CHAPTER 3

UNCERTAINTY ANALYSIS IN ECOLOGICAL STUDIES:

An Overview

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3.1 INTRODUCTION

Large-scale simulation models are essential tools for scientific research and environmental decision-making because they can be used to synthesize knowledge, predict consequences of potential scenarios, and develop optimal solutions (Clark et al. 2001, Berk et al. 2002, Katz 2002). Modeling is often the only means of addressing complex environmental problems that occur at large scales (Klepper 1997, Petersen 2000). For example, investigations of global climate change (Wobbles et al. 1999), regional assessments of net primary productivity and carbon dynamics (Jenkins 1999, Peters et al., Chapter 7, Law et al., Chapter 9), and landscape analysis of fire spread (Hargrove et al. 2000) rely heavily on simulation modeling at various scales. However, uncertainty in simulation modeling is often overlooked even though it is a fundamental characteristic of modeling that can be caused by incomplete data, limitations of models, and lack of understanding of underlying processes (Beck 1987, Reckhow 1994, Clark et al. 2001, Berk et al. 2002, Katz 2002, Stott and Kettleborough 2002, Urban et al., Chapter 13). If simulation results are to be useful, researchers must show the reliability of the model output by providing information about model adequacy and limitations, prediction accuracy, and the likelihood of scenarios (Clark et al. 2001, Katz 2002).

Uncertainty affects every aspect of modeling (Reckhow 1994, Klepper 1997, Jansen 1998, Katz 2002, Stott and Kettleborough 2002, Urban et al., Chapter 13). Data may contain errors that result from problems with sampling, measurement, or estimation procedures (O'Neill and Gardner 1979, Regan et al. 2002). Incomplete data are a common problem, especially in spatial modeling at broad scales. Models are imperfect because they are simplifications of real systems and always have errors in their assumptions, formulation, and parameterization. Moreover, effects of these errors on model adequacy are often insufficiently evaluated (Beck 1987, Reckhow 1994). In fact, most large-scale models are not fully validated, partly

J. Wu, K.B. Jones, H. Li, and O.L. Loucks (eds.)
Scaling and Uncertainty Analysis in Ecology: Methods and Applications, 43–64
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because validation data are not available (sometimes no data can be collected under the existing technological and logistical constraints) and partly because techniques for validating spatial models have not been perfected. Although the importance of uncertainty in modeling is well recognized, few studies of ecological modeling provide critical information about uncertainty, confidence levels or likelihood associated with simulation results (Reckhow 1994, Clark et al. 2001, Rypdal and Winiwarter 2001, Katz 2002). This lack of discussion and reporting is unfortunate because predictions that are not accompanied by information about uncertainty are of limited value in policy- or decision-making. Researchers must adopt a new modeling philosophy that requires that uncertainty in models and modeling be understood, quantified when possible, and reduced to an acceptable level when feasible.

Scaling is the translation or extrapolation of information from one scale to another in time or space or both (Blöschl and Sivapalan 1995, Wu 1999, Wu and Li, Chapters 1 and 2). For example, scaling is needed to resolve most of the large-scale management problems because most of our knowledge and data is obtained by means of small-scale research. In the process of scaling, errors in data and models may be propagated into results. It is not adequate simply to ask how to scale: one must ask how to scale with known reliability and uncertainty even when ecological systems and models involved are often complex. Thus, uncertainty analysis is an essential part of scaling because it provides critical information about the adequacy of models or algorithms used in the scaling process and about the accuracy of scaling results (Katz 2002).

In this overview, we will focus on the major concepts and techniques of uncertainty analysis associated with up-scaling methods (i.e., those that extrapolate information from fine scales to coarse scales; Wu and Li, Chapters 1 and 2). Specifically, we will identify sources of uncertainty in the scaling process and illustrate approaches to and techniques of uncertainty analysis. Because translating or extrapolating is usually done with the help of models (Wu and Li, Chapter 2), scaling can be regarded as a special case of modeling (i.e., modeling with changing scales). Therefore, most discussion of uncertainty in modeling is directly applicable to uncertainty in scaling. Also, it should be noted that most of the techniques of uncertainty analysis discussed below are more suitable for ecological models with low to intermediate complexity than for highly complex models like the general circulation models employed in climate change research (Allen et al. 2000, Forest et al. 2002, Stott and Kettleborough 2002).

3.2 UNCERTAINTY AND RELATED CONCEPTS

The term uncertainty implies some kind of error, inexactness, unreliability, and imperfection in our knowledge and understanding of the systems under investigation (Funtowwicz and Ravetz 1990, Petersen 2000, Regan et al. 2002, Katz 2002). Some degree of uncertainty is unavoidable in modeling and scaling because there are always errors associated with the stochastic nature of ecological processes, system complexity caused by spatial heterogeneity and nonlinear relationships, unreliability and unavailability of data, and/or imperfections of models (Mitchell and Hulme

1999, Katz 2002, Regan et al. 2002, Stott and Kettleborough 2002, Groffman et al., Chapter 10, Urban et al., Chapter 13). However, many of the uncertainties in simulation modeling should be quantified and reduced, and different sources of uncertainty be ranked with respect to their relative contributions to errors in model output. The term uncertainty is sometimes used to mean levels of risk involved in a scenario, action, or inaction defined by policy or management decisions, but such usage may require caution because risk implies probability and consequence that can be themselves uncertain (Pate-Cornell 1996, Katz 2002). All of these uncertainties should be studied thoroughly and systematically (Reckhow 1994), but they may require different treatments. Some uncertainties can be quantified and reduced (e.g., input uncertainty; Katz 2002), some can be quantifiable but hard to reduce (e.g., natural variability of data; Nauta 2000, Regan et al. 2002), some may be unquantifiable (e.g., model uncertainty; Beck 1987, Klepper 1997, Regan et al. 2002, Stott and Kettleborough 2002), and some may have only insignificant effects on model output in a particular modeling exercise (e.g., omission of minor processes or variables; Katz 2002).

Uncertainty analysis is the process of assessing uncertainty in modeling or scaling to identify major uncertainty sources, quantify their degree and relative importance, examine their effects on model output under different scenarios, and determine prediction accuracy (Jansen 1998, Katz 2002). Uncertainty analysis is employed primarily to determine whether the estimated prediction uncertainty is acceptable for a particular model application and, if it is not, to highlight factors whose uncertainty is pivotal in policy considerations and to recommend ways of reducing prediction error (Jansen 1998, Katz 2002). Specifically, uncertainty analysis addresses questions like: What is the magnitude of error in large-scale estimates? How is error propagated in the scaling process? Which factors are most critical, most poorly understood, or least predictable? How can errors be reduced? What is the probability that an event or scenario will occur? Uncertainty analysis can increase the credibility of modeling even when much of uncertainty may not be reduced (Rykiel 1996, Rypdal and Winiwarter 2001). Thus, understanding, quantifying, reporting, and ultimately reducing uncertainty in large-scale assessment is of great interest to policy makers.

Sensitivity analysis and scenario analysis are closely related to uncertainty analysis (Saltelli et al. 2000, Melching and Bauwens 2001, Katz 2002). The similarity is that they all involve in running models under perturbations (e.g., changes in model structure, parameters, or input data) and may use similar techniques (e.g., Monte Carlo simulation). Sensitivity analysis quantifies the rate of change in model output when one or more input variables and parameters are varied by a fixed amount or proportion while the others are held constant (Klepper 1997, Katz 2002). A more formal approach to sensitivity analysis with various statistical sampling methods may also be used (Saltelli et al. 2000). Sometimes, the absolute rate of change is converted into a relative measure to make comparisons among different parameters more meaningful (i.e., absolute vs. relative sensitivity). Sensitivity analysis is often used as a model-testing tool to examine model behavior in terms of the most sensitive parameters. A scenario is a possible future boundary condition (represented by a set of key input values or sometimes by trajectories of

key input values) on the basis of which simulations are run (Clark et al. 2001). In other words, a scenario is the IF in the WHAT-IF questions of simulation modeling. In scenario analysis, all of the inputs are changed simultaneously. Scenarios are model input rather than predictions, but they may be defined by results of previous simulation studies. Scenario analysis usually focuses on policy-relevant possibilities of future conditions (e.g., best case vs. most likely case vs. worst case), and is an effective means of communicating a large amount of technical information obtained by simulations with large, complex models (Wobbles et al. 1999, Clark et al. 2001, Katz 2002). Both sensitivity and scenario analyses may best be regarded as necessary precursors to full-fledged, probability-based uncertainty analysis (Katz 2002).

3.3 SOURCES OF UNCERTAINTY

Uncertainty in modeling may come from many different sources, which in turn may be classified into many different categories (O'Neill and Gardner 1979, Funtowwicz and Ravetz 1990, Jansen 1998, Petersen 2000, Katz 2002, Stott and Kettleborough 2002, Urban et al., Chapter 13). However, most classifications of uncertainty sources consider similar sets of factors when viewed as a whole. In this overview, we discuss three main sources of uncertainty: models themselves, input data, and scaling algorithms (O'Neill and Gardner 1979, Jansen 1998, Katz 2002, Urban et al., Chapter 13). Note that uncertainty in scaling algorithms may be regarded as part of model uncertainty, but we separate them here because it presents a unique problem and is a focus of this book.

3.3.1 Model

Model uncertainty has two basic components, model structure and model parameters (Figure 3.1; Morgan and Henrion 1990, Klepper 1997, Katz 2002). Model structure uncertainty is caused by the modeling processes of simplification and formulation. Model simplification is essential to modeling and is the identification and selection of the processes, relationships, and variables that are the most important to the system of interest and the modeling objectives. Simplification is done by assuming that some processes may be ignored because they explain an insignificant amount of variability in model predictions. Model simplification may also reflect a failure to understand certain processes. Model formulation focuses on the mathematical translations of relationships and the designs of algorithms and computer codes. Because many of the assumptions and subjective judgments must be made during model construction but are not often reported, most hidden error is created in the process of model formulation. Therefore, model structure uncertainty is the failure to include relevant processes and the unreliability caused by deficiencies in confidence, quality, and scientific basis of the equations and algorithms that represent the selected processes and their interactions.

Model parameter uncertainty is introduced by the modeling process of parameterization of models (Morgan and Henrion 1990, Klepper 1997, Katz 2002).

Model parameterization is the estimation and calibration of parameters. Calibration produces a set of optimal parameter values by forcing selected model outputs to agree with testing data. Model parameter values are built into models and may be fixed or change in space and time. Model parameter uncertainty results from imperfect knowledge about the parameters, lack of data or understanding, and errors in the estimation and calibration processes. Given the large number of parameters involved in ecological models, the first step in uncertainty analysis is often to perform sensitivity analysis to identify the parameters that may have significant effects on model output. Uncertainty analysis requires that statistical distributions (or ranges, means, variances) of parameters be known. However, a common problem in uncertainty analysis is that the accuracy of measurements and/or estimates of parameters are unknown. Modelers often have no information about the variability of parameters and have to make assumptions about parameter distributions (Urban et al., Chapter 13).

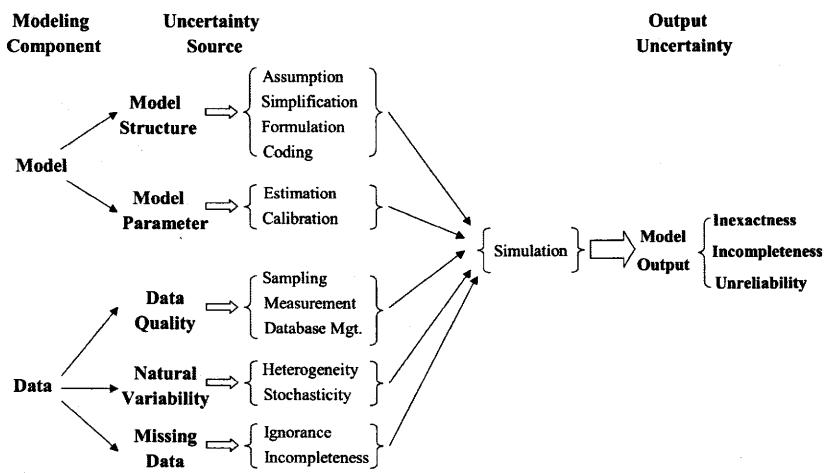

Figure 3.1. Sources of uncertainty in scaling and modeling.

A lesser known but perhaps more critical problem in model parameterization is the use of free (or fuzzy) parameters in model functions (Petersen 2000, Berk et al. 2002). Free parameters are those whose values are arbitrarily assigned or tuned in model calibration to make the model output fit the testing data. Problems arise when a model contains many free parameters that have no physical meanings and thus are not subject to evaluations by observation or measurement. Although the use of free parameters is often unavoidable when models are complex, their overuse can introduce large uncertainty into model output, and their uncertainty can severely diminish the value of the calibrated model (Petersen 2000). Thus, if models require intensive calibration of key parameters before they can be applied to new sites, they are of limited use in large-scale spatial simulation or scaling because data needed for

such calibration may be unavailable and because model predictions may have high uncertainty due to the calibration. Reducing the number of free parameters in models should alleviate these problems and improve models (Petersen 2000) but poses a daunting challenge to model developers.

3.3.2 Input Data

Input data are those required to run models for specific applications. Input data are usually from measurements or observations and are composed of systems attributes and driving variables. Systems attributes define the simulation settings about characteristics of the modeled system and its environment (e.g., evapotranspiration rate, leaf area index, spatial distribution of vegetation). Systems attributes are often fixed as constants even though they may have a range of values and change over time. Uncertainty in systems attributes is a major focus and is relatively easy to handle in uncertainty analysis. Driving variables define the environmental conditions (e.g., climate variables) that change in space and time, but are not affected by the model. Driving variables are often not examined in uncertainty analysis, but treated as part of the simulation conditions. This is primarily due to technical difficulties involved. However, if variability of a driving variable needs to be considered, it can be done via scenario analysis.

Data uncertainty can be caused by unknown data quality, high natural variability of the system, or lack of information (Figure 3.1; O'Neill and Gardner 1979, Jansen 1998, Regan et al. 2002). Data quality is affected by instrument or measurement errors, sampling errors, and database management errors. Data quality is always a concern in modeling and it becomes a major problem in uncertainty analysis when errors in sampling or measurement for observed data and errors in interpolation or aggregation for estimated data are not reported (Berk et al. 2002, Regan et al. 2002). The data employed in modeling exercises are usually collected for other purposes, and this often causes difficulties in model construction and testing because they may not adequately represent key characteristics of the modeled system. In such cases, critical reviews of data quality should be required before model simulations. A related problem is inappropriate use of data outside their intended purpose or domain. For example, whether model testing data are obtained independently and at the appropriate scale is a question of data quality.

Variability in ecological systems may result from spatial heterogeneity of environmental conditions or from randomness in interactions of different processes. Natural variability of data is a critical factor in uncertainty analysis that must be considered because modeling only with average values can produce severe bias in predictions, especially for nonlinear models (O'Neill 1979, Scherm and van Bruggen 1994). Spatial variability in systems attributes and driving variables need to be effectively incorporated into simulation modeling. We will discuss this point in the next section. Natural variability in data is the most studied in uncertainty analysis.

Lack of information is a pervasive problem in ecological research, especially in large-scale modeling where the emphasis is on synthesis. Unavailability of large-scale and long-term data greatly hinders uncertainty analysis and model evaluation

because large-scale processes often cannot be predicted directly from fine-scale data (Clark et al. 2001). Thus, it is imperative to obtain experimental and observational data at landscape or regional scales. Other data availability concerns include inadequacy of resolution and duration of observational studies, and gaps in temporal and spatial coverage (Clark et al. 2001). Techniques for dealing with missing data must be developed for scaling; at the present state of knowledge, data requirements often cannot be met and uncertainty analysis must be conducted with key data missing (Berk et al. 2002). Missing data is the uncertainty source that cannot be quantified (Funtowwicz and Ravetz 1990).

3.3.3 Scaling Algorithm

Scaling algorithms are a new source of uncertainty. One perspective of scaling is that it is an uncertainty problem of error propagation. This is partly because the factors that cause problems in scaling (e.g., spatial heterogeneity, nonlinearity) are also those that contribute greatly to uncertainty (Schulze 2000). Scaling in space brings forward two causes of uncertainty: mismatch of scales in model or data and spatial heterogeneity of system variables and parameters. Mismatch of scales is an issue of model adequacy and occurs when models are applied at scales different from those for which they have been developed or when the support of a model (or data) changes with changing scales. Support refers to the nature of the modeled entities, such as size, shape, orientation, and heterogeneity (Heuvelink 1998a, Wu and Li, Chapter 1), and changes of the support may cause changes in parameter values and even in functional forms of the model (Heuvelink 1998a, Katz 2002). Models are often developed for application at a specific scale or domain of scales (Reynolds et al. 1993, Heuvelink 1998a, Katz 2002). Thus, when a model is applied outside its designed domain of scales, the uncertainty of model structure may increase as a consequence of loss of model adequacy (Rykiel 1996). Spatial heterogeneity and its representation in scaling algorithms is a major source of scaling uncertainty. Ecological processes and phenomena exhibit both stochastic and patterned variations over a wide range of spatial scales. Such spatial heterogeneity increases system complexity and raises questions about the adequacy or representativeness of sampling methods and data. The problem of accounting for spatial heterogeneity explicitly in scaling (or modeling in general) is a critical challenge and remains to be resolved (Hunsaker et al. 2001, Lowell and Jaton 1999, Groffman et al., Chapter 10, Urban et al., Chapter 13). The scale-specific nature of models and data and the heterogeneous characteristics of the system must be considered in scaling.

3.4 METHODS OF UNCERTAINTY ANALYSIS

Uncertainty analysis focuses on effects of uncertainty from different sources on model output under multiple scenarios. Uncertainty analysis is not employed routinely in ecological studies mainly because the existing techniques are neither widely known nor universally applicable and effective. This section reviews the

existing techniques of uncertainty analysis and points out their key characteristics and deficiencies. We discuss: (1) model evaluation to examine model structure uncertainty, (2) examination of error propagation to quantify uncertainties in model parameters and input data, and (3) prediction accuracy and error partitioning to present scaling (or model output) uncertainty.

3.4.1 Model Evaluation: Model Structure Uncertainty

Model structure uncertainty can affect model output significantly, but it is often not addressed in traditional uncertainty analysis (Morgan and Henrion 1990, Klepper 1997, Katz 2002, Regan et al. 2002). Models that are to be employed to solve real-world problems should first be subjected to model testing. Uncertainty analysis remains important even if model uncertainties have been dealt with by means of sensitivity analysis during model testing. It is critical to establish prediction confidence, especially when models must be applied to new sites or systems. A complete analysis of uncertainty that deals with all major sources of uncertainty should be pursued whenever possible (Reckhow 1994). Thus, it is a good practice to treat evaluation of model adequacy as part of uncertainty analysis (Heuvelink 1998a).

We use the term model evaluation in preference to the controversial term model validation (Oreskes et al. 1994, Rykiel 1996). Because models are always imperfect, it is the adequacy, not the validity, of models that is to be determined. Beldring (2002) defined two important aspects of model evaluation: scientific evaluation and performance evaluation. Scientific evaluation examines the extent to which the model's behavior is consistent with prevailing scientific theory and determines whether the model can describe the physical processes of interest. Performance evaluation determines the degree to which model-predicted values agree with a corresponding set of reliable and independently obtained observations. Model evaluation is usually done in the process of model construction, but a more detailed, systematic analysis should also be performed in model applications to ensure a model's practical value.

In practice, model evaluation examines the degree of adequacy in a model's assumptions, simplifications, formulations, and predictions (Rykiel 1996). Model adequacy is defined operationally by the following criteria of model behavior and prediction accuracy (Cale et al. 1983, Oreskes et al. 1994, Rykiel 1996, Beldring 2002): (1) Models should be consistent with prevailing scientific theory and concepts; (2) Models should have no detectable flaws in internal structure and logic chain; (3) Models should contain all necessary components, critical variables and processes to achieve the objectives; (4) Models should yield predictions that agree with observations; (5) Models should incorporate well-tested submodels with sound (acceptable) algorithms or formulations; (6) Models should be used within the domain of designed applicability and scales; (7) Models should be tested for multiple state variables, in multiple years, and at multiple locations (systems); (8) Models should produce results with acceptable confidence levels. This last criterion is added because of the recognition of the important roles that uncertainty analysis plays in establishing credibility of models. However, specifics about the

implementation of this criterion still need to be developed because what constitutes an acceptable confidence level will depend on the objectives of a particular application. Although any deviation from these criteria can cause serious problems, a determination of model adequacy is in essence a judgment that takes into account the objectives of the study and the characteristics of the system of interest (Rykiel 1996).

Some of the model structural errors identified in model evaluation can be eliminated, as when modifications of the model can successfully remove the inconsistencies with theory and the logic flaws in model formulation and algorithms. Some can be quantified, as when outputs from alternative models can be contrasted to determine differences in their agreements to observations (Jansen 1998). Some can be reduced, as when mismatch of scales in models and data can be avoided or corrected and when missing critical variables and processes can be included. Unfortunately, some model structural uncertainty is not quantifiable and cannot be reduced or eliminated because it reflects imperfections that are inherent in all models (Beck 1987, Klepper 1997, Katz 2002, Stott and Kettleborough 2002). However, there are ways to cope with this unquantifiable uncertainty. Some techniques, like the Bayesian Forecasting System (Krzysztofowicz 1999a), combine all of the untreatable uncertainty and provide some measure of it as a whole. Also, good model testing can go a long way in reducing uncertainty. The key is to perform model evaluation thoroughly and systematically.

Model comparison can provide a benchmark for and insight into model uncertainty, especially when no data are available for model testing (Klepper 1997, Jain et al. 1997, Berk et al. 2002). One model may be compared with another to identify possible problems. Large differences in key model behavior indicate a need for detailed analysis and evaluation of the model under study. Similar to the hierarchical modeling approach to scaling (Reynolds et al. 1993), a fine-scale mechanistic model can be used as a surrogate for reality in testing models of lesser complexity (Jansen 1998, Urban et al., Chapter 13). However, model uncertainty cannot be quantified through such inter-model comparison alone because the true system values and formulations are still unknown. Moreover, similarity of model predictions is not a sufficient indicator of the new model's predictive quality (Jansen 1998). Thus, model comparison is useful but limited in its capability to determine model uncertainty.

3.4.2 Error Propagation: Uncertainties in Model Parameters and Input Data

Errors propagate from model parameters and input data to model outputs in the process of modeling or scaling. In essence, to quantify errors and their propagation is to determine how variances or standard deviations of random variables get combined and manifested in the model predictions or large-scale estimates of some state variables. The variability in the state variables (i.e., model output) is then used as a measure of the output uncertainty. Many techniques can be used to analyze uncertainties in model parameters and input data. These include applications of probability theory, Taylor series expansion, Monte Carlo simulation, generalized likelihood uncertainty estimation, Bayesian statistics, and sequential partitioning

(Gardner and O'Neil 1983, Gardner et al. 1990, Rastetter et al. 1992, Heuvelink 1998b, Jansen 1998, Wiwatenadate and Claycamp 2000, Katz 2002). In this section, we will describe these major techniques of uncertainty analysis. Other techniques (e.g., the fuzzy set method, Franks and Beven 1997, Scherm 2000; the Rosenblueth's method of approximation, Heuvelink 1998b; the fingerprinting techniques of climate variability, Allen et al. 2000, Forest et al. 2002, Stott and Kettleborough 2002) also exist. We refer the reader to the cited literature for methods not covered here.

To demonstrate these techniques, we suppose a simple system with three random variables, X, Y, and Z, in which Z is a monotonous function of X and Y:

$$Z = \Phi(X,Y). \tag{3.1}$$

We use μ_Z, σ_Z^2, μ_X, σ_X^2, μ_Y and σ_Y^2 to denote the means and variances of Z, X and Y. Note that X and Y can be either predictive variables or model parameters, and that Φ is a model to estimate output Z from inputs X and Y.

3.4.2.1 Probability theory

Probability theory method employs probability theory of moments of linear combinations of random variables to define means and variances of random functions (Wiwatenadate and Claycamp 2000). The essence of this approach is to calculate analytically the mean and variance of the output as a function of random variables of input, using the basic statistics of the random variables as follows. For the case of Z as an addition or subtraction function of X and Y, i.e.,

$$Z = \Phi(X,Y) = X \pm Y, \tag{3.2}$$

the mean and variance of Z can be calculated by the equations

$$\mu_Z = \mu_X \pm \mu_Y \tag{3.3}$$

$$\sigma_Z^2 = \sigma_X^2 + \sigma_Y^2 \pm 2 \cdot \sigma_{XY}. \tag{3.4}$$

For the case of multiplication, i.e.,

$$Z = \Phi(X,Y) = X \cdot Y, \tag{3.5}$$

similar equations can be used to calculate the mean and variance of Z, i.e.,

$$\mu_Z = \mu_X \cdot \mu_Y, \tag{3.6}$$

$$\sigma_Z^2 = \sigma_X^2 \cdot \sigma_Y^2 + (\mu_Y)^2 \cdot \sigma_X^2 + (\mu_X)^2 \cdot \sigma_Y^2. \tag{3.7}$$

Here, X and Y are assumed to be independent. If X and Y are correlated, the variance equation can get complicated. Similar equations can also be derived for the case of division (or ratio), but the variance equation may not always exist.

The probability theory method is powerful. Its main advantage is that it is analytical and provides exact solutions, i.e., it has neither estimation error nor approximation error. For example, it works when one knows the functional form and the basic statistics of the random variables (e.g., means, variances). For example, when dealing with relationships from literature, one does not have to have the raw data for X and Y. Thus, use of the probability theory method to study error propagation is straightforward for simple linear models. The disadvantage of the method is that it does not apply to nonlinear functions. However, it may be used to deal with uncertainties in complex models when combined with other techniques.

3.4.2.2 Taylor series expansion

The Taylor series method uses the Taylor series expansion at the point of (μ_X, μ_Y) to estimate the mean and variance of a simple function of random variables (Rastetter et al. 1992, Heuvelink 1998b). The idea of the Taylor series method is to first approximate the model by a linear function and then solve analytically for the combined error from the error propagation. In most situations, the first or the second order Taylor approximation is sufficient. Higher order Taylor methods are seldom used because the gain in reduced approximation errors may be greatly outweighed by the increased complexity.

Where the second order Taylor approximation is employed, the method can be presented as follows. For the same system defined by Equation 3.1, the mean of Z is defined by applying the original function with the means of the component random variables, and the variance of Z is estimated by the Taylor series expansion, i.e.,

$$\mu_Z \approx \Phi(\mu_X, \mu_Y), \tag{3.8}$$

$$\sigma_Z^2 \approx \left[\partial\Phi/\partial X\right]^2 \cdot \sigma_X^2 + \left[\partial\Phi/\partial Y\right]^2 \cdot \sigma_Y^2 + 2 \cdot \left[\partial\Phi/\partial X\right] \cdot \left[\partial\Phi/\partial Y\right] \cdot \sigma_{XY}, \tag{3.9}$$

where $\partial\Phi/\partial X$ and $\partial\Phi/\partial Y$ are partial derivatives of Z with respect to X and Y, and σ_{XY} is the covariance. If X and Y are independent (i.e., $\sigma_{XY}=0$), then a simplified equation can be obtained by eliminating the covariance term in Equation 3.9.

The Taylor series method is a useful alternative to the probability theory method, which cannot be employed when the random function Φ is complex. One important characteristic of the method is that the function can be of any kind; but obviously, different types of equations will have different approximation errors. Thus, the main

advantages of the method are that it is analytical, is flexible in terms of functional forms, and can be applied to models of moderate complexity. The main disadvantages are that it requires that models be presented as differentiable functions and that the approximation errors are usually unknown. The Taylor series method has been used in ecological modeling for carbon dynamics in peatland (Bubier et al. 1999) and for water quality in a Florida watershed (Zhang and Haan 1996).

3.4.2.3 Monte Carlo simulation

The Monte Carlo method computes output statistics (means, variances) by repeating simulations with random sampling of input variables and model parameters (Gardner and O'Neil 1983, Gardner et al. 1990, Rastetter et al. 1992, Heuvelink 1998b, Jansen 1998, Katz 2002). The basic procedures are to define input distributions, sample randomly from the input distributions, run simulations with repeated samplings, and determine probability distribution for the output.

The method can be presented as follows. For a model of any complexity (e.g., Equation 3.1), a realization of Z is obtained by

$$Z_i = \Phi(X_i, Y_i) \tag{3.10}$$

with X and Y being defined by

$$X_i = \{ X \mid X \sim N(\mu_x, \sigma_x) \} \tag{3.11}$$

$$Y_i = \{ Y \mid Y \sim N(\mu_y, \sigma_y) \} \tag{3.12}$$

where X_i and Y_i are values obtained from samples of normal distributions, and all other terms are the same as defined previously. With repeated sampling of size N, the statistics of the output can be calculated by

$$\mu_Z = \sum_i Z_i \Big/ N \tag{3.13}$$

$$\sigma_Z^2 = \sum_i (Z_i - \mu_Z)^2 \Big/ N - 1. \tag{3.14}$$

Notice that both X and Y are assumed to be independent and have normal distributions. Joint distributions are required if the independence assumption does not hold.

The Monte Carlo method is the most commonly used technique for uncertainty analysis because it has no strict requirement about the exact formulation of the function and is therefore easily implemented and generally applicable. The function can be either a simple empirical model or a complicated dynamic model; the steps of

Monte Carlo error analysis effectively remain the same because the method treats the function as a black box (i.e., only input and output are considered) and studies the resulting outputs by systematically sampling from the input space. The main disadvantages of the Monte Carlo method are that the results are not in an analytical form and that joint distributions for correlated variables are often unknown or difficult to derive. The Monte Carlo method is computationally intensive, but one can employ sampling schemes to reduce the computation burden. A common sampling scheme is the Latin hypercube sampling in which the range of a variable is stratified and each stratum is sampled once with an equal probability (McKay et al. 1979). The Monte Carlo method has been used to study uncertainty related to forest dynamics (Gardner et al. 1990), water quality (Gardner and O'Neil 1983, Zhang and Haan 1996), soil acidification at the European scale (Kros et al. 1999), and nitrate leaching at a regional scale (Hansen et al. 1999).

3.4.2.4 Generalized likelihood method

Generalized likelihood uncertainty estimation (GLUE) is a statistical technique for simultaneously calibrating the parameter and estimating the uncertainty of predictive models (Beven and Binley 1992, Zak and Beven 1999). It operates on the assumption that many parameter sets may be equally acceptable in producing reasonable simulations of the observed data. The method can be presented as follows (Zak and Beven 1999, Brazier et al. 2000). First, a likelihood measure is selected to determine the goodness of fit in comparing observations with model predictions. This measure is chosen on basis of its appropriateness in relation to the model, the observed data, and the objectives of the study. For example, if the absolute error is chosen as the likelihood measure, the likelihood function for a single observation is given by

$$L(Z \mid Z_{Obs}) = \left[1 - \left(\left|Z_{Obs} - Z\right| / Z_{Obs}\right)\right]^N \tag{3.15}$$

where Z_{Obs} is the observed value of the predicted variable Z, and N is the shaping factor of the likelihood function (Zak and Beven 1999). Second, Monte Carlo simulations are run with all parameter sets, using the following equations,

$$X_i = \{X \mid X \sim U(a,b)\} \tag{3.16}$$

$$Y_i = \{Y \mid Y \sim U(c,d)\} \tag{3.17}$$

where X and Y are uniformly distributed parameters with ranges of (a,b) and (c,d), respectively. Third, a predetermined threshold, L^*, is used with the likelihood measure to identify and exclude those parameter sets that perform poorly (i.e., having a likelihood of zero or below the threshold). This process defines an acceptable parameter space, R_a, which is composed of values of all physically

reasonable parameter sets from the potential parameter space in Monte Carlo simulations, i.e.,

$$X_i^*, Y_i^* \in R_a \tag{3.18}$$

given that

$$L\left(Z_i^* \mid Z_{Obs}\right) > L^*. \tag{3.19}$$

Finally, the simulation results with acceptable parameter sets are then to define likelihood weighted distributions of predicted results from which uncertainty bounds are derived.

GLUE is a hybrid technique for parameter calibration and output uncertainty assessment that combines Monte Carlo simulations and likelihood analysis. The advantage of GLUE is that it provides a probabilistic distribution of model prediction so that output uncertainty is defined. The probabilistic distribution is enhanced by the selection of the acceptable parameter space because only physically reasonable parameter sets are used. The disadvantage of GLUE is that it does not explicitly consider the effects of individual parameters on model predictions because it considers only sets of parameter values. However, sensitivity analysis may be performed to determine the relative importance of model parameters and the processes they represent. The same sensitivity analysis can also be used to reduce the number of parameters used in GLUE by selecting only those that show significant effects on model predictions (Zak and Beven 1999). Another disadvantage is that the applicability of GLUE is limited by the need for observations against which model predictions can be compared in the likelihood analysis. Such observations are often unavailable in scaling projects. GLUE has been used primarily in hydrological modeling (Zak and Beven 1999, Brazier et al. 2000).

3.4.2.5 Bayesian statistics

Bayesian statistical methods quantify uncertainty by calculating probabilistic predictions. The procedure has three stages: (1) determination of the prior probability distribution for model parameters, (2) construction of a likelihood function for the statistical model, and (3) derivation of the posterior probability distribution for the parameters by using the Bayes rule to adjust the prior distribution based on the observed data (Katz 2002). The Bayes rule states that the posterior probability distribution is proportional to the prior probability distribution multiplied by the likelihood, i.e.,

$$P\left(Z \mid Z_{Obs}\right) = P(Z) \cdot P\left(Z_{Obs} \mid Z\right) \Big/ P\left(Z_{Obs}\right) \tag{3.20}$$

where $P(Z \mid Z_{Obs})$ is the posterior probability distribution for the predicted variable Z given the observations Z_{Obs}, $P(Z)$ is the prior probability distribution of Z, $P(Z_{Obs} \mid Z)$ is the conditional distribution of the observations, and $P(Z_{Obs})$ is the marginal distribution of the observations. The probabilistic predictions generated by Bayesian statistical methods are used to define modeling uncertainty.

One example of such methods is the Bayesian Forecasting System (BFS) developed for deterministic hydrologic models by Krzysztofowicz (1999a, 1999b). The BFS first identifies the random inputs whose uncertainty significantly affects the model outputs and varies from forecast to forecast. Then, the BFS decomposes the total uncertainty into input uncertainty and model uncertainty. Krzysztofowicz (1999a, 1999b) proposed that model uncertainty should be the combined uncertainty from all other sources, including imperfections of the model, incorrect estimates of parameters, and incorrect estimates of deterministic inputs. The BFS has three components (steps): (1) the input uncertainty processor, which runs simulations with parameter values of the random inputs and defines the uncertainty in model output caused by the input uncertainty; (2) the model uncertainty processor, which yields the posterior density based on the prior density and the likelihood function; and (3) the integrator, which integrates input uncertainty and model uncertainty into a predictive distribution. The characteristics of Bayesian statistical methods in general and BFS in particular are that they are a process of learning from data, require prior probability distributions and observations, and provide probabilistic predictions in the form of posterior distributions.

3.4.2.6 Sequential partitioning

The sequential partitioning method is not a new technique, but rather a hybrid approach based on a new strategy (Rastetter et al. 1992). It may apply a combination of probability theory, Taylor series, and Monte Carlo methods in clearly defined steps or modules in the process of modeling or scaling up. The sequential partitioning method should be useful to deal with uncertainty in complex models when other methods are difficult to implement. The procedures employed vary from situation to situation, but the general approach is as follows. Complex models are first divided into independent compartments or modules, and appropriate techniques are used to identify the most critical variables in each module. Various methods are then employed to examine uncertainty associated with the critical variables from different compartments. For example, to study uncertainty in net ecosystem productivity, one may first use the Monte Carlo method to determine uncertainties related to the processes of photosynthesis and respiration separately, and then apply the probability theory method to combine the findings of these analyses. As all of the previously discussed methods of uncertainty analysis have limitations and as ecological models are getting too complex, the sequential partitioning method may be a promising alternative, given that successful division of complex models into independent compartments can be achieved. This approach requires the full access to the source codes of the models, a requirement that often cannot be met (Urban et al., Chapter 13).

3.4.3 Presentation of Prediction Uncertainty

Uncertainty from different sources is manifested in model output, and effective communication of the manifestations of uncertainty in modeling is a critical component of uncertainty analysis. In this section we use some examples to show how results of uncertainty analysis can be summarized and reported as output uncertainty, prediction accuracy, and error contributions of critical factors.

Output uncertainty is usually presented quantitatively as the probability distribution or statistical characteristics of model predictions. In the BFS and GLUE approaches, the uncertainty of each model prediction is defined by the probability distribution of model output. Thus, no additional analysis is needed. In other approaches (e.g., Taylor series, Monte Carlo simulation), the variance of an output variable is a common measure of error (Heuvelink 1998b, Rypdal and Winiwarter 2001). Often, the confidence levels for predicted values of system variables are presented as indicators of degree of uncertainty, and coefficient of variation (CV) is used to compare uncertainties associated with different variables or different applications. There are no simple criteria for judging the acceptability of estimated prediction uncertainty in model applications. However, a clear indicator of unacceptable uncertainty is that the simulation results cannot be used to determine the basic status of the system being modeled. For example, high uncertainty may prevent researchers from unequivocally answering the following questions: Is the system a carbon sink or source? Does a system perturbation generate a positive effect or negative effect or no effect at all on the processes of interest? Failure to answer such questions will limit effective applications of simulation modeling to resource management.

Many measures of prediction accuracy can be used in uncertainty analysis (Kvalseth 1985, Armstrong and Collopy 1992, Mayer and Butler 1993, Beldring 2002). For example, the Nash-Sutcliffe modeling efficiency index, R^2, is often used to assess the goodness of fit between model predictions and observations. The index is defined as (Nash and Sutcliffe 1970):

$$R^2 = 1 - \sum_i \left(Z_i - \hat{Z}_i\right)^2 \Big/ \sum_i \left(Z_i - \mu_Z\right)^2 \tag{3.21}$$

where Z_i is the observed value of Z and $\hat{Z}_i$ is the simulated value of Z. The values of R^2 range from minus infinity to 1.0, with higher values indicating better agreement. Other error measures include root mean square error (RMSE) and mean absolute percentage error (MAPE). In addition, the goodness of fit may also be revealed by graphic displays of results, such as the plot of observed (Z) against predicted ($\hat{Z}$) values or the plot of residual ($Z_i - \hat{Z}_i$) against predicted values. The selection of an error measure depends on the situation. None of the error measures is best in all circumstances (Armstrong and Collopy 1992).

Determining how much error each of the critical factors contributes to the total uncertainty is important because this information may indicate how uncertainty can best be reduced. The questions to resolve are: What is the ranking of the relative

contributions of factors to the total uncertainty of model output? Which factor is the most critical uncertainty source? The usual approach is to use the variance of the output distribution as a measure of prediction uncertainty because the variance can often be decomposed into meaningful parts. When the output variance can be partitioned, the analysis of uncertainty contributions becomes essentially a form of analysis of variance (Heuvelink 1998b). Although partitioning of variances is not always possible, it can be achieved by many techniques of uncertainty analysis. Notice that, for models with multiple outputs, rankings of input parameters as sources of uncertainty are not unique, but output specific (Klepper 1997). If a single set of ranks is of interest, one can use the ranks of output variables as weights to derive a composite ranking of input parameters for the model. Below, we discuss methods of partitioning variance and determining error contributions in association with sensitivity analysis, probability theory, Taylor series, and Monte Carlo simulation procedures.

Klepper (1997) described a simple technique for determining the relative importance of output variables to input parameters in sensitivity analysis. The basic procedure is to run Monte Carlo simulations with parameter values sampled from the parameter space, obtain a linear regression model of the output variable on the corresponding parameters, and calculate relative sensitivity as an aid to interpretation of the results. For the simple system defined in Equation 3.1, the regression model is in the form

$$Z = a + b \cdot X + c \cdot Y \tag{3.22}$$

where a, b, and c are the regression coefficients. The relative sensitivity is given by the standardized regression coefficient, i.e.,

$$S_X = b \cdot \sigma_X / \sigma_Z \tag{3.23}$$

$$S_Y = c \cdot \sigma_Y / \sigma_Z \tag{3.24}$$

where S_X and S_Y are the relative sensitivity indices of variables X and Y, respectively. Equations 3.22, 3.23, and 3.24 can easily be extended to a general system with more variables and parameters. This approach is effective if the coefficient of determination of the regression model is high; otherwise, additional analyses are needed.

For the analytical methods of uncertainty analysis (i.e., probability theory, Taylor series), variance partitioning is straightforward because the prediction error is already decomposed and treated as a function of the variances of the independent variables. The relative contribution of a variable to the total uncertainty is defined by the fraction of the terms associated with its variance (e.g., Equations 3.4, 3.7, and 3.9). For example, the relative contribution by variable X as calculated by the Taylor series method (see Equations 3.8 and 3.9) can be expressed as

$$U_X = f\left(\sigma_X^2\right)/\sigma_Z^2 \tag{3.25}$$

$$f\left(\sigma_X^2\right) = \left(\partial\Phi/\partial X\right)^2 \cdot \sigma_X^2 + \left(\partial\Phi/\partial X\right) \cdot \left(\partial\Phi/\partial Y\right) \cdot \sigma_{XY} \tag{3.26}$$

where U_X is the relative contribution to the total uncertainty by variable X, and $f\left(\sigma_X^2\right)$ is uncertainty associated with variable X. Equation 3.26 assumes that the covariance is shared equally by the two variables involved. Similar equations can be derived for Y. This analysis can also be extended to a general system with more variables and parameters.

When the Monte Carlo simulation method is employed, error contributions of critical factors must be determined indirectly because the variances are not given in an analytical form. Similar to the regression method discussed for sensitivity analysis, correlation analysis can be used with simulation results. Melching and Bauwens (2001) used correlation coefficients between model parameters (or variables) and model outputs to rank the importance of the parameters in predicting pollutant loading in streams. A more complicated method requires that, in addition to the Monte Carlo simulation that considers the uncertainty of all factors (i.e., σ_Z^2), new simulations be conducted to define the uncertainty caused by a particular factor (Katz 2002).

Katz (2002) described two approaches, the absence effect approach and the presence effect approach. The absence effect approach requires a new simulation with the uncertainties of all factors but one (e.g., X) to calculate the top-marginal variance, which is defined as the expected reduction of prediction variance if the uncertainty of factor X is assumed to become perfectly known (Katz 2002). The procedure is represented by the following equations:

$$U_{-X} = \sigma_{-X}^2 / \sigma_Z^2 \tag{3.27}$$

$$\sigma_{-X}^2 = \sigma_Z^2 - \sigma_{ALL-X}^2 \tag{3.28}$$

where U_{-X} is the relative error contribution of the factor X, σ_{-X}^2 is top-marginal variance of X, σ_Z^2 is the variance caused by all factors, and σ_{ALL-X}^2 is the output variance calculated without factor X. Similarly, the presence effect approach uses a different new simulation to consider the uncertainty only from factor X in calculating the bottom-marginal variance, which is defined as the prediction variance caused by the factor of interest when all other factors are assumed to be perfectly known (Katz 2002). The equation for the error contribution is given by

$$U_{+X} = \sigma_{+X}^2 / \sigma_Z^2 \tag{3.29}$$

where U_{+X} is the relative error contribution of the factor X and σ^2_{+X} is the bottom-marginal variance of X. For linear models with independent sources of uncertainty, U_{-X} and U_{+X} are the same and the sum of uncertainty contributions from all sources is equal to the total prediction variance. For complex models, however, both the absence and presence effect approaches should be used to define the range of the relative error contribution of a particular factor (Katz 2002).

3.5 CONCLUDING REMARKS

Future research should focus on bridging data gaps and developing new techniques of uncertainty analysis so that uncertainty in complex models can be assessed effectively. Lack of good data is the most critical obstacle to uncertainty analysis (Berk et al. 2002). Conducting well-designed field experiments and observations, especially at large scales, to meet the data requirements for uncertainty analysis should be a top priority. However, the problem of inadequate data may be partially resolved by improving the way data are reported; the variability of key variables and parameters (e.g., variance, range) should be presented together with the mean values. Another challenge in uncertainty analysis is the high complexity of models needed to address environmental assessment and resource management issues at large scales. This difficulty may be resolved by the sequential partitioning method discussed above and the disintegrated uncertainty analysis approach recommended by Katz (2002). Both approaches imply a strategy of keeping uncertainty analysis simple and doable by assessing uncertainties in individual model components separately. Nonetheless, effective techniques should be developed to conduct uncertainty analysis with complex systems when data are incomplete and models are insufficiently verified. For example, quantitative information about spatial heterogeneity should be incorporated into scaling procedures to reduce uncertainty and improve predictions.

Development of new techniques or innovative ways of using existing techniques should also be directed at creating capabilities of providing ideal outputs of uncertainty analysis – those that can fully characterize the uncertainty involved in modeling or scaling. These desirable outputs of uncertainty analysis include: (1) measures of model adequacy, (2) full probability distributions of model outputs (e.g., density function, probability-weighted values), (3) reliability of model results (e.g., accuracy, confidence level, error), (4) relative contribution or importance of each factor as an error source to total uncertainty, (5) the likelihood of different scenarios (probability or ranking), and (6) identification of the least understood or predictable components of the model (critical factors).

It is imperative that prediction uncertainty be treated as a critical issue and uncertainty analysis as a mandatory component in scaling because uncertainty in scaling is inevitable and should be assessed thoroughly to ensure the credibility and reliability of scaling results. Important sources of uncertainty in scaling include scaling algorithms, model parameters, quality and natural variability of data, and heterogeneous environment. These uncertainties must be quantified and reduced to ensure that scaling results are used effectively in policy- and decision-making. The

existing techniques of uncertainty analysis (e.g., Taylor series expansion, Monte Carlo simulation, Bayesian statistics) can provide basic information about prediction accuracy, effects of uncertainty from different sources on scaling results, and the relative importance of individual sources of uncertainty even though they have some major limitations. The use of uncertainty analysis in ecological studies has been rather limited. However, with recognition of the importance of uncertainty analysis in both research and application, uncertainty analysis will become an integral part of modeling and scaling.

ACKNOWLEDGEMENTS

The authors wish to thank Helen Regan, Devendra Amatya, and Debra Peters for their valuable suggestions to an earlier draft of the manuscript. JW acknowledges support from EPA (STAR R827676-01-0) and NSF (DEB 9714833, CAPLTER). This paper has not been subjected to the Agencies' required peer and policy review and therefore does not necessarily reflect the views of the agencies and no official endorsement should be inferred.

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