x_i \]

We assume the weights \( a_i \) are not uncertain. Applying (14) and (15) we obtain the following expressions for the mean and variance of a weighted sum:

\[ E[y] = \sum_{i=1}^{n} a_i E[x_i] \]  \hspace{1cm} (16)

\[ \text{Var}[y] = \sum_{i=1}^{n} a_i^2 \text{Var}[x_i] + 2 \sum_{i=1}^{n} \sum_{j \neq i}^{n} a_i a_j \text{Covar}[x_i, x_j] \]  \hspace{1cm} (17)

These expressions are exact no matter what the distribution over \( X \), provided only that it has a finite mean and covariance matrix. If the distribution over \( X \) is a multivariate normal for the weighted sum model, the resulting output distribution will be exactly normal. But even if the inputs are not normal, according to the central limit theorem, the distribution of \( y \) will tend to become normal for large \( n \), for any reasonable distributions on the \( x_i \), provided they are independent.

8.3.4. Products of Powers with Log Transform

These results may easily be extended to another important class of models, namely, products of powers of uncertain variables. (This also comprises ratios of powers, which are simply products with negative powers for terms in the denominator.)

\[ y = \prod_{i=1}^{n} x_i^{a_i} \]

By applying a log transform to this, the function becomes a weighted sum of the uncertain inputs. The weights are simply the powers of the variables:

\[ \ln(y) = \sum_{i=1}^{n} a_i \ln(x_i) \]

Hence, we can obtain expressions for the mean and variance of the log of the output in terms of the mean and variance of the log of the inputs:

\[ E[\ln(y)] = \sum_{i=1}^{n} a_i E[\ln(x_i)] \]  \hspace{1cm} (18)

\[ \text{Var}[\ln(y)] = \sum_{i=1}^{n} a_i^2 \text{Var}[\ln(x_i)] + 2 \sum_{i=1}^{n} \sum_{j \neq i}^{n} a_i a_j \text{Covar}[\ln(x_i), \ln(x_j)] \]  \hspace{1cm} (19)

The mean of the log of a random variable is the same as the log of its geometric mean, and the variance of the log is the same as the log of its geometric variance. By analogy with the weighted sum, these expressions are exact, provided the geometric means and geometric covariance matrix for \( X \) are finite.

If the distribution over \( X \) is multivariate lognormal (i.e., \( \ln(X) \) is multinormal), the distribution of \( y \) will be exactly lognormal. Similarly, according to the central limit theorem, for any reasonable independent distributions on the \( x_i \), the distribution of \( y \) will tend to become lognormal for large \( n \).

The lognormal approximation for multiplicative models is widely used. For example, in risk assessments that involve evaluating the impact of a pollution release on human health and the environment, the risk is often modeled as the product of the probability of release with the amount of release, the fraction of the release that reaches the receptor location, the amount of exposure realized by the target organisms at the receptor, and the dose-response relationship representing the health or environmental effect. The uncertainties in each component of the release, transport, fate, exposure, and health effect assessments can be combined using the lognormal model.

8.3.5. Products of Powers with Relative Error

It is also possible to apply the Gaussian approximation for direct error propagation in a product-of-powers model. This avoids the effort of having to transform to and from the log space, and allows use of arithmetic means and variances instead of the less familiar geometric means and variances. However, the results are only approximate, and it only works when the uncertainties are small relative to the means of the variables. It leads to a particularly simple formulation in terms of relative error, that is, the ratio of the standard deviation to mean for each variable. This approach is widely used for error propagation in engineering and the physical sciences.

As above, we are interested in error propagation for a product-of-powers model:

\[ y = \prod_{i=1}^{n} x_i^{a_i} \]

By applying (14) to the product-of-powers model we estimate the expected value of \( y \) as the product of the powers of the means of the \( x_i \):

\[ E[y] \approx \prod_{i=1}^{n} E[x_i]^{a_i} \]  \hspace{1cm} (20)
In order to apply (15) to estimate the variance, we will first need the partial derivatives:

$$\frac{\partial y}{\partial x_i} = \frac{a_i}{E[x_i]} \times \prod_{j=1}^{n} E[x_j]^j$$

Using (20) we get

$$\frac{\partial y}{\partial x_i} = \frac{a_i}{E[x_i]} E[y] = \frac{a_i}{2} y^0$$

Using these partial derivatives in the Gaussian approximation for the variance of $y$, equation (15), we get:

$$\text{Var}[y] \approx \sum_{i=1}^{n} \text{Var}[x_i] \left( \frac{a_i}{2} y^0 \right)^2$$

Dividing by $y^0$ we get:

$$\frac{\text{Var}[y]}{y^2} \approx \sum_{i=1}^{n} \frac{a_i^2 \text{Var}[x_i]}{2}$$

This may be looked at in terms of the relative error (also known as relative standard deviation or coefficient of variation), that is, the ratio of standard deviation to the mean for each variable:

$$h(x) = \frac{\text{Var}[x]}{x^2} \quad (21)$$

Substituting this into the previous expression, we get the following simple and useful formula:

$$h(y)^2 \approx \sum_{i=1}^{n} a_i^2 h(x_i)^2 \quad (22)$$

In other words, we can estimate the relative error of a product of powers by the root sum of squares of the relative error of its components, weighted by the squares of their powers.

As an example, consider the following model:

$$z = \frac{r^2}{\sqrt{u}}$$

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Suppose we are given the accuracy of $r$, $s$, $t$, $u$ as their percent standard deviation (i.e., relative error times 100):

$$h(r) = 1\% \quad h(s) = 1\% \quad h(t) = 3\% \quad h(u) = 2\%$$

What is the accuracy of $z$? Applying (22), where the $a_i$ are the powers of the four variables, we get:

$$h(z)^2 \approx (1 \times 1)^2 + (2 \times 1)^2 + (-1 \times 3)^2 + (-0.5 \times 2)^2,$$

$$h(z)^2 \approx 15$$

$$h(z) \approx 4\%$$

Note that in a simple product of a set of uncertain variables, if the coefficients of variation of two uncertain quantities differ by more than a factor of 3, the smaller relative uncertainty may generally be ignored. Its relative variance will be about an order of magnitude less (actually a factor of $3^2$). In this way the propagation process through a cascaded chain of models may often be greatly simplified.

8.3.6. Higher Order Approximations

So far we have considered only first order approximations to the general function and treated only the mean and variance of the distributions. These work well for small uncertainties with smooth, well-behaved functions, but may not work so well for large uncertainties that are typical in many areas of policy and risk analysis. One way to improve the accuracy of the approximation is to use higher order terms from the Taylor expansion. Effectively, this allows us to approximate the function by quadratic, cubic, or higher order surfaces, fitted at the nominal scenario.

If the function actually is a quadratic or cubic and so on, this approach can provide exact results. Seiler has developed tables of correction factors that provide better approximations or exact expressions for a variety of common functions (Seiler, 1987). These include products of two, three, and four terms, powers of single terms, and more complex combinations. A very simple example is the exact expression for a weighted sum where, unlike in our earlier analysis, the weights $a_i$ are also uncertain.

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

If we can assume the variables $x_i$ and weights $a_i$ are all independent, the following is the exact expression for the variance:

$$\text{Var}[y] = \sum_{i=1}^{n} \left[ (E[a_i])^2 \text{Var}[x_i] + (E[x_i])^2 \text{Var}[a_i] + \text{Var}[a_i] \text{Var}[x_i] \right] \quad (23)$$
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The first two terms are the first order (linear) approximation; the third is the correction term. As Seiler (1987) points out, the correction is always positive, thus increasing the final error. For more complex functions, the propagation may be done in multiple stages.

Unfortunately, the algebraic complexity increases rapidly with the complexity of the function. For example, the exact expression for the product of four normal variables contains twenty-eight terms. So unless the function is one of the simpler cases, this method of moments employing higher order terms can rapidly become intractable.

8.3.7. Finding Derivatives

To employ the method of moments, we need to calculate the partial derivatives of the model. Given a computer implementation of the model, it is often relatively easy to compute this numerically. Conceptually, the simplest way is to take each uncertain input \( x_1 \), one at a time, perturb it slightly from the nominal scenario, by \( \Delta x_1 \). The derivative is estimated as the ratio of the change in output to the change in the input:

\[
\left[ \frac{\partial y}{\partial x_1} \right]_{x_0} \approx \frac{f(x_0 + \Delta x_1) - f(x_0)}{\Delta x_1}
\]

(We assume all inputs other than \( x_1 \) are left unperturbed.) Higher order derivatives are computed similarly from their standard definitions in terms of small perturbations. Of course, for computation the actual perturbation must be sufficiently large not to get lost in the imprecision (e.g., round off error) of the computation.

In practice, it may be preferable to use larger perturbations, comparable to the range of variation for each input. In this case, we are no longer fitting a hyperplane (or higher order surface) tangential to the actual response surface at the nominal scenario, but rather to intersect more distant points of the response surface. This may actually produce a better fit in many cases when averaged over the domain of the inputs.

This one-input-at-a-time perturbation will require evaluation of the model for the base case, and then once for each uncertain input for a first order approximation, and an additional evaluation for each input and each pair of inputs for a second order approximation. If there are very many uncertain inputs, and the model is expensive to evaluate, the cost may become prohibitive. To mitigate this, one may be able to do some initial screening based on inspection of the model to eliminate some of the uncertain inputs as contributing negligibly to the overall uncertainty. Another approach possibility is to use a factorial design in selecting scenarios for evaluation, which can allow estimation of the low-order derivatives from a smaller number of evaluations.

8.3. Analytic Methods

A way to reduce the computational effort is to perform symbolic differentiation on the model, chaining through it to obtain the partial derivative of the output(s) with respect to each uncertain input. The final step is to evaluate them, using the values for the nominal scenario (generally the means of the inputs).

For a simple model this is often not hard to do by hand, but for complex models it can be extremely arduous. For models used in nuclear engineering and safety analysis, this process has required many person-months of analysis (Iman and Helton, 1988). In cases of such complexity, one might also worry about the reliability of the analysis. Would errors necessarily be discovered?

Nowadays another possibility is to perform the symbolic differentiation by computer program (Roll, 1981; Oblow, 1983a). Typically in large engineering applications where there is interest in systematic sensitivity and uncertainty analysis, models have been implemented as large FORTRAN programs. Oblow (1983b) describes a program named GRESS, which takes FORTRAN source code as input, and via symbolic differentiation generates additional code to compute and chain the derivatives through the model. With this extended model, a single additional run will be sufficient to compute the required first order derivatives.

For complex dynamic models that need to be solved by sophisticated iterative techniques, there are a variety of approaches to improving the efficiency for computing their sensitivities. This is the field of differential sensitivity theory. Such approaches employ specialized numerical procedures, utilizing knowledge of the model structure, to minimize the computational effort. Techniques include adjoint methods (e.g., Koda, Dogru, and Seinfeld, 1979; Cacuci et al., 1980; Cacuci, 1981a, 1981b; Hall, Cacuci, and Schlesinger, 1982) and Green's function methods (e.g., Hwang et al., 1978; Dougherty, Ilwong, and Rabitz, 1979). These techniques tend to be rather complex to use and time-consuming to implement, although availability of programs such as GRESS for automatic symbolic differentiation of the model could help significantly. While they may be useful for very large: dynamic models, for example in atmospheric modeling, they seem unlikely to be necessary for most applications in policy and risk analysis. Consequently, we will refer the interested reader to the references for more detailed description.

8.3.8. Moments and Other Properties of Distributions

One feature of the method of moments, which is sometimes cited as an advantage, is that it does not require specification of the entire probability distribution of the input parameters, but only the first few moments, typically only the mean and variance. Whether this is really an advantage depends on the form in which the input uncertainties are given. If they are given in the form of mean and standard error, then, of course, it is an advantage, provided
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no higher moments are wanted. In nuclear power safety studies and other risk analysis for complex engineering systems, failure frequencies are typically given as a median, \( m \), and uncertainty factor, \( f \). To translate these into mean and variance requires some strong assumptions about the shape of the distribution. Commonly, the distributions are assumed lognormal, with median at \( m \) and 95th percentile at \( m \times f \). Moments can be derived accordingly. However, other distributions that may be fit have quite different moments, especially if they are symmetrical (Muritz et al., 1983). The method of moments cannot avoid this problem any more than other methods.

A related problem, peculiar to the method of moments, is how to obtain percentiles from the moments computed for the outputs. The Chebyshev inequality provides confidence bounds based on the computed variance. Generalizations of this inequality by Markov and Cantelli (Mallows, 1956; allow use of higher moments as well. Such confidence intervals are usually highly conservative (i.e. much wider than necessary), although in some cases, because of inaccuracies in the method of moments, they may instead be too narrow (Muritz et al., 1983). An alternative approach is to fit a distribution to the moments, such as a lognormal, and obtain appropriate percentiles from that. This may give better results but relies on knowledge about what will be an appropriate form for the distribution.

8.3.9. Advantages and Disadvantages of the Analytic Methods

First order or Gaussian approximation is very widely used in engineering and the physical sciences, particularly in the relative error form for products of powers. Higher order approximations, often known as the method of moments, have been applied quite widely to the analysis of complex models. The approach has two important advantages:

- Once the algebraic analysis has been performed, the numerical calculations are usually relatively simple.
- It provides a very clear and direct approach to uncertainty analysis, generally decomposing the variance of each output into the sum of the contributions from each input.

However, it suffers from three disadvantages:

- The complexity of the algebra can increase rapidly with the complexity of the model, particularly if higher order terms will be required.
- Because it primarily produces moments of distributions, usually only the mean and variance, it is hard to obtain reliable estimates for the tails of output distribution.
- It is basically a local approach and will not be accurate if the uncertainties are large, if the model is not smooth (for example the response surface has discontinuities), or if important covariances terms are omitted.

8.4. Discrete Distributions and Decision Analysis

We introduced the use of discrete probability distributions to approximate continuous ones, and their combination into probability trees as a basic idea, in...
cumulative distribution and the stepwise cumulative function representing the discrete distribution. This area is crosshatched in Figure 8.9.

It has been observed that this approach, minimizing the integral of the absolute difference between the cumulative distributions of the discrete distributions and the continuous one, may not be the best approach. It typically leads to substantially understating the variance, by 15% to 30%, depending on the shape of the underlying distribution. It is usually better to have the side points farther away from the midpoint. Several authors have proposed methods which maintain the first few moments as accurately as possible in the discrete approximation (Keffer and Bodily, 1983; Miller and Rice, 1983). It may not always be worthwhile to go to the effort of finding the optimal approximation, unless one has software that does it automatically. But it is as well to remember that the conventional approach can lead to significant underestimation of the uncertainty.

8.4.2. The Method of Discrete Probability Distributions

In an attempt to moderate the exponential complexity of the probability tree approach to propagating uncertainties, Kaplan proposed an alternative, which he calls the method of discrete probability distributions (DPD) (Kaplan, 1981). This was developed for application to uncertainty analysis of fault trees in the risk assessment of nuclear power. We illustrate with an example.

Consider a simple redundant safety system $S$ consisting of three subsystems, $A$, $B$, and $C$, as in Figure 8.10. These are arranged in parallel so that $S$ fails (is unavailable) only if all three of $A$, $B$, and $C$ are unavailable simultaneously. If the unavailability rates of the three subsystems are denoted $a$, $b$, and $c$, respectively, assuming the three subsystems are independent, we can compute the unavailability rate, $s$, for the entire system as the product $s = a \times b \times c$. Suppose we are given probability distributions over the unavailability rate for each subsystem, and the rates are considered independent. How can we propagate these uncertainties to obtain the probability distribution over the unavailability rate $s$ for the entire system?

The first step of the DPD method is to discretize them, let's say each into a five point discrete distribution, as illustrated in Figure 8.11. Suppose we represent the DPDs for $A$ and $B$ as:

$$f(a) = \{[a_1, \alpha_1], [a_2, \alpha_2], [a_3, \alpha_3], [a_4, \alpha_4], [a_5, \alpha_5] \}$$

$$f(b) = \{[b_1, \beta_1], [b_2, \beta_2], [b_3, \beta_3], [b_4, \beta_4], [b_5, \beta_5] \}$$

where each pair $[a_i, \alpha_i]$ is a value and corresponding probability, so $\alpha_i = Pr(a = a_i)$, and similarly for $b$. We then obtain a corresponding distribution for $a \times b$.
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taking the cross products of the values and of the probabilities, obtaining a DPD with \(5 \times 5 = 25\) value-probability pairs:

\[a_i \times b_j, \alpha_i \times \beta_j\] for \(i = 1\) to 5

This is essentially just the standard approach with probability trees, but the next step is different. The DPD for \(a \times b\) is condensed, that is, the twenty-five-point distribution is approximated by a five-point distribution. Thus, when using the result of this to obtain the cross product for \(a \times b \times c\), the resulting DPD has only twenty-five points, rather than \(5 \times 5 \times 5 = 125\) points. This may itself be condensed before participating in further computations. In this way the potential combinatorial explosion is moderated.

When combining two DPDs, the quantities they represent are assumed to be independent. Information about how combined quantities depend on their components is lost in the process of condensation. Thus, if two quantities, \(x\) and \(y\), both depend on a common third quantity, \(k\),

\[z = a \times b,\quad y = b + c \times d\]

straightforward application of the method to compute \(x \times y\) will ignore their correlation and produce incorrect results. Sometimes the order of the calculations can be rearranged to eliminate multiple occurrences of the same parameter in different places, so that each parameter only appears in the expression for a single higher order quantity. But this kind of rearrangement can require considerable ingenuity (Martz et al., 1983), and in some cases it is impossible. In more complex situations, more than three variables may need to be combined without intermediate condensation, and the complexity reduces to the standard combinatorial approach. This puts a severe limitation on the applicability of the method.

Another major deficiency of the DPD method is the difficulty of performing uncertainty analysis with it to compare the contributions of different sources of uncertainty. Because the discrete probability distributions are condensed after each step in the computation, the information about which input scenarios are responsible for which outputs is lost. Thus, it does not provide any simple way to compute the degree to which each input has contributed to the uncertainty in the output.

8.4. Discrete Distributions and Decision Analysis

severely limit the complexity of the models they can handle. They generally approach the problem by conducting systematic deterministic sensitivity analysis to identify which uncertain inputs and decisions may have significant impact on the results, and which are unlikely to do so. The most commonly used measure of uncertainty importance is nominal range sensitivity, the effect on the output of holding each input from low to high level, holding the rest at nominal values (described in Section 8.2). It usually turns out that only a handful of the variables account for most of the variation in consequence. Only those need to be modeled as uncertain in the probabilistic analysis, and the rest are treated as fixed at their nominal value. In this way a model that may have many dozens of uncertain variables and decisions may be reduced to one that has less then a dozen or so, and therefore become computationally tractable for decision tree programs running on microcomputers.

So far, in our discussion of sensitivity and uncertainty analysis, we have been content to talk of effects on outcomes. Decision analysis, with its emphasis on decision making, provides some important distinctions to sharpen these ideas. For example, suppose you are interested in buying a particular new model of car which is available from two different dealers, one of whom asks for a price which is a thousand dollars less than the other. You may be somewhat uncertain just how good the car will turn out to be, and consequently uncertain about how you will feel about the entire transaction. But, assuming the car and options will be identical from the two dealers, it is obvious that uncertainty about the quality of the car is irrelevant to which dealer you choose. The point is that the importance of an uncertainty depends on how much it could affect the decision, not simply the outcome.

In the terminology of control theory, a measure of sensitivity or uncertainty importance is called open loop if it is a measure of how far an assumption or uncertain quantity affects the outcome utility (or other outcome measure) for a fixed decision (Howard, 1971). If, on the other hand, the decision may be adjusted to optimise the outcome reflecting the change in assumption or input value, the measure is called closed loop. Closed loop sensitivity is generally a more powerful and relevant measure, but often more difficult to compute. Open loop sensitivity is a weaker measure, in that open loop sensitivity in a variable is necessary but not sufficient for closed loop sensitivity. But uncertainty about the car quality exhibits open loop sensitivity, but not closed loop sensitivity. Uncertainty about the relative prices of the two dealers would produce both open and closed loop sensitivity, because it could affect both the outcome and which decision is best.

One closed loop measure of uncertainty importance, well known in decision analysis, is the expected value of perfect information (EVPI). The EVPI is a measure of the importance of uncertainty about a quantity in terms of the expected improvement in the decision that might be obtained from knowing
the value of the quantity exactly. The measure of improvement is the expected
difference in expected value of the outcome (utility) before and after the true
value of the quantity becomes known. In the car example, the EVPI for the
car quality would be zero with respect to the decision of which dealer to buy
from. The EVPI of the relative prices of the two dealers might be quite large
if there was significant uncertainty about which would be cheaper. Note that
EVPI (and any closed loop measure of uncertainty importance) is specific to a
particular decision variable.

Another closed loop measure of uncertainty importance, namely the expected
value of including uncertainty (EVIU) is discussed in more detail in Chapter 12.
The EVIU is a measure of the value of explicitly modeling uncertainty in a
quantity instead of assuming some fixed value.

Decision analysis generally tend to use easy-to-compute open loop sensitivity
measures, such as range sensitivity, for initial screening of variables to find out
which are important. They sometimes go on to examine closed loop sensitivity
measures, particularly the EVPI, for a few of the variables explicitly modeled
as uncertain. Modelers such as policy and risk analysis from other traditions
have generally placed less emphasis on decisions for focusing modeling, and
have stayed with simple open loop measures. In practice EVPI is generally
computed using discrete decision trees, although analytic approaches derived
from Taylor expansions have been developed both for the EVPI (Howard,
1971) and for the EVIU (Henrion, 1982, and Chapter 12). The use of other
computational approaches for uncertainty propagation, such as Monte Carlo
sampling, for closed loop sensitivity measures does not seem to have been
reported hitherto.

8.5. Monte Carlo and Other Sampling Methods

One can view the combinatorial scenarios and probability tree approach as a
way of sampling points from the uncertain input domain, that is the subset of
the \(n\)-dimensional space defined by the ranges of the \(n\) uncertain parameters.
The combinatorial scenarios define points at all the vertices of a regular
rectangular grid in that space. (This is illustrated in Figure 8.5 for a two-
dimensional case.) There are many other ways of sampling from that space,
of which the best known and simplest is Monte Carlo simulation. To avoid
having to assess the relative likelihood of different points with the input
space, uniform distributions are sometimes used.\(^2\) More often, probability
distributions may be assessed for each uncertain parameter, using the kind
of techniques described in the previous chapters. In crude Monte Carlo

\(^2\) We note, and duck, the philosophical arguments about the difference between representing your
beliefs by a uniform distribution and using a uniform distribution because you don’t know the
distribution.
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8.5. Monte Carlo and Other Sampling Methods

We rearrange this in terms of \(m\)

\[
m > \left(\frac{2ca}{w^2}\right)^2
\]

(24)

To use this, we should first make small Monte Carlo runs, with, say, ten values to get an initial estimate \(s^2\), the variance. From this, we can then use this expression (24) to estimate how many samples are needed in total to reduce the confidence interval to the requisite width \(w\).

For example, suppose we wish to obtain a 95% confidence interval for the mean that is less than twenty units wide. Suppose your initial sample of ten gives \(s = 40\). The deviation \(c\) enclosing a probability of 95% is about 2. Substituting these numbers into (24) we get

\[
m > \left(\frac{2 \times 2 \times 40}{20}\right)^2 = 8^2 = 64
\]

To get a total of sixty-four runs, another fifty-four runs should be done in addition to the ten already done.

8.5.3. Estimating Confidence Intervals for Fractiles

Another criterion for selecting sample size is the precision of the estimate of the median and other fractiles, or more generally, the precision of the estimated cumulative distribution. In Section 5.3.3 we saw how to obtain a confidence interval for \(Y_p\), the \(p^{th}\) fractile of \(Y\). Without loss of generality, we assume the sample \(m\) values of \(y\) are re-labeled so that they are in increasing order,

\[y_1 \leq y_2 \leq \cdots \leq y_m\]

Sample value \(y_i\) is an estimate of fractile \(Y_p\), where \(p = i/m\).

According to equation (7), the following pair of sample values constitutes the confidence interval with confidence \(\alpha\):

\[
(y_i, y_k)
\]

(25)

where

\[
i = \left[ mp - c \sqrt{mp(1-p)} \right]
\]

\[
k = \left[ mp + c \sqrt{mp(1-p)} \right]
\]

(26)

and \(c\) is the deviation enclosing probability \(\alpha\) of the unit normal, and \(\lfloor x \rfloor\) means rounding \(x\) down and \(\lceil x \rceil\) means rounding it up.
8. Monte Carlo and Other Sampling Methods

8.5 How Many Runs Are Enough?

In typical applications for the uncertainty analysis of reliability models for nuclear power plants, analysts have used very large numbers of Monte Carlo runs, over 18,000 runs in one example (Jackson et al., 1981). As just seen, this allows sufficient accuracy that we can be more than 95% confident that the true percentile of the distribution is between the estimates for its two neighboring percentiles, for instance, \((x_{90}, x_{50})\) is a 95% confidence interval for \(x_{50}\). Before either expending all this computer time or giving up in disgust at the prospect of doing so, it is a good idea to consider whether this much precision is really needed. For example, in nuclear safety reliability codes, the input values and uncertainty factors for most of the component failure rates are based largely on expert judgment. The difference between an uncertainty factor of 10 and one of 12 is unlikely to be subjectively discriminable to the expert assessor. In such a case, the degree of precision in the propagation of these uncertainties is probably pointless. The approximation uncertainty contributed by the finite number of runs will be totally dominated by the empirical uncertainty from the input parameters. Thus, in most uncertainty analyses of quantitative policy models, a few hundred or sometimes only a few tens of runs may be quite sufficient.

Where computing costs do turn out to be a significant issue, there may be several ways of reducing them. Sometimes the computation involved in the model itself can be reduced by some reordering of expressions. One example of this is in fault tree analysis, where a fault tree is reduced to its minimal cut-sets. Substantial savings may be obtained by omitting those cut-sets that are shown by initial analysis to make negligible contributions to the top event frequency. It can also pay to look at the Monte Carlo code itself. Early work was much concerned with improving the efficiency of random sampling. But examination of one widely used code, SAMPLE, developed for the Reactor Safety Study (Rasmussen et al., 1975), revealed that most of the effort was consumed in sorting the output values to produce the cumulative probability distribution. Replacement of the sorting algorithm, which required time of order \(O(n \log n)\), by a categorizing algorithm to generate the histogram, requiring time of order \(O(n)\), improved overall performance by an order of magnitude or more for an \(n\) of thousands (Jackson, 1981).

8.5.5 Variance Reduction Techniques

Another way to reduce the computational effort for sampling schemes is to improve their statistical efficiency by one of a number of variance reduction techniques (Rubinstein, 1982; Johnson, 1987). These techniques use structural knowledge or other information about the model to reduce the variance in estimates of the mean, or other parameters of interest of the output distribution.
The controlled variate method may be used if there is a simplified approximation to the full model that is cheaper to run. For example, an analytic model based on a Taylor series expansion (method of moments) might be used. Input scenarios may be computed in the usual random way (or using a stratified approach, as described in the next section). Let the exact model be \( y = f(X) \), and the approximate one be \( y' = f'(X) \). Each input scenario \( X_i \) for \( i = 1, \ldots, n \) is fed into both complete and approximate models producing outputs \( y = f(X) \) and \( y' = f'(X) \). With the simple model it is easy to calculate the approximate mean output \( E[y'] \). The mean from the complete model can then be calculated in terms of the difference from the approximate model, instead of directly:

\[
E[y] = E[y'] + \frac{1}{m} \sum_{i=1}^{m} (y_i - y'_i)
\]

If the approximate model is any good at all the variance of the difference \( y_i - y'_i \) will be less than the variance of \( y_i \) alone. Hence, the variance in the sample mean will be less than if it was calculated directly. A given precision should thus be attainable with fewer runs. Analogous techniques may be used for estimating other parameters of the output.

8.5.6. Stratified Sampling and Latin Hypercube Sampling

It is important to understand that the value of Monte Carlo methods is not primarily the randomness of the sampling but the resulting equidistribution properties of the sets of points in the parameter space. Once it is recognized that a primary objective is to produce a more uniform distribution of points in parameter space, then systematic or stratified sampling techniques become appealing. In stratified sampling the sample space for an input parameter is divided up into strata, and input values are obtained by sampling separately from within each stratum instead of from the distribution as a whole. One version of this, which is being used increasingly widely, has the impressive name of Latin hypercube sampling (LHS) (Iman, Davenport, and Zeiger, 1980). It is more straightforward than it sounds.

To generate \( m \) samples using LHS, each input distribution is divided up into \( m \) equiprobable intervals. In standard LHS, a single value is sampled at random from within each of these intervals, according to the probability distribution. This produces a sample of \( m \) values for each input distribution that are more uniformly spread out than for standard random sampling. An alternative, midpoint LHS, produces yet more uniform sampling. In this case, we choose the median of each of the \( m \) probability intervals. This is repeated for all the probabilistic inputs. A scenario is generated by selecting one value at random from each of the inputs, but without replacement, from the \( m \) sample values for each input.

8.5. Monte Carlo and Other Sampling Methods

We end up with \( m \) scenarios, with each value from each input being used only once.

In Latin hypercube sampling, because the sample scenarios tend to be more evenly spread out over the input domain, the sample from each input will represent the mean, variance, and other parameters of the distribution more accurately than with unstratified random sampling. With midpoint LHS, the mean and variance of the sample will often be almost exact. If the model is roughly linear, the mean of the output will converge more rapidly. The same is true if the uncertainty in the output is dominated by one or two inputs. On the other hand, if there are many uncertain inputs contributing and the model is highly nonlinear, LHS may not be much better than crude Monte Carlo.

If LHS is sometimes much better and never worse than crude Monte Carlo, why should we ever use the latter? One reason is that the statistics may be harder to compute with LHS. With standard LHS, the sample scenarios and hence the outputs are random, but they are not completely independent. Thus statistics for estimating the precision of the results for Monte Carlo, as discussed in preceding paragraphs, will be inaccurate for LHS. Typically they will underestimate the true precision. Of course, if one would rather have higher precision, even if unsure exactly what level of precision, this is not a problem.

In general, midpoint LHS performs considerably better than standard LHS, but it is subject to a rather subtle, if rare, problem. If the model exhibits periodicity with respect to an input with a wavelength comparable to that induced by the \( m \) equal probability intervals, midpoint LHS could produce misleading results. As a worst case, consider this model:

\[
z \sim \text{Uniform}(0,100)
\]

\[y = \cos(2\pi z)\]

The expectation of \( y \) should be zero (averaging over an integral number of cosine wave patterns with amplitude 1). Suppose we perform midpoint LHS with a sample size of 100. Then \( z \) will be divided up into 100 equiprobable intervals, whose midpoints are \((0.5, 1.5, 2.5, \ldots, 99.5)\). Evaluating \( y \) at each point will give a cosine of an odd number of radians, which yields \(-1\). Hence, it will estimate the mean \( E[y] \) as \(-1\). Although it is important that models be aware of this danger, such periodic behavior is very unusual in policy and risk analysis models, and should be predictable.

8.5.7. Generating Correlated Input Variables

As mentioned in Section 6.4.6, when two input quantities are judged to be probabilistically dependent, it is often best to try to structure the model to model the dependence explicitly, by adding, if necessary, the common factor that causes
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the dependence. In this way the need to assess the probabilistic dependence directly is avoided. However, in some cases this may not be practical, and the dependence may be expressed directly as correlations. How can we generate sample values for dependent uncertain inputs with a specified correlation?

It is not hard to generate correlated normal distributions. Suppose we wish to generate random samples for two variables \( x \) and \( y \) with unit normal distributions and correlation \( r \). We define an auxiliary variable, \( z \). We generate a sample of values for \( x \) and \( z \), from independent normal distributions, either in the standard way, or using Latin hypercube sampling. We use these to compute a corresponding sample for \( y \),

\[
y := x z \sqrt{1 - r^2}
\]

where the notation := denotes a replacement statement. The sample for \( y \) will also be from a unit normal with the specified correlation to \( x \). If we wish \( x \) and \( y \) to have mean and standard deviation other than 0 and 1, respectively, say, \( \mu_x, \sigma_x, \mu_y, \sigma_y \), we can transform them appropriately:

\[
x := \mu_x + \sigma_x x
\]

\[
y := \mu_y + \sigma_y y
\]

These transformations will not affect their correlations. Given a \( n \times n \) covariance matrix (which must be positive definite), this approach can easily be generalized to generate \( n \) correlated normal variates (Scheuer and Stoller, 1962).

If we want to generate correlated continuous random variables with other kinds of marginal distributions, the situation becomes trickier. In fact, it is not generally possible to generate two random variables, each with an arbitrary marginal distribution and with any specified Spearman correlation. But Iman and Conover (1982a) have shown how it is possible to generate variables with specified rank-order correlation. They describe a method for generating \( n \) variables with arbitrary strictly increasing cumulative functions and specified rank order correlation matrix. They start by generating \( n \) unit normal variables with the specified correlation matrix. They then transform each input sample from the unit normal to the desired marginal distribution. This transform will not necessarily preserve the Pearson correlations exactly, but any strictly monotonic transform is guaranteed to preserve the rank-order correlations.

Just as the mean or variance of a random sample will not be identical to the exact mean and variance of the parent distribution, so the rank correlation matrix for the results of the generation method just described will not be precisely that specified. Even samples generated from uncorrelated distributions are likely to have nonzero correlation, just because of random noise. Iman and Conover (1982b) describe a technique that, when combining sample values for the inputs

8.5. Monte Carlo and Other Sampling Methods

to form scenarios, can control the resulting correlations. Thus, it produces results whose correlations are more exactly those specified. This may be used even for variables that are intended to be uncorrelated, since it can reduce incidental correlation from the sampling process to nearer zero. In effect this increases the uniformity of the sampling process, not simply over each individual input dimension but also over the joint domains of pairs of inputs. This reduces the consequent noise in the simulation process, and increases sampling efficiency.

8.5.8. Importance Sampling

In crude Monte Carlo or standard Latin hypercube sampling, all input values are generated equal, in the sense that the probability of any value being generated is proportional to the probability density at that point. If one is more interested in some parts of the output distribution than others, it is often possible to use importance sampling to generate more sample points to illuminate these aspects of special interest, and fewer in other parts (Clark, 1961).

For example, in a safety analysis of a reactor vessel, events that could lead to a failure are likely to be of particular interest. To examine this more efficiently, one may artificially inflate the probability of choosing input values that are likely to lead to this, so that even if the prior probability of vessel failure is very small, one can still simulate a significant number of events that lead to failure. Thus, one might adjust the sample generation process so that inputs that lead to higher internal pressure and inputs that lead to lower vessel strength are sampled disproportionately. The adjustment to the probability of each input value is termed its importance weight. The importance weight of the corresponding output value is the product of importance weights of all the input values that lead to it. To estimate the true probability distribution for the output value, you must restore the actual probability of each sample that is inversely proportional to its importance weight. This approach, which has been shown to be widely used in scientific applications, has considerable (so far largely unrealized) potential for uncertainty propagation in risk analysis problems with low probability, high consequence risks, where the extreme upper tail of the distribution is often of much greater interest than the rest of it.

8.5.9. Measures of Uncertainty Importance

Monte Carlo and other random sampling techniques have occasionally been criticized for not supporting attribution of uncertainties (e.g., Cox and Baybut, 1981). But in fact a variety of rather powerful measures of uncertainty importance are available. One useful approach is to compute the correlation between the sample of output values and the corresponding sample of values for each input. Let us consider \( n \) samples from the output and a single input,
8. The Propagation and Analysis of Uncertainty

denoted as $y_k, x_k$, for $k = 1$ to $m$. We compute the sample correlation as:

$$U_p(x,y) = \frac{\sum_{k=1}^{m} (x_k - \bar{x})(y_k - \bar{y})}{\sqrt{\sum_{k=1}^{m} (x_k - \bar{x})^2 \times \sum_{k=1}^{m} (y_k - \bar{y})^2}}$$

The correlation gives an estimate of the linear contribution of each input to the output uncertainty: It is inherently a global measure of uncertainty importance, averaging the effect of each input over the joint probability distribution for all other inputs.

Several related approaches have been demonstrated based on regression analysis of the output samples with respect to the uncertain inputs. Consider a least squares regression model fitted to estimate the output $y$ as a linear function of the inputs $x_j$. (Note that the index $j$ is over the $n$ inputs, where $k$ was over the $m$ sample values for one input).

$$\hat{y} = b_0 + \sum_{j=1}^{n} b_j x_j$$

The $b_j$ regression coefficients are measures of the linear sensitivity of $y$ to the inputs $x_j$ (Draper and Smith, 1981). They have the disadvantage that they depend on the units or scale of measurement of $y$ and $x_j$. A more useful measure of uncertainty importance, known as the standardized regression coefficient (SRC), may be obtained by multiplying each coefficient by the ratio of the estimated standard deviations of $x_j$ to $y$:

$$U_{SRC}(x_j, y) = \frac{b_j \times s_y}{s_j}$$

It is often useful to perform stepwise regression, producing a sequence of linear models consisting of 1, 2, 3, up to $n$ of the input variables respectively. Inputs are added one at a time to maximize the improvement in fit of the model according to $R^2$ value. The sequence in which they are selected is a useful measure of their uncertainty importance, as is the increment in $R^2$ they produce. Iman and colleagues (Iman and Conover, 1980; Iman and Helton, 1988) have also suggested the use of partial correlation coefficients. These are measures of the contribution of each uncertain input to the output uncertainty, after removing the effects attributable to the other inputs. They are particularly useful when there are significant correlations between the inputs.

Correlations, whether partial or not, and regression coefficients are a measure of the strength of linear relationship between input and output. They do not necessarily provide a good measure of nonlinear monotonic relationship. If the distributions of input or output are far from normal, particularly if they have one or two long tails, they are liable to distortion from the effect of outliers. One way to avoid this problem is to rank order the sample values for each input and for the output, and examine rank-order correlations. This is a good measure of the strength of monotonic relations, whether linear or not. It may also be useful to examine the effects of squares, products, and higher order combinations of inputs in the regression analysis to see if there are important nonmonotonic and interaction effects.

To understand more about the nature and strength of relationships between inputs and outputs of a model, it is often useful to examine scatter plots of one against the other. These can provide a lot of insight, show nonlinear effects, thresholds, and so on. and may be useful in suggesting relationships to test with regression (Iman and Davenport, 1982). For more details and illustrations of the use of these various measures, see Iman and Conover (1980, 1982); Iman and Davenport (1982); Iman and Helton (1985, 1988).

8.6. Fourier Amplitude Sensitivity Test

An approach that examines sensitivity to inputs, averaged over the input parameter space (although it does not provide a measure for attribution of probabilistic uncertainty), is the Fourier Amplitude Sensitivity Test (FAST), (Cukier et al., 1973; Schabib and Schuler, 1973; Cukier, Schabib, and Schuler, 1975; Cukier, Levine, and Schuler, 1978). The essence of this technique is to generate a curve in the parameter space that is a periodic function of each parameter, with a different frequency for each. The problem is to generate $x_{ij}$, for each parameter $x_i$, and each model run, $j = 1 \ldots m$:

$$x_{ij} = E[x_i] + v_i \sin(\omega_i x_j), \quad i = 1 \ldots n$$

where $v_i$ are positive constants chosen so that the parameter values vary between assigned upper and lower limits; $\{x_i\}$ is a set of integer frequencies chosen so there is no interference (correlation) between the parameters; $x_j$ is a parameter selecting points along the $n$-dimensional search curve. Equally spaced values, $s_j$, are chosen to generate the $x_{ij}$. The relative contribution of each input parameter to the range of the output can be measured by a discrete Fourier analysis of the output. The contribution of each input is measured by the contribution of its characteristic frequency, as specified by $\omega_i$, to the outputs.

8.7. Response Surface Methods

For large, computationally expensive models it is sometimes useful to build a simplified response surface, which is an approximation of the full model (Myers, 1971; Downing, Gardner, and Hoffman, 1985). The response surface is generally fitted to a moderate number of model runs. If many model runs
are needed for some application, then instead of expensively evaluating the whole model, it is possible to substitute the simplified response surface model and greatly reduce the computational cost. For example, if a large number of Monte Carlo runs are required for uncertainty propagation and analysis, these may be economically carried out using the response surface. This approach may be particularly useful for real time tasks, such as real time control of a complex system, a manufacturing process or aerospace vehicle. A response surface model can be fitted to a large and sophisticated model of the system; but when rapid response is required to predict the effect of control measures in real time, the simple response surface model may be used. This response surface approach has been developed for uncertainty analysis of some very large computer codes for simulation of the liquid metal fast breeder reactor (Vaurio, 1982). Another example involves a regional photochemical air pollution model (Milford, Russell, and McRae, 1988).

There are three key issues in response surface modeling: first, how to select the small sample of scenarios with which to run the large model. Second, how to screen the uncertain inputs and identify which ones need to be modeled explicitly. And third, how best to fit a response surface to these results. In complex engineering models, there may be tens or hundreds of uncertain inputs, and it may initially be unclear which of these are of any significance. Usually, inspection of the model structure and/or judgment from experience may be sufficient to rule out at least some of the inputs as possibly having significant impact on the output uncertainties. Discovering which of the rest are important must rely on examination of the model behavior.

A simple selection approach, perturbing one input at a time, keeping the rest at nominal values, is highly inefficient. It will require at least as many runs as uncertain inputs, and even then is restricted to modeling local behavior around the nominal scenario, ignoring nonlinearities and interactions between inputs. Combinatorial scenarios will cover a larger part of the model behavior, but require far too many model runs in general. Fractional factorial designs (FFD) (Box, Hunter, and Hunter, 1978) have been quite popular. These select a subset of the combinatorial scenarios. There is an extensive statistical literature on FFD, on how best to choose scenarios to be able to estimate higher order behavior with minimal runs. (See Box and Hunter, 1961a, 1961b, for a good expository article on two-level fractional factorials.) Others (e.g., Vaurio, 1982) have used Monte Carlo and related random sampling techniques, which they suggest as a convenient and reliable way to cover the input domain.

The main purpose of the sampling process is to identify those uncertain inputs that contribute most to the output, that is, essentially to perform uncertainty analysis. Usually just a few uncertain inputs are found to contribute the majority of the uncertainty in the output. The simplified response surface need model only the effect of these, and can generally ignore the other inputs. The

8.8. Selecting a Method

techniques for uncertainty analysis described in Section 8.5.9 may be used for this task in identifying which variables should be used in the response surface. A variety of correlation and stepwise regression techniques have been used (Vaurio, 1982). Depending on the model, it may be wise to examine quadratic and higher order relations to see if there are significant nonmonotonic relations or interactions. Vaurio (1982) also describes methods to test the significance of possible discontinuities in model behavior.

Once the important parameters are identified, the problem is to construct a response surface model that most accurately reproduces the output values as a function of them. The most common scheme is simple linear and quadratic regression models, fit to the test scenarios (Iman and Helton, 1988). For models with complex behaviors, more sophisticated fitted surfaces may be appropriate. Regionwise quadratics have been found to give good results, using a different quadratic function for different quadrants of the input hyperspace. The inputs and outputs may be transformed before trying to fit them. Of course, the more complex the functions to be used, the better the fit is likely to be, but the more effort and ingenuity is required of the analyst in devising it. The availability of flexible surface-fitting software can make this process much easier (Vaurio, 1980a, 1980b).

One difficulty with response surface methods is obtaining a reliable guide to the accuracy of the results. Statistical measures of goodness of fit of the surface to the selected points, such as R-square, or the maximum residuals, give a lower bound on the likely error. But they depend partly on the degrees of freedom of the surface: If the number of parameters is comparable to the number of points fitted, then a high degree of fit has little significance. If it is important to get a better idea of the accuracy, a small number of independent additional runs of the full model may be performed for validation. These should be chosen for scenarios distinct from the scenarios to which the response surface was originally fit. The response surface may guide selection of points that are expected to generate outcomes in particularly interesting regions.

8.8. Selecting a Method

As we have seen, there exists an almost overwhelming variety of different methods for representing, propagating, and analyzing uncertainties. They have been developed and applied in a wide range of modeling domains, in policy and risk analysis as well as more traditional areas of science and engineering. These include financial investment planning, physics, chemical engineering, nuclear engineering and safety analyses, ecological modeling, and atmospheric modeling, to list but a few. In the beginnings of uncertainty analysis, traditions about which method to use grew up within the shelter of different application areas. This resulted in a degree of isolation and incompatibility of views between
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analysis even though they were working on methodologically similar kinds of problems. However, in recent years there has been more extensive sharing of ideas between disciplines, which has led to a number of reviews and comparative experiments, applying different techniques to the same problem to identify their relative advantages and disadvantages. At least for some kinds of application, a degree of consensus about the appropriateness of particular techniques now seems to be starting to develop.

This last section of this chapter is intended to distill the findings from our discussion and from other comparative literature to help guide analysts confronted with the need to select a method for a particular problem at hand. After a brief discussion of the criteria for comparison, we examine the pros and cons for some of the key choices. Among those comparative studies we have found particularly useful have been Martz et al. (1983), and Iman and Helton (1985, 1988).

8.8.1. Criteria

As a counter to the natural tendency for one's thinking to be dominated by just one consideration, it is useful to list out the full range of criteria that may be relevant to choice of method. These criteria may be organized into the following four groups:

- **Uncertainty about the model form**: What is the relative importance of uncertainty about the form of the model versus the contributions of parameter uncertainty? If model structure and relationships are disputed or poorly known, extensive evaluation of parameter uncertainty within a specific model may be pointless and misleading. If the model structure is well characterized, parameter uncertainty analysis is typically appropriate.

- **The nature of the model**: How large is it, in terms of the number of uncertain inputs, and the computational cost of a single run? How large are the uncertainties? Is the response surface smooth, monotonic in its inputs, and is it reasonably approximated by simple functional forms? Or does it show complex, nonmonotonic, or discontinuous behavior?

- **The requirements of the analysis**: What is the main purpose of the analysis? Are significant actions to be based directly on its results? Is the uncertainty analysis intended to guide refinement of the model and/or decisions about what additional information to collect? Is the central tendency (mean or median) of the outputs the main interest, or is a solid characterization of the uncertainty also important? How precise an estimate of the full distribution is necessary? Are extreme tails of the output of importance? How much precision is needed in the identification and ranking of the main contributors to the uncertainty?

- **Resources available**: How much time (calendar time and staff time) is available to conduct the analysis? What kinds of skills and experience do the analysts have? What kinds of computing resources, and, in particular, what kind of software is available?

In technical comparisons of methods, it is easy to focus on computation costs, since they are often the simplest to quantify. But as computer resources continue to diminish in cost, for all but the most colossal models they will tend to be dominated by the other costs, particularly human resources. Thus, for models of moderate size (i.e., modest computational cost per run), the most important questions may be about the amount of human effort a method requires, to set up and run the uncertainty analysis, and to interpret the results.

8.8.2. When to Use the Method of Moments

When a model is simple and the uncertainties are small relative to its nonlinearities, the first order method of moments, that is, the Gaussian approximation and particularly its relative error formulation for products of powers, is very useful. In these cases, the application of the approach is straightforward, and lends itself to quick, back-of-the-envelope calculations. It provides a clear basis for uncertainty analysis, by partitioning up the variance of the outputs as the sum of the contributions for each input. This kind of approach is widely used in the physical sciences and deserves to be more widely known and used among policy and risk analysts. It is especially helpful in developing intuitions about how uncertainties combine and propagate.

Having said this, it is important to acknowledge that the uncertainties in policy and risk analysis are often rather large compared to nonlinearities in the models. Hence, first order approximations, representing the response surface as a hyperplane, can be quite inaccurate. Although there have been attempts to develop techniques using higher order approximations (e.g., Seiler, 1987), these get algebraically complicated rapidly as the complexity of the model increases. Moreover, it is hard to discover just how good or bad a given approximation may be to the actual model, and subsequently how safe it is to rely on the results. The basic problem is that these schemes are local, looking at perturbations around the nominal scenario, and may not work well globally.

An apparent advantage of the method of moments is that it requires only the first few moments of input distributions, typically the mean and variance, without needing complete specification of the entire distribution. But concomitantly, it provides only these moments for the output distributions. In applications such as nuclear safety analysis, where the tails of the distributions are of particular interest, this can be a serious deficiency.

There has also been considerable research on the development of adjoint methods for differential sensitivity analysis for complex dynamic models. However, analysts who have attempted to use these have reported they can be extremely difficult to implement, often requiring an effort for the uncertainty analysis comparable with the original model development effort (e.g., Iman and Helton, 1988). To remedy the analytic complexity of obtaining partial derivatives in complex models, one may employ automated systems for symbolic differentiation. In contrast, Monte Carlo and other sampling techniques are generally rather easy to apply to existing computer models. It is mainly a
matter of putting an outer repetition loop around the program to run it for multiple scenarios.

It is increasingly apparent that quite few sample runs are often sufficient, particularly with more efficient sampling strategies. Therefore, the computational advantages of the method of moments, in requiring fewer model runs, are less obvious. Moreover, for all but the most enormous models, the time the analyst spends implementing the model, and setting up and interpreting the uncertainty analysis, is more important than the computational cost. It is now clear that sampling methods provide measures of uncertainty importance that are at least as useful as differential methods. Finally, the difficulty of estimating the accuracy of the approximation is a major drawback of the method of moments. For all these reasons, it increasingly appears that sampling techniques are the technique of choice over the method of moments for all except simple near-linear models with small uncertainties.

8.8.3. Discrete Probability Tree vs. Monte Carlo

Among practicing decision analysts by far the most common approach to uncertainty analysis is using discrete probability distributions to form probability trees or, more generally, decision trees. Currently, the use of Monte Carlo approaches is considerably less frequent. Among the advantages of the discrete probability tree enumeration schemes are the following:

1. Provided the model is quite small, with not more than three or four uncertain quantities and decisions, the tree can be a clear and appealing representation. It is easy to explain, and the computations can be carried out with pencil and paper or hand calculator.
2. It is generally easier to express probabilistic dependencies among variables as discrete conditional probability distributions, than to express them in terms of correlations between continuous variables.
3. It is generally much easier to apply Bayes' rule to reverse conditioning in discrete probability trees than it is for continuous variables.

On the other hand, Monte Carlo and other sampling methods have some important advantages over tree schemes:

1. If uncertain quantities are continuous, there is no need to discretize them for sampling schemes. (If they are already discrete, this also poses no problems for Monte Carlo.)
2. The imprecision in the propagated distributions and uncertainty measures can be estimated easily by standard statistical methods, and improved simply by taking additional samples. The imprecision due to the discretization for tree-based methods is much harder to estimate.
3. Measures of uncertainty importance are more powerful than those typically used in tree enumeration schemes.
4. The computational effort is essentially linear in the number of quantities represented as uncertain, rather than exponential as it is in tree enumeration schemes.

In summary, tree enumeration schemes are appropriate for models that have a modest number of uncertain inputs. Typically, if there are more than a dozen or so uncertain inputs, they are likely to be computationally intractable. If there are complex probabilistic dependencies to be represented, and especially if Bayesian inference is required, then tree representations have important advantages. If there are not, then Monte Carlo methods may be more appealing. The advantages of its linear computational complexity and easily measurable precision are important, and the wider availability of flexible Monte Carlo software may lead to wider use of the technique for decision analysis.

If there are complex dependencies and Bayesian inference is required, and there are many uncertain quantities, it may be hard to find any tractable scheme. But by careful sensitivity analysis of deterministic models or uncertainty analysis of simplified models, it may be possible to identify a small number of uncertain inputs that dominate the uncertainty in the results. Then the use of the uncertain inputs can be treated as deterministic, and tree enumeration schemes may be rendered tractable.

8.8.4. What Type of Sampling Scheme to Use?

The various alternatives to crude Monte Carlo sampling, including the controlled variate, Latin hypercube sampling, and importance sampling schemes, all improve convergence rate at little extra cost, other than a slightly more complex program. Given software that provides these alternatives in a form that can be easily applied, there seems little reason not to use one of them. Latin hypercube sampling seems to be particularly valuable. Although it can introduce slight bias in the estimates of moments, in practice this seems negligible. Midpoint LHS is still better than standard LHS, as long as one can be sure the model does not contain any high frequency behavior, which is extremely unlikely in policy and risk models. The Iman and Conover (1982a) scheme for reducing incidental correlation between uncertain inputs to near zero is valuable in further improving the uniformity of sampling. Importance sampling appears to have been little used in policy and risk analysis, but it has considerable potential in cases where particular regions of the model domain are of special interest, as in the upper tails of failure frequencies in nuclear reliability analysis.

8.8.5. When to Use Response Surface Methods

For models that are very expensive to run, response surface methods (RSM) become attractive. The initial effort to develop a good response surface may be significant, but once it is available a wide variety of sensitivity and uncertainty analyses may be performed, provided they stay within the domain of the input space for which the surface was fit. The functional form and coefficients of the surface should themselves give considerable insight to which inputs are contributing most uncertainty and in what ways. The analytical effort in developing a response surface may be greatly eased by the use of flexible
software for screening input variables and exploring the fit of different surfaces, such as SCRREEN and PROSA-2 (Nuño, 1980a). Given an appropriately well-behaved function, moment methods and RSM may in many cases give greater accuracy for similar computational effort (or equivalently the same accuracy for less computational effort) than Monte Carlo. However, with Monte Carlo it is easy to use standard statistical tests to find out just how accurate the output distribution is, in terms of confidence intervals on moments and fractiles. But with the former methods, except in very simple cases it is difficult to find out just how accurate the results are, and whether, in fact, this is one of the cases in which results are poor, at least in certain parts of the domain.

8.8.6. The Importance of Software

In most cases, a major factor in selecting an approach to uncertainty propagation and analysis is the effort spent setting up and conducting the analysis. This can be much affected by the availability of easy-to-use and flexible software to support the approach. Lack of software or computing resources will tend to favor approaches that can be done without special programs, primarily Gaussian approximation or probability trees for small models. Several packages are now available running on microcomputers to perform decision analysis that can support uncertainty analysis using probability trees (three are reviewed in Henrion, 1985). There are also a number of packages to support Monte Carlo analysis, including Latin hypercube sampling and correlational uncertainty analysis. These include EFP3 (Execoum, 1983), Demos (Henrion and Morgan, 1985), and packages for Latin hypercube sampling (Ivan, Davenport, and Zeiger, 1980; Iman and Shortencarier, 1984; Iman, Shortencarier, and Johnson, 1985). New software packages for decision analysis and Monte Carlo simulation are becoming available all the time. Issues in the design and use of computer packages for uncertainty analysis are addressed in more detail in Chapter 10.

References


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References


