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Sensitivity Analysis as an Aid in Modelling and Control of (Poorly-Defined) Ecological Systems

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Sensitivity Analysis as an Aid in Modelling and Control of (Poorly-Defined) Ecological Systems

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INTRODUCTION

Theories useful for developing mathematical models or for designing control systems are, for the most part, pertinent to well-defined systems, i.e., those for which a valid model structure is available and for which parameter values can be accurately specified. As Young (1978) has pointed out, strategies for building models of well-defined systems are rarely (or never) suitable for application to poorly-defined systems in which uncertainties in measurements, model structure and parameter estimates are likely to exert a dominant influence. Similar constraints apply to the application of control theory to poorly-defined systems. Conventional methodologies cannot be readily used to solve a variety of important problems that fall into the category of "poorly-defined systems."

Problems in the ecological sciences are often poorly-defined (in the sense of our use of the term). This fact may be attributed to a variety of reasons. Biological processes and complex chemical reactions that take place in these systems are not well understood, at least in quantitative terms. Data are limited in quantity and quality and non-stationarity is the rule rather than the exception. Nevertheless, the ultimate goal of many efforts relating to modelling ecological systems is to develop a firm basic understanding of processes and an ability to control these systems. Sensitivity analysis is a term descriptive of a range of methods that can be used to address the general problem of modelling and control of ecological systems.

We report here a brief literature review of the use of sensitivity analyses in modelling ecological systems and on recent work of the authors in collaboration with R. C. Spear on the development of a generalized sensitivity analysis procedure.

PREVIOUS WORK ON SENSITIVITY ANALYSIS

In the analysis of ecological systems, including closed or partly closed micro ecosystems, there is no alternative to utilizing some type of *simulation model* as the mathematical format into which assumptions regarding causal relations and parameter values are summarized. By *simulation model* we mean one whose structure and parameters are explicitly related to physical, chemical or biological processes. Data in the literature on algal growth rates as a function of nutrient level, for example, are often given in terms of Michaelis constants, a fact which points out that simulation models are constrained to be written in the language of the various disciplines which have studied the component processes of the system. This constraint immediately leads to the result that most simulation models will be complex with many parameters, state variables and nonlinear relations. Under the best of circumstances such models have many degrees of freedom and, with judicious fiddling, can be made to produce virtually any desired behavior, often with both plausible structure and parameter values. Because of this problem, simulation modelling has limited importance in cases where understanding

of functional relationships is fragmentary and where extensive data sets that quantify the system behavior are lacking.

In spite of the problems cited above the potential utility of information yielded by simulation models in planning experiments has been recognized. For example, with reference to ecological models, Jeffers (1972) states that

> "much time can be saved in the early stages of hypothesis formulation by the exploration of these hypotheses through mathematical models. Similarly mathematical models can be used readily to investigate phenomena from the viewpoint of existing theories, by the integration of disparate theories into a single working hypothesis, for example. Such models may quickly reveal inadequacies in the current theory and indicate gaps where new theory is required."

Similarly, Mar (1974) in his review of multidisciplinary modelling studies pointed out that

> "The strategy to construct models without data and then employ sensitivity analysis to identify critical components where research and new data would enhance model performance is not commonly practiced."

Stenseth (1977), while roundly criticizing simulation modelling, admits that a simple model, when used to explore or to generate hypotheses, can be a valuable research tool.

The use of parameter sensitivity in models of ecological systems has typically been for the purpose of analyzing system responses (e.g., Waide and Webster 1976; Wolaver 1980). These efforts are oriented, for the most part, toward linear systems models and thus to broad generalities in ecology and not to specific problems. These particular applications are

thus not strictly pertinent to analysis of regenerative life support systems.

Several workers (e.g., Adams 1972; Maddock 1973; McCuen 1976; Meyer 1972) have suggested that parameter sensitivity analysis can be used to guide future data collection efforts and/or to order research priorities. Such techniques might be useful in conducting research on poorly-defined systems. Traditional parameter sensitivity analysis, however, pertains to a particular point in the parameter space (the vector space spanned by all possible combinations of parameter values). This requires that point estimates of all parameters be available which in turn, for complex ecological models, implies that sufficient input-output data for strenuous model calibration exist, and this is an unrealistic assumption for ecosystem simulation.

This problem of an inherent inability to specify the "nominal" values of parameters has significant implications in terms of control of ecological systems in general and of regenerative life support systems in particular. For example, O'Neill et al. (1980) deduce from a sensitivity analysis of a nonlinear ecological model that small parameter errors yield significant errors in trajectories of state variables. Similar conclusions can be drawn from other work (e.g., Beck et al. 1979; Fedra et al. 1980; Halfon 1979). This indicates that control schemes for poorly-defined systems must be robust in the sense of not depending upon precise and accurate estimates of parameter values. We will develop below a robust technique -- referred to as a generalized sensitivity analysis --

for overcoming the problem cited above but first we present a formal treatment of a class of modelling problem.

Mulholland and Sims (1976) have proposed a means of solving large-scale dynamical optimization problems. Their technique, as applied to the problem of regenerative life support system (RLSS) control, can be formalized as follows:

Let

$$\dot{\underline{x}} = \underline{f}\ (\underline{x}(t),\ \underline{V}(t),\ \underline{P}(t)) \tag{1}$$

be a model representation of a RLSS with state vector $\underline{x}$ simulating real system components $\underline{X}$, $\underline{V}$ the set of controlled parameters, and $\underline{P}$ the set of uncontrolled parameters and environmental variables. Because it may be difficult to formulate control laws based upon this large-scale system, a new vector, $\underline{y}$, of smaller dimension than $\underline{x}$ is defined. This reduced dimension vector serves as an indicator of the overall system performance, and can be related to $\underline{x}$ through some vector-valued function

$$\underline{y} = \underline{\rho}(\underline{x}). \tag{2}$$

For example, y_1,and y_2 may be the concentrations of oxygen and carbon dioxide in the RLSS.

Next an equation is chosen to insure the good performance of $\underline{y}$,

$$\dot{\underline{y}} = \underline{g}(\underline{y},\underline{\mu}) \tag{3}$$

where $\underline{\mu}$ is an auxiliary control vector. For example $\underline{\mu}$ may involve the use of auxiliary oxygen tanks and carbon dioxide scrubbers subject to the failure of biological control at the $\underline{V}$ level. The function $\underline{g}$ might be selected such that

$$\dot{y}_1 \begin{cases} < 0 \text{ if } [O_2] > 30\% \\ > 0 \text{ if } [O_2] < 20\% \end{cases}$$

$$\dot{y}_2 \quad < 0 \text{ if } [CO_2] > 3\%.$$

Differentiating equation (2) with respect to time, yields

$$\dot{\underline{y}} = (d\underline{\rho}(\underline{x})/d\underline{x}) \cdot (d\underline{x}/dt) = (d\underline{\rho}(\underline{x})/d\underline{x}) \cdot \underline{f}(\underline{x},\underline{V},\underline{P}).$$

From equations (2) and (3)

$$\dot{\underline{y}} = \underline{g}(\underline{\rho}(\underline{x}), \underline{\mu}).$$

The control law, $\underline{V}(t) = \underline{h}(\underline{x},\underline{P},\underline{\mu})$ can therefore be calculated from the equality

$$\underline{g}(\underline{\rho}(\underline{x}),\underline{\mu}) = (d\underline{\rho}/d\underline{x}) \cdot \underline{f}(\underline{x},\underline{V},\underline{P}). \qquad (4)$$

The implementation of the above outlined control scheme requires the development of a model to simulate the RLSS behavior. Construction of such a model traditionally proceeds in three steps.

First a scenario must be selected, that is, it must be decided what aspect of the system is to be modelled (e.g. energy flux, carbon flux, phosphorous flux, etc.). This decision will depend on the control goals and the practicality of measurement.

Second, a model structure must be selected. This includes both a decision on the number of state variables and the form of interactions between variables. Unfortunately, no reliable means of objectively selecting a model structure exists and the modeller must therefore rely on experience and trial and error (Jørgensen 1979). Often models of subsystems are developed and calibrated, but these calibrations are not always valid when the submodels are linked in a conglomerate (Jørgensen 1979).

A second approach is to start with a simple system and increase complexity until reliable simulation is achieved. Jørgensen and Meyer (1977 and 1979) suggest that a new component should be added to a system only if it contributes significantly to the ecological buffering capacity (β), where β is defined as the change in system loading divided by the change in the state variable being added. Williams (1971) found that the reliability of his simulations of a cedar bog lake increased as he added more components and incorporated nonlinear interactions.

Perhaps the most fervent argument in systems ecology is that between the proponents of linear models and nonlinear models. In this context, a linear model is any set of first order differential equations

$$d\underline{x}/dt = A\ \underline{x}(t) + \underline{Z}(t) \tag{5}$$

where the elements in the coefficient matrix A are independent of the state vector $\underline{x}$. (They may, however, be time dependent.) The most attractive feature of linear models is that their behavior is well understood and techniques to analyze them already exist (Waide and Webster 1976). Patten (1975) has hypothesized that macro scale ecological interactions are intrinsically linear. However, it is generally conceded that ecosystems, at least on the fine scale, show nonlinear behavior. Nonlinear models can be linearized for a small envelope about the equilibrium state ($\underline{X}_o$) by using a truncated Taylor series expansion of the form:

$$\dot{X} \cong f(\underline{X}_o) + \sum_i ((\delta \underline{f}/\delta X_i \,|\, X_{io}) \cdot (X_i - X_{io})) \tag{6}$$

where $\dot{\underline{X}} = \underline{f}(\underline{X})$ is the nonlinear model. Bledsoe (1976) is

strongly critical of the Taylor series approximation and linear ecosystem modelling in general claiming it to be a borrowed technique which "imposes the mathematics on the biology rather than letting the ecosystem itself dictate the way in which the model is to function." Nonetheless, much of the work in systems ecology is based on linear models (e.g., May 1972, 1973, 1975; Wolaver 1980; Lewis 1977).

Ulanowicz et al. (1978) attempted constructing an empirical model based on a fit to a quadradic polynomial. They then conducted stability and sensitivity analyses. Their attempts are no more reflective of the system biology than the models criticized by Bledsoe (1976). Tiwari et al. (1978) on the other hand, have based their model almost exclusively on the underlying biology, using Michaelis-Menten, and Q_{10} terms, donor, recipient and third party controls, and stochastically varying parameters,forcing functions and initial conditions. The result is a very complex model which may be difficult to incorporate in the control scheme described above.

The third step in developing a model is calibration. As indicated above, this is a problem of considerable difficulty for ecological systems. Often only qualitative data are available and even small measurement errors in the quantitative data can lead to wide discrepencies in the model. Several techniques have been proposed to overcome this problem.

For some simple models or submodels, parameters can be estimated from a least squares fit to the real system. However, as mentioned above, such calibrations may not be valid

when submodels are incorporated into the conglomerate. In addition, there may not be a unique solution to such a fit or, especially for more complex systems (many degrees of freedom), the curve fitting may not reflect biological reality.

In light of the discussion above we contend that simulation models for RLSS control can be useful only in a probabilistic context. That is, given the model and the inherent uncertainties in structure and parameter values the only meaningful analysis must focus on the probabilities of various behaviors. Most importantly, it must focus on the probable structures and parametric relations which appear consistent with that behavior which is associated with the desired characteristics of the system under consideration. One method for applying simulation models in a probabilistic context is to use Monte-Carlo techniques. (For example, see Tiwari and Hobbie (1976a,b) and Tiwari et al. (1978) for an application of Monte-Carlo simulation in ecological modelling.) The methodology developed below adjoins the notion of qualitative or semi-quantitative descriptors of the behavior of the system to Monte-Carlo simulation to obtain a usable technique for the analysis and control of poorly-defined ecological systems such as those of an RLSS.

A GENERALIZED SENSITIVITY ANALYSIS

a. Class of Mathematical Models. For clarity of exposition we restrict our attention to a specific class of models and introduce nomenclature which will be required subsequently. Assume the processes are to be modelled by a set of first

order ordinary differential equations. (Different mathematical structures can be dealt with in an analogous way). Let these equations be given in the form:

$$\frac{d\underline{x}(t)}{dt} = \dot{\underline{x}}(t) = \underline{f}[\underline{x}(t), \underline{\xi}, \underline{z}(t)]$$

where $\underline{x}(t)$ is the state vector and $\underline{z}(t)$ a set of time variable functions which include input or forcing functions. The vector $\underline{\xi}$ is a set of constant parameters described more fully below. Thus for $\underline{\xi}$, $\underline{z}(t)$ and $\underline{x}(o)$ specified, $\underline{x}(t)$ is the solution of the system of equations and is a deterministic or a stochastic function of time as determined by the nature of $\underline{z}(t)$. For simplicity of exposition, $\underline{z}(t)$ will be treated hereafter as a deterministic function of t. Under this assumption, there are two types of uncertainty with which we will deal: uncertainty in the model structure, i.e. in the functions, $\underline{f}$, and uncertainty in the parameter values $\underline{\xi}$. Different model structures would pertain to competing hypotheses on system functioning (e.g., phosphorus limitation vs nitrogen limitation in a eutrophication problem); we use the term scenario to indicate a particular structure.

For a given scenario each element of the vector $\underline{\xi}$ is defined as a random variable the distribution of which is a measure of our uncertainty in the 'real' but unknown value of the parameter. These parameter distributions are formed from data available from the literature and from experience with similar structures. For example, the literature suggests that the maximum growth rate of *Chlorella vulgaris* is almost

certainly between 1.5 and 2.5 $days^{-1}$ at water temperatures near 25°C. Interpreting these limits as the range of a rectangularly distributed random variable, and forming similar *a priori* estimates for the other elements of $\underline{\xi}$, results in the definition of an ensemble of models for a given scenario. Some of these models will, we hope, mimic the real system with respect to the behavior of interest.

b. The Problem-Defining Behavior. Turning now to the question of behavior, recall that for a given scenario every sample value of $\underline{\xi}$, drawn from the *a priori* distribution, results in a unique state trajectory, $\underline{x}(t)$. Following the usual practice, we assume that there are a set of observed variables $\underline{y}(t)$, calculable from the state vector which are important to the problem at hand. So, for each randomly chosen parameter $\underline{\xi}^*$, there corresponds a unique observation vector $\underline{y}^*(t)$. Since the elements of $\underline{y}(t)$ are observed (that is, we assume that they are measured in the real system) it is sensible to define behavior in terms of $\underline{y}(t)$. For example, suppose y_i is the concentration of phytoplankton in a body of water and the problem in question concerns unwanted algal blooms due to nutrient enrichment. Then there is some value of y_i above which a bloom is defined to have occurred and the behavior is defined by this critical value.

In general a number of behavior categories can be used. Without loss of generality, however, we can consider the case for which behavior is defined in a binary sense, that is, it either occurs or does not occur for a given scenario and set

of parameters $\underline{\xi}$. It follows that a rule must be specified for determining the occurrence or non-occurrence of the behavior on the basis of the pattern of $\underline{y}(t)$. It is also possible that the behavior might depend on the vector $\underline{z}(t)$. For example, suppose one element of $\underline{z}(t)$ were water temperature. We might be interested only in extreme values of $\underline{y}(t)$ when adjusted or controlled for temperature variations. In any event, the detailed definition of behavior is problem-dependent and, for present purposes, it is sufficient to keep in mind that a set of numerical values of $\underline{\xi}$ leads to a unique time function $\underline{y}(t)$ which, in turn, determines the occurrence or non-occurrence of the behavior conditioned, perhaps, by $\underline{z}(t)$.

c. The Analysis Procedure. We have now presented the class of models to be studied, defined the scenario concept and described how we propose to deal with parametric uncertainty. For a given scenario, behavior and set of parameter distributions $\underline{\xi}$, it is possible to explore the properties of the ensemble via computer simulation studies. In particular, a random choice of the parameter vector $\underline{\xi}$ from the predefined distributions leads to a state trajectory $\underline{x}(t)$, an observation vector $\underline{y}(t)$ and, via the behavior-defining algorithm to a determination of the occurrence or non-occurrence of the behavior. A repetition of this process for many sets of randomly chosen parameters results in a set of sample parameter vectors with which the behavior was observed and a set for which the behavior was not observed. The key idea is then to attempt to identify the subset of physically, chemically or biologically meaningful parameters which appear to account

for the occurrence or non-occurrence of the behavior. More traditional sensitivity analyses of large ecological models inevitably show that a surprisingly large fraction of the total number of parameters is simply unimportant to the critical model behavior. We maintain that this unimportant subset or conversely the critical subset, may be tentatively specified rather early in any study.

Ranking the elements of $\underline{\xi}$ in order of importance in the behavioral context is accomplished through an analysis of the Monte-Carlo results. The essential concept can be best illustrated by considering a single element, ξ_k, of the vector $\underline{\xi}$ and its *a priori* distribution as shown in Figure 1. Recall that the procedure is to draw a random sample from this parent distribution (a similar procedure is followed for all other elements of $\underline{\xi}$), run the simulation with this value and record the observed behavior and the total vector $\underline{\xi}$ therewith associated. A repetition of this procedure results in two sets of values of ξ_k, one associated with the occurrence of the behavior B, and the other with not the behavior, $\bar{B}$. That is, we have split the distribution $f(\xi_k)$ into two parts as indicated in the figure. This particular example would suggest that ξ_k was important to the behavior since $f(\xi_k)$ is clearly divided by the behavioral classification. Alternatively, if the sample values under B and $\bar{B}$ appeared both to be from the original distribution $f(\xi_k)$ then we would conclude that ξ_k was not important.

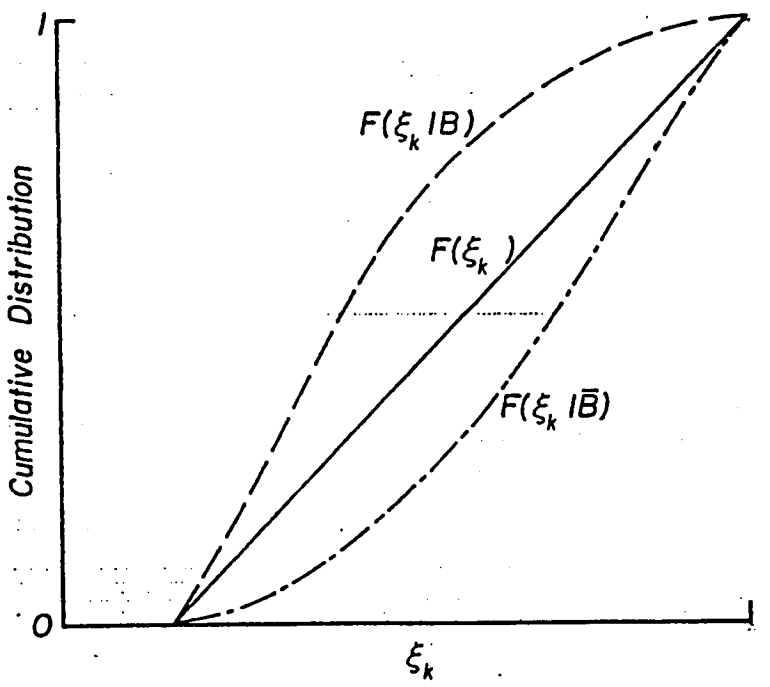

Figure 1.

d. Sensitivity Ranking of Parameters. For the case where $\underline{Z}(t)$ is a deterministic function of time, the parameter space is clearly divided by the behavioral mapping; that is, there is no ambiguity regarding whether a given parameter vector results in B or $\bar{B}$. Our analysis then focuses on the description of the region of parameter space associated with the behavior and our aim is to delineate what parameters or combinations of parameters are most important in distinguishing between B and $\bar{B}$. The hypersurface dividing the parent space cannot usually be determined analytically for environmental systems because of model complexity and a statistical analysis of the Monte-Carlo results must be used to make inferences regarding sensitivity rankings. In general, all of the moments of the distribution under the behavioral classification are necessary to describe completely the shape of the two subspaces, but, as with similar types of problems in the field of pattern recognition, examination of the first two moments should be sufficient in practical application.

We will restrict the discussion to the case for which the parameter vector mean is zero and the parameter covariance matrix is the identity matrix. (A suitable transformation can always be found to convert the general problem to this case.) The problem of identifying how the behavior mapping separates the parent parameter space can then be approached by examining induced mean shifts and induced covariance structure.

For example, considering only shifts in the mean and variance of the individual parameters, we can base a sensitivity ranking on a direct measure of the separation of the cumulative distribution functions, $F(\xi_k|B)$ and $F(\xi_k|\bar{B})$. In particular, we utilize the statistic

$$d_{m,n} = \sup_x \; | \; S_n(x) - S_m(x) \; |$$

where S_n and S_m are the sample distribution functions corresponding to $F(\xi_k|B)$ and $F(\xi_k|\bar{B})$ for n behaviors and m non-behaviors. The statistic $d_{m,n}$ is that used in the Kolmogorov - Smirnow two sample test and both its asymptotic and small sample distribution are known for any continuous cumulative distribution function $F(\xi_k)$. Since S_n and S_m are estimates of $F(\xi_k|B)$ and $F(\xi_k|\bar{B})$ we see that $d_{m,n}$ is the maximum vertical distance between these two curves and the statistic is, therefore, sensitive not only to differences in central tendency but to any difference in the distribution functions. Thus, large values of $d_{m,n}$ indicate that the parameter is important for simulating the behavior and, at least in cases where induced covariance is small, the converse is true for small values of that statistic.

In general, however, ranking on the basis of the separation in the distribution functions along the original axes of the parameter space (the individual parameter values) is not sufficient. It is possible, for example, that the first and second moments for a single parameter might exhibit no separation and yet this parameter could be crucial to a successful simulation by virtue of a strong correlation with other parameters under the behavior (see Fig. 2). The induced

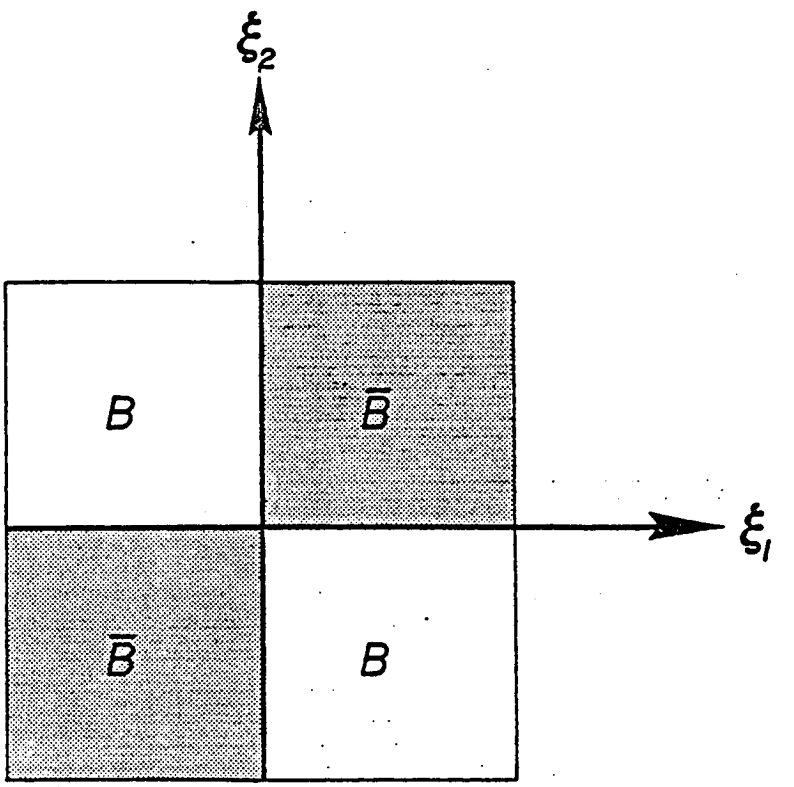

Figure 2.

covariance structure must therefore be included in a general sensitivity ranking. (This point is discussed fully by Hornberger and Spear 1980b).

e. Extension to Control System Design. There is an obvious appeal to the notion of extending the sensitivity concept to the problem of controlling systems that are parametrically ill-defined. The most straight-forward extension to the control problem is to consider the design of a controller that will deliver a high probability of adequate performance under the uncertainty in knowledge of the process parameters manifested by these *a priori* distributions. Here the binary classification notion of the sensitivity approach is retained in the form of adequate or inadequate system performance. Moreover, since this performance is to be based on the simulation results it can be defined in very practical terms and requires only an algorithmic definition rather than an analytically tractable formulation.

The simplest approach to controller design would appear to involve the specification of one or more candidate controller structures together with a set of control parameters for each structure. Each parameter set would then be assigned a distribution of allowable values and the problem is to select from within this set of allowable values the one specific set of control parameter values that maximize the probability of adequate performance P(B). Then, the controller structure with the highest P(B) is the best of the candidates with the particular value of P(B) allowing the designer to decide if the risk can be accepted and the design implemented or greater

knowledge of the process will be needed.

The procedure has been successfully applied to two problems in the control of poorly-defined ecological systems during the past two months by the authors in collaboration with Professor Robert C. Spear of the University of California. One of these problems deals with control of water quality in a river and the other with control of a biological waste treatment plant. Details of this work will be included in the later reports on this contract.

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16. Abstract

This report presents a literature review of the use of sensitivity analyses in modelling non-linear, ill-defined systems, such as ecological interactions. Included are discussions of previous work, and a proposed scheme for generalized sensitivity analysis applicable to ill-defined systems. This scheme considers: classes of mathematical models, problem-defining behavior, analysis procedures, especially the use of Monte-Carlo methods, sensitivity ranking of parameters, and extension to control system design.

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