PARAMETER UNCERTAINTY AND MODEL PREDICTIONS:

A review of Monte Carlo results

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INTRODUCTION

Uncertainty in ecological models (O'Neill and Gardner 1979) is due to a number of factors. The total error associated with model predictions can only be assessed by a validation process (Caswell 1976, Mankin et al. 1977) which tests the model against independent data (Shaeffer 1979). However, such validation experiments are often infeasible, and modeling research has focused on individual factors that contribute to total error. These factors include assumptions in model construction (Harrison 1978, Cale and Odell 1979, O'Neill and Rust 1979), measurement errors (O'Neill 1973, Argentesi and Olivi 1976), and errors in formulating ecosystem processes (O'Neill 1979^a).

Of the factors contributing to total error, parameter variability has received the greatest emphasis. Many studies have taken advantage of the availability of analytical methods derived from sensitivity analysis (e.g., Argentesi and Olivi 1976, Lettenmaier and Richey 1979). This approach estimates the error in some system output, such as a state variable, by taking the partial derivative of the variable with respect to each parameter.

In the series of studies reviewed in this paper, we approached the study of parameter variability by Monte Carlo analysis, i.e., repeated simulations of the model with randomly selected parameter values. At the beginning of each simulation (or at intervals during the simulation), parameter values are chosen from specific frequency distributions. This process is continued for a number of iterations sufficient to converge on an estimate of the frequency distribution of the output variables.

Our goal in these studies was not merely to establish error bounds around model predictions, but to explore the general properties of error propagation in models. In our opinion, the Monte Carlo approach is uniquely suited to this exploration because (1) the technique is relatively free of restrictive assumptions; (2) the sources of model error must be explicitly considered; and (3) the method can be quickly implemented, allowing the comparison of many different models. The present paper will review the results of our recent studies with a view toward testing the implicit assumptions of analytical methods and pointing out counter-intuitive results produced by the Monte Carlo approach.

Two Sources of Parameter Variability

Differences in the assumed sources of error lead to differences in formulating the problem and interpreting the results. Figure 1 illustrates the interplay between two sources of error: natural variability in the ecosystem and error in parameter estimation. Figure 1a shows the simple case with no natural variability and no measurement error. In this case, the "true" behavior of the system can be represented by a frequency distribution which is a single vertical line of height 1.0. Assuming that there are no errors in model construction, as we will throughout this paper, the model predicts the distribution perfectly and there is no need for error analysis. This case, of course, never actually occurs but will serve as a reference for more realistic cases.

In Fig. 1b, the ecosystem has natural variability but there is no measurement error. In this case, we must represent ecosystem behavior by a distribution representing the statistical population of behaviors of which the ecosystem is capable. This is an important point to keep in mind: natural variability in the ecosystem implies a population of possible behaviors. The Monte Carlo implementation of the model explicitly accounts for this variability and exactly predicts the distribution. The deterministic model, in contrast, still predicts a single value and, even without measurement error, this prediction is incorrect. This bias or shift in the predicted value results from attempting to represent the variable system by a deterministic model. The error results from the fact that

$$E [f(A)] \neq f[E(A)] \quad (1)$$

whenever $f(A)$ is a nonlinear function. In other words, the expected value of a function, $E[f()]$, with a set, A , of randomly varying parameters is not equal to the value of the function using the expected value of each of the parameters. The two are equal only when $f(A)$ is simply the sum or product of the A 's or when the function is linear (O'Neill 1979b), but these cases do not appear particularly relevant for ecological models. Even a system of linear differential equations produces an $f(A)$ which is an exponential function.

Figure 1c depicts the situation in which the ecosystem has no natural variability but parameter values for the model are measured with error. In this case, the deterministic model shows a shift in the predicted value because the parameters are incorrect. The value from

the Monte Carlo implementation of the model is also incorrect, but it is possible to make a probabilistic statement about the magnitude of the error.

Figure 1d shows the most common situation in which there is both natural variability and also uncertainty in model parameters. The deterministic model is incorrect because (1) incorrect parameters are used, and (2) bias is introduced by the model (Eq. 1). The expected value of the Monte Carlo iterations is also incorrect due to measurement errors. However, the shift or bias in the expected value will be less than the deterministic model, and an estimate of the uncertainty associated with the prediction is possible.

SENSITIVITY ANALYSIS AS AN APPROXIMATION TO ERROR ANALYSIS

In many studies, error analysis is approached by sensitivity analysis (Argentesi and Olivi 1976, Lettenmaier and Richey 1979). This approach estimates the error in model predictions by evaluating the partial derivative of some model output (typically, the value of a state variable) with respect to each of the parameters. However, this method only approximates the error on model predictions because of three implicit assumptions:

(1) The expected behavior of the model is equal to the behavior of the model using the expected parameter values (Argentesi and Olivi 1976).

(2) The total error can be approximated by examining the contribution due to each parameter taken separately.

(3) Small perturbations in the parameters approximate errors resulting from large uncertainties, i.e., higher order effects are absent.

Since some version of the sensitivity analysis approach is the most commonly applied method for error analysis, it is important that we examine the extent to which these assumptions are valid.

It should be clear from our discussion of Fig. 1 that a deterministic model of a variable system always yields a biased prediction of the expected behavior. Thus, the first assumption of sensitivity analysis is ordinarily violated. However, the magnitude of the bias can vary significantly. In one study (Gardner et al., in press) comparing six phytoplankton-zooplankton models, all of the models were calibrated to a single hypothetical data base. As a result, bias was small, ranging from 1 to about 10% of the total uncertainty in the model prediction. In contrast, a study of a marsh hydrology model (Gardner et al., submitted) showed that the deterministic prediction can be in error by an order of magnitude due to bias! In the majority of our applications, however, the bias has been small (approximately 10%). It seems reasonable to conclude, therefore, that violation of the first assumption of sensitivity analysis will not lead to serious problems. If the first-order approximation of Hahn and Shapiro (1968) is used, the assumption will be violated only in unusual cases.

Our past duties do not provide a direct test of the second assumption that each parameter contributes independently to total error. We can, however, approach the question by comparing partial and

simple correlation coefficients calculated between individual parameters and total model variability. When all parameters are simultaneously varied, the partial correlation coefficient indicates the direct contribution of that parameter to the variance of the predicted value. If there are no interaction terms between parameters, the partial correlation coefficient will approximate the individual sensitivity coefficient. The simple correlation coefficient represents the direct relationship between a parameter and predicted values when all parameters are varied simultaneously. Comparison between simple and partial correlations is a test of the second assumption if we assume that no higher order interaction terms are present. If the partial is not equal to the simple, this indicates that the variance of the other parameters has altered the relationships between parameters and predictions.

The comparison of partial and simple correlation coefficients is possible for the analysis we performed of the marsh hydrology model (Gardner et al. submitted, Huff and Young, submitted). For most parameters, the partial and simple coefficients are similar and the second assumption appears valid. Where they diverge, it is usually only for a portion of the simulated annual cycle. The few exceptions that were found among the 14 parameters had unusually high variances. For example, the greatest divergence occurs for a parameter with a coefficient of variation of 48%. Our analysis indicates that the sensitivity coefficients are conservative. That is, the effect of simultaneously considering all parameters is a decrease in the correlation between an individual parameter and total model error.

The third assumption is that the uncertainty on model output can be characterized by examining small variations in the parameters; that is, large variations, more characteristic of ecological measurements, will not significantly alter parameter sensitivities. We can address this assumption directly, based on unpublished analyses of the marsh hydrology model. In separate Monte Carlo simulations, we assumed all parameters to have (1) a coefficient of variation of 1% and then, (2) variations characteristic of real field measurements. By comparing the partial correlation coefficients generated by these two runs, we can examine how larger variations alter sensitivity patterns. In general, the partial correlation coefficients are similar between the two sets of simulations, and the assumption appears valid for this model. The exceptions, however, were dramatic. Figure 2 shows the partial correlation coefficient between the parameter FC (field capacity of the soil) and total model error for the 1% case (dashed line) and the case in which all parameters were varied at realistic levels (solid line). Allowing all parameters to take on large variations obviously has an important effect on the sensitivity of model output to this parameter. In general, when the coefficients diverge (Fig. 2), sensitivity analysis would indicate that the model is more sensitive to a parameter than would be indicated by a Monte Carlo analysis.

In an analysis of a phytoplankton-zooplankton model (O'Neill et al. 1980, Gardner et al., in press), increasing the variance associated with individual parameters from 4 to 10% of their means results in complex changes in the predicted values. The deterministic system is characterized by an increase in populations in the spring, a decline

during the summer months, a fall recovery, and a winter decline. Prediction error (sum of squared deviation from the deterministic solution) increases in the spring and fall when the populations are changing rapidly (Fig. 3). Because all populations are declining during warm summer months, the errors at this point are at a minimum.

Increasing variability of the parameters, from 4. to 10%, changes the magnitude of variation and the pattern of variability throughout the year (Fig. 3). Herbivore errors increased approximately 10-fold and carnivores approximately 5-fold. Increase in parameter variability resulted in a smoothing and broadening of the peaks of variability, and because the relationship between populations is nonlinear, the pattern of response of the fall carnivore populations is most affected.

At the present stage of our understanding, the assumptions of sensitivity analysis do not appear to cause serious problems. This is a consoling result because most analyses will be limited to this approach. However, we observed some important exceptions to the rule. The marsh study (Gardner et al., submitted) showed that sensitivity analysis (1% variation) could lead to erroneous decisions. Based on the sensitivity analysis, one would be led to believe that model uncertainty could be significantly reduced by increasing the accuracy of a small subset of parameters. The error analysis (i.e., realistic variances) revealed that increased accuracy and precision in measuring this subset of parameters would have little practical effect on model error. Sensitivity analysis has many practical and theoretical uses for model examination, but caution must be exercised because the assumptions can be violated under some circumstances.

Establishing the Domain of Applicability of an Analysis

Unless consideration is given to the different sources of parameter variability (Fig. 1), considerable ambiguity can be introduced into the interpretation of results. The inferences which can be drawn from any particular error analysis study are dependent on the selection of nominal values for the parameters and the definition of their statistical properties (e.g., distributions, variances, maxima and minima, etc.). Any assumptions implicit in the choice of these statistical properties will strongly influence the inferences drawn from the analysis. If variances are measured for a specific system in a specific year, conclusions should not be drawn about other systems and future years. If study objectives call for inferences about a particular system, variances characteristic of an entire class of systems should not be used. The problems associated with the formulation of a particular case and inferences which can be drawn are illustrated by two recent studies.

In our analysis of the marsh hydrology model (Gardner et al., submitted), the statistical distributions were assumed to be normal, with variances and extreme values estimated a priori from available information on marsh systems. One parameter, W , set the upper limit above which overland flow occurs and excess water drains rapidly into an adjacent lake. When this value is allowed to vary from iteration to iteration, it determines directly the maximum water level of the marsh and, hence, the actual water level and storage when the soils are saturated. The initial investigation set the mean of W at 15.2, the

variance at 48% of the mean, and the minimum and maximum at 0.0 and 30.0, respectively. The resulting relationship between W and predicted water level in the spring (March, April, and May) was quite strong, with W the second most significant contributor to water level variability (R^2 from 44 to 77%).

This result had very little practical meaning for any single marsh. For an individual marsh system the variability of W would be smaller and result largely from spatial heterogeneity and measurement error. The uncertainty of the nominal value of W is obviously much less "within" a marsh than the "between marsh" value used in the simulation. When the Monte Carlo experiment was repeated with the variance of W reduced from 48 to 1%, the statistical relationship between W and predicted water level during saturated periods disappeared.

The second example concerns the frequency distribution of predicted dose to the thyroid of infants from a chronic release of radioiodine-131 (O'Neill et al., submitted). The model includes a Gaussian plume atmospheric dispersion, the movement through the foodchain into milk, and the subsequent dose (resulting from ingestion) to the thyroid gland of infants. The extreme value for a particular parameter, B , which describes the transfer of radioisotope from the soil to pasture forage, proved to be troublesome. The parameter B , is dependent on the nature of the soil and is quite variable between sites. In addition, there are few measured values of B . Variability of B at a local site is restricted to the variability of the local soils within the area and yet we can only characterize the universal

variability of B across all soils. This point was not apparent when we began our investigation but we soon realized that allowing the maximum value of B to change by orders of magnitude from 1 to 1000 resulted in a change in the correlation of B with dose from 0.06 to 0.32 and a shift in the mean and maximum predicted dosages as well (Table 1). Like W in the marsh model, B has a small effect on the predicted value when variances characteristic at one site are used, but when either the region grows or knowledge of the parameter is insufficient, then the results must be cast in a different light.

Meaningful insights must come from a meaningful definition of parameter values and distributions. The approach must be applied uniformly across all parameters of the model, otherwise meaningless relationships between parameters and predictions will be obscured. It is most helpful to define first the level of resolution that the model will consider, then define the statistical properties of parameters within that framework.

Frequency Distributions of Parameters

Any real system (Fig. 1c) contains natural variability, and system behavior is most realistically, represented as a frequency distribution of potential behaviors. The distribution of system behaviors is the result of the mathematical characteristics of the model and the distributions of model parameters. The factors used to select a parameter distribution should include the probabilistic properties of specific processes in the model, the empirical distribution of available data, and any information on the expected distribution of

system behaviors. In our experience this information is seldom available, even for a portion of the parameters of the model. Approximations must be made based on the best available information (Morgan et al. 1978).

Under such circumstances we concur with Tiwari and Hobbie's (1976) recommendation that the triangular distribution be selected. The few parameters necessary for this distribution (mode, maximum, and minimum) can usually be inferred from the physical process under investigation. Tiwari and Hobbie point out that the choice of any other distribution involves additional assumptions. The triangular distribution is the least biased assumption under conditions of minimal information. In addition, under many circumstances, the results generated by the triangular distribution resemble results using a variety of more complex distributions.

For purely analytical studies (e.g., no statements about real confidence limits are expected), we prefer normal distributions because covariances can be specified with relative ease and the symmetrical distribution of parameters aids in interpreting the often skewed frequency distributions of predicted values. The effects of altering the distributions of parameters by changes in the variance, by specifying covariance terms, or by selecting another distribution can make a serious difference in the predicted results.

For instance, in a multiplicative chain model (prediction is calculated as the simple product of a number of coefficients and variables), prediction errors can be calculated analytically (Shaeffer 1979) if parameters are lognormally distributed. The choice of a

lognormal distribution has been justified for a number of reasons, including the fact that extreme values are more likely and predicted frequency distributions will be conservative. However, the shape of the frequency distribution of predictions is largely determined by the mathematics of the model rather than by the assumed distribution of model parameters. The mean and variance of the distribution are affected by the choice of a particular parameter distribution.

The effect of altering the parameter distributions is illustrated by holding the parameter means and variances constant, but changing the frequency distributions from lognormal to normal distributions for the radiation dose model (Shaeffer 1979, O'Neill et al., submitted). When parameters are lognormally distributed, the mean, the 95 percentile, and the maximum value of dose from 1000 iterations are 0.86, 2.9, and 9.5 rem/year. When the parameters are normally distributed, the mean is 1.4, the 95 percentile is 4.5, and the maximum is 109.5 rem/year (calculations based on an arbitrary release of 1 Curie per year of radioiodine-131).

Examination of lognormal distributions with different variances (Hahn and Shapiro 1958) shows that as variance increases, the peak of the distribution shifts farther to the left, i.e., more values lie below the mean. The complementary normal distribution is symmetrical, and a proportionately larger fraction of the values lies above the mean. The practical result is that the normal distribution predicts a slightly higher mean dose and a much higher extreme dose. For this example, the choice of distribution for parameters affects the mean, variance, and extreme value, and a choice of lognormal distribution for

conservative results is a poor one. However, no matter what parameter distribution is used, the predictions appear to be lognormally distributed.

Another factor which affects the frequency distribution of predicted values is the method chosen to simulate the problem. We recently studied density independent Leslie models of striped bass populations which predict abundances in each of 15 age classes for 40 years, based on age-specific fecundities (F_i) and survival (P_i) parameters.

Leslie matrix models (Leslie 1945, 1943) tend to predict population behavior that approaches infinity or zero through time. The probability of choosing random parameter values for the matrix that will result in a stable age distribution is very small. One way of forcing the model to produce a stable result is to calculate the survival from eggs to young-of-the-year, P_0 , based on the remaining parameters (Van Winkle et al. 1978). If parameters are chosen randomly only at the beginning of a Monte Carlo run, if P_0 is calculated to ensure a stable age distribution, and if the parameters remain unchanged for the 40 years of the simulation, the predicted mean population size is equal to the deterministic solution of the model and the coefficient of variation is 5.9%. If parameter values are chosen each year of the simulation (and P_0 recalculated each year), the mean is 35% greater than the deterministic solution and the coefficient of variation is 19%. The upward shift of the mean results from the continual adjustment of P_0 to reach a new, stable age distribution based on current parameter and age distribution.

If we make P_0 a random variable, like the other parameters of the model, a stable age distribution is no longer guaranteed. Now the predicted mean population size is 140% greater than the deterministic solution and the coefficient of variation is 254%! The shift to a higher mean value results from exponential increase in the population for some parameter combinations. This exponential increase can result in very large populations for a few iterations, resulting in an increased mean.

The fish population model also reflects an important advantage of the Monte Carlo approach. The simulation in which all parameters, including P_0 , are assumed to vary randomly, predicts an increased mean population size. Using an analytical approach which reflects only the shift in the mean, this result indicates that the fish population would be larger than the deterministic prediction. The Monte Carlo simulation produces a complete frequency distribution of predictions. It is clear from this distribution (Fig. 4) that the most likely result of parameter uncertainty in this model is extinction. In this case, the mode of the distribution is of greater significance because the mean is strongly influenced by a few large numbers. The frequency distribution reveals that most populations will lie well below the mean value. In this respect, dealing only with the means and variance is deceptive, and the frequency distribution of predicted behaviors is needed to arrive at a reasonable understanding of the result.

CONCLUSIONS

Much of this paper has been concerned with showing that prediction error is a complex phenomenon that requires careful analysis to avoid

error bounds on a prediction, but it will may be the most effective approach to exploring the mechanisms involved in propagating uncertainty and the factors involved in minimizing and controlling these uncertainties.

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FIGURE LEGENDS

- Figure 1. Comparison of frequency distributions of the real system ("truth") with the deterministic model solution ("model") and the deterministic model with variable parameters ("analysis model"). Four situations are illustrated: (a) The real system is deterministic, the model is deterministic and unbiased. No analysis is necessary. (b) The real world is variable, the model is deterministic, the analysis model is coincident with "truth." (c) The real system is deterministic, the model is deterministic and biased, the analysis model is variable and less biased. (d) The real world is distributed, the model is deterministic and biased, the analysis model is more variable than the real world and less biased than the deterministic model.
- Figure 2. The partial correlation coefficient between FC (the estimated soil capacity for water) and the predicted water level in a marsh system through 240 days of the year. The solid line is based on 500 iterations with parameters varied at realistic levels; the dotted line is based on 500 iterations with parameters varied at 1%.
- Figure 3. The daily total error of coupled herbivore-carnivore system when parameters are varied at either 4 or 10% of their mean value. The total sum of squares are calculated as the daily mean of the sum of squares deviation from the deterministic system.

Figure 4. The cumulative probability of predicted levels of a Leslie model of striped bass populations when all parameters of the model are varied at 10% (N case) or when P_0 (the probability of survival from eggs to young-of-the-year) is calculated for each iteration (N-1 case). Each line represents the results obtained from 1000 iterations.

Table 1. Relationship between the maximum value of B and the predicted dose to thyroid of infants from chronic release of radioiodine-131*

B max	Predicted dose (rem/year)			r**
	Mean	95 percentile	Maximum	
1.	0.87	2.9	9.4	0.06
10.	0.88	2.9	9.6	0.07
100.	1.03	3.4	11.5	0.14
1000.	2.47	9.0	53.6	0.32

*Values of B were generated from a triangular distribution with minimum value equal to 0.0, expected value of 0.2, and maximum value as indicated in the table. Each row summarizes the results of 1000 Monte Carlo iterations. The expected value from the deterministic system is 0.72 rem/year.

**r is the simple correlation coefficient between B and the predicted dose.

ORNL-DWG 79-19190

PARTIAL CORRELATION
COEFFICIENT

WATERLEVEL WITH FC

ORNL-DWG 79-19192

TOTAL ERROR

ORNL-DWG 79-19494