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Intrinsic Uncertainties in Modeling Complex Systems

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Abstract

Models are built to understand and predict the behaviors of both natural and artificial systems. Because it is always necessary to abstract away aspects of any non-trivial system being modeled, we know models can potentially leave out important, even critical elements. This reality of the modeling enterprise forces us to consider the prospective impacts of those effects completely left out of a model – either intentionally or unconsidered. Insensitivity to new structure is an indication of diminishing returns.

In this work, we represent a hypothetical unknown effect on a validated model as a finite perturbation whose amplitude is constrained within a control region. We find robustly that without further constraints, no meaningful bounds can be placed on the amplitude of a perturbation outside of the control region. Thus, forecasting into unsampled regions is a very risky proposition.

We also present inherent difficulties with proper time discretization of models and representing inherently discrete quantities. We point out potentially worrisome uncertainties, arising from mathematical formulation alone, which modelers can inadvertently introduce into models of complex systems.

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Contents

Introduction

Models are necessary for understanding and predicting the behaviors of both natural and artificial systems. They are however often expensive and time-consuming to build, and assessing their usefulness for a particular purpose is a challenging endeavor. Models are always incomplete because modelers only include the elements they think are essential for capturing the key features of a system, which are selected from among the salient features they recognize. Even within these constraints, researchers are often surprised by behaviors manifested in models that reveal themselves to be sensitive in unexpected ways to variations in parameters. This reality of the modeling enterprise forces us to consider the potential impacts of system features that are truly unknown; i.e., elements left out of the model altogether.

This work complements the standard uncertainty quantification paradigm already applied to models routinely, in which the input parameters are varied systematically to understand their effects on the outputs. In this discussion, we call unknown parameter values the "known unknowns" because the existence of the effects they represent may be well known to modelers (and captured in the model), but the magnitude of their impacts can be very uncertain. By contrast, the approach we describe here examines the potential effects of what is not there at all; it's an approach to tackling the "unknown unknowns".

In principle, the effects of structural information not included in a model are completely unknowable. It would be very valuable nevertheless to be able to constrain the errors of models that we know to be incomplete structurally. To make progress, we consider what we would see in a hypothetical, generic model if we were to include a new known with finite bounds on its structure and impact, and then to ask how big of a change the new known can possibly make. The primary goal of this (in practice iterative) procedure is to be able to guide the model construction process and identify when the point of diminishing returns has been reached.

We approach the problem of the "unknown unknowns" mathematically by injecting into the structure of a model a hypothetical new element with estimated bounds on its magnitude. The initial model has been validated against a set of discrete measurements made within a sample region in which the system's behavior is understood well. If the new element affects first-order model results, the original model was incomplete, in the sense that it was sensitive to a structural element left out of the original system. Including the new element in the model is therefore essential for ensuring the robustness and accuracy across a larger range of scenarios, and hence its usefulness. If the model can be shown to *not* be sensitive to new structure, however, the model is complete relative to the effects of structural change. Insensitivity to new structure is an indication of diminishing returns from further modeling effort. The system's behavior may not be fully captured, but adding new components to the model will not significantly improve its accuracy (or usefulness).

This paper presents a method for quantifying the potential error in the output of a model fit to hypothetical sample data. The focus here is to identify a way to conceptualize the measurement of unknown unknowns (deep uncertainty) useful across modeling types. We start with a functional analysis of an unconstrained case that reveals the open-endedness of the general problem and the role of application-specific constraints to bound the problem mathematically.

The mathematical question posed by this approach is, given a model and an extended model (derived from the original model plus a new term), if the behavior of the two systems are within a tight threshold over the initial sample space, how far can they diverge across a forecast space? Our goal here is to provide a rigorous framing of the problem through which to identify the critical features that must be addressed by any specific application. The ideas presented are expected to be applicable to models of many variables, although our treatment here focuses for simplicity and clarity on a single-valued function of one independent variable.

Functional Formulation of the Problem

We now present a mathematical formulation of this problem in terms of generic functions of one variable. Let $f(x)$ be some function that describes the behavior of an engineered system as it is designed to operate, or the true behavior of a natural system. Let $F(x) = f(x) + \mathbf{c}g(x)$ be the operation of the system with the inclusion of an additional structural element $\mathbf{c}g(x)$, which can also be thought of as a perturbation superposed on the original model. The vector $\mathbf{c}$ consists of the coefficients of the terms of the function $g(x)$, or for our purposes it can be considered a single scalar value applied to $g(x)$. For now, we have left out structural alterations that involve a multiplication or other functional composition of the unknown term because, as we will see, simple addition is sufficient to demonstrate the key point of this study.

Sample Space Condition

The domain for x is divided into two regions. The region from a to b is the sample space, and the region from b to d is the forecast space. The sample space is the region in which the difference between f and F are tested for and measured. The behavior of F is constrained to be within $\varepsilon > 0$ of f over the region from a to b for some measure: $\|F - f\|_a^b \leq \varepsilon$. If we are dealing with continuous functional models, then one could require an integral error constraint; e.g.,

$$\int_a^b |F(x) - f(x)|\, dx \leq \varepsilon. \tag{1}$$

If f represents a set of discrete set S of observation points $\{a = a_1, a_2, \ldots a_S = b\}$, rather than a continuous function within the sample region, the integral constraint becomes a discrete sum:

$$\sum_{i=1}^{S} |F(a_i) - f(a_i)| \leq \varepsilon. \tag{2}$$

F and f are meant to be able to represent models that may or may not be expressed as integrable functions, so this final norm is the most general expression of the requirement. It also has the feature of testing the distance for a finite set of sample points rather than being continuous over the sample space. The analogy is that we are testing the behavior of our system F against the assumed/known true behavior f at each of the tested/sample points $\{a_1, a_2, \ldots a_S\}$, and our measuring tool has a detection threshold of ε.

Elimination of $f(x)$

Because the error generated by the new structural element is calculated by $\|F - f\| = \|f(x) + \mathbf{c}g(x) - f(x)\| = \|\mathbf{c}g(x)\|$, the error caused by the additional factor is by construction independent

of the base model behavior.[1] Only the *difference* in behavior matters. Thus the constraint on how inaccurate a model may become in the sampling space due to the additional element can be calculated with

$$\max_{a \le x \le b} \mathbf{c}g(x) < \varepsilon \text{ or } \forall a_i : \mathbf{c}g(a_i) \le \varepsilon. \tag{3}$$

Forecasting Error Calculation

Given that the behavior of the additional element $\mathbf{c}g(x)$ is below our detection threshold ε in the sample space from a to b, we then evaluate its behavior in the forecasting region from b to d. As before, the evaluation can be done treating g as a continuous function or by measuring it at some set of observation points $\{ b = b_1, b_2, \ldots b_T = d \}$. We are looking to determine the degree of error contributed by $\mathbf{c}g(x)$ in this forecasting region. So, using Equation 1 to define the error over a closed interval, our measure of the magnitude of the forecasting error becomes

$$\int_b^d \mathbf{c}g(x) \text{ or } \sum_{i=1}^{T} \mathbf{c}g(b_i). \tag{4}$$

[1] With respect to particular applications, one might care about the *proportion* of error generated by $g(x)$ compared to the magnitude of f, in which case one must also evaluate f across the sample and forecasting spaces. Of course, the error is still independent of f, but once f and g are constrained by particular domain concerns, then the relationship of the magnitude between f and F can be included in a robustness analysis of the behavior of the system. We also discuss below that external elements that are not additive generate errors that do depend on the model itself.

Arbitrarily Large Forecasting Errors

We will now show that given this formulation, it is possible to be arbitrarily large in the forecasting error for all values of ε when the elements of $g(x)$ are not constrained. Let $g(x) = e^{kx}$ for some constant value k. Because e^{kx} is a monotonically increasing function, the maximum error is given by $\max_{a \le x \le b} \mathbf{c}g(x) = \mathbf{c}g(b) = \mathbf{c}e^{kb}$. We must ensure that this is no greater than ε at its greatest maximum, which it reaches at the sample region limit (at $x = b$). Setting $\mathbf{c} = \frac{\varepsilon}{e^{kb}}$ ensures that the additional element is at the detection threshold in the sample space for any values of a, b, ε, and k.

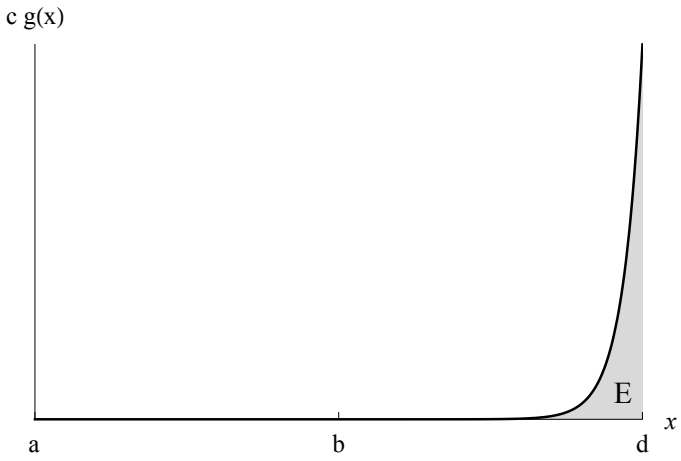

Figure 1. Generalized plot of the error level E when the added element $g(x) = e^{kx}$.

Let E be the target error level (greater than zero) in the forecasting region. For this additional functional element, we then have

$$\|\mathbf{c}g(x)\| = \int_b^d \mathbf{c}g(x) = \int_b^d \frac{\varepsilon e^{kx}}{e^{kb}} = \frac{\varepsilon(e^{kd} - e^{kb})}{k(e^{kb})} = \frac{\varepsilon}{k} \cdot [e^{k(d-b)} - 1] = E. \tag{5}$$

Our claim is that for such a system, there exists a k for any forecasting region $x = d > b$ and any target $E > 0$ such that $\|\mathbf{c}g(x)\| \ge E$.

First, we recognize that the Taylor series expansion is equal to the exponential function, and that the full expansion is greater than the power series truncated to the third term for any $x > 0$:

$$e^x = \sum_{n=0}^{\infty} \frac{x^n}{n!} = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \frac{x^4}{4!} + \ldots > 1 + x + \frac{x^2}{2}. \tag{6}$$

We then apply the transformation to our error condition:

$$\frac{\varepsilon(e^{k(d-b)}-1)}{k} > \frac{\varepsilon[k(d-b)+\frac{1}{2}k^2(d-b)^2]}{k} = \frac{\varepsilon}{2}(b-d)(bk-dk-2) \geq E. \tag{7}$$

Finally we rearrange this expression to find the condition for k. For $g(x) = e^{kx}$, any value of k satisfying

$$k \geq \frac{2 \cdot [\varepsilon(b-d)+E]}{\varepsilon(b-d)^2} \tag{8}$$

will produce an error value greater than E for $0 < b < d$, $\varepsilon > 0$, and $\mathbf{c} = \frac{\varepsilon}{e^{kb}}$. This analysis demonstrates, without restricting the functional form of the error term added to the original system, that the error term is essentially unbounded outside of the sample region.

Although there are other functions (than the exponential we chose) for which the potential error amount is also unbounded, that is not true for all functional forms one might choose for $g(x)$. If one restricts the elements that compose the added function $g(x)$, then in many cases the ε-condition prevents arbitrary growth within the domain from b to d. The collection of elements that may form the basis set of $g(x)$, as well as appropriate bounds for the sampling and forecasting regions, are problem-specific and cannot be generalized.

Application of This Framework

We recognize that once we have identified a specific problem, the details of that application domain will typically impose stronger constraints on the problem's mathematical specifications than our example function, $g(x) = e^{kx}$, which leads to theoretically unbounded errors (see Equation 8). Those constraints could then bound the degree to which an ε-tested system's behavior could deviate from expected/true behavior outside a control region.

To demonstrate the use of this framework in order to understand the error bounds of a constrained system, we will run through the analysis for the first five terms of the Taylor series expansion of the exponential function. We perform this analysis for demonstration purposes only, noting that for a particular application, the form of $g(x)$ may be determined from additional knowledge about the system. For example, in a physical model, energy conservation could provide useful guidance about the form and magnitude of the new term.

In the previous proof, we used the first three terms of the Taylor series to replace e^{kx} in the integral of $\mathbf{c}g(x)$. In this case, we will use the Taylor series expansion as an example constrained polynomial for our choice of $g(x)$. In that case, we have

$$\mathbf{c}g(x) = c_1 + c_2 x + c_3 \frac{x^2}{2} + c_4 \frac{x^3}{6} + c_5 \frac{x^4}{24}. \tag{9}$$

This function is continuous and everywhere differentiable. So we can once again use the maximum value across the sampling space as the ε-constraint and apply the integral form as our error metric (Equation 1). However, because there are multiple terms, and some of the c_i values may be negative, this is not necessarily a monotonically increasing function. This application also differs from the exponential function case above in that there is no parameter k to fit. The task in this case is to find values for the coefficients that maximize the integral over the domain from b to d, while keeping the value below ε between a and b.

One could also perform a standard parameter-sweep sensitivity analysis on the five coefficients in order to uncover the range and distribution of errors, rather than just searching for maximal error cases. This would be useful for determining confidence levels over the space of potential errors from any structural addition of this kind. Equation 9 also includes (through the use of zero coefficients) the addition of structures that are simpler than the maximal one with respect to the number of terms. By including multiple alternative additions and exploring all possible combinations of those additional elements from a restricted set of basis elements, unknown structure can be explored more thoroughly. The choice of basis elements, as we have noted, remains problem-specific.

Finally, we point out that the same conceptual framework for understanding error bounds from unknown structural features can be extended to models that are not equation based. Adding new structure and assessing its maximum impact is potentially applicable to agent-based models and other non-functional modeling approaches. Probing a model's sensitivity to external perturbations

can lead to surprising insights about its projected behavior in poorly understood regimes.

Discrete and Differential Formulations

We compare here continuous and discrete models for dynamical systems, both of which have been used in diverse fields such as biology [4], social dynamics, and economics. For example, see the many applications of non-linear dynamics discussed in [1]. Our discussion is not intended to be conclusive but rather thought-provoking and to elicit discussion about how models should be properly formulated for different types of complex systems. Detailed analysis and/or proof of the conjectures made herein is left for future work.

In this discussion, a typical differential model is a dynamical system of coupled first-order differential equations specifying the derivative of each independent variable with time (or whatever the independent variable happens to represent). These differential equations must be integrated to obtain the time development of the system. By contrast, a discrete dynamical model involves either integer-valued dependent variables (discrete space) or a coupled system of finite time-differenced equations (discrete time). Finite-differenced systems are known variously as recursion relations or iterated maps [6, p. 348]. They prescribe the evolution of a dynamical system assuming fixed-sized time steps. As with differential equations, interesting phenomena with maps can be revealed by examining solutions under parameter variations.

We note both types of models can (and typically do) have non-linear terms. Many simple systems can be captured fully with linear equations or linear approximations of non-linear interactions, but we do not restrict our discussion to linear systems here. Although the forms of the equations on paper appear to be similar, discrete models can behave very differently from similar systems of differential equations. For example, structural features of discrete maps make them in general more susceptible to chaotic behavior. An example is the logistic map, discussed in depth by [6, p. 353-69], which exhibits chaotic behavior for values of the parameter $r \geq 3.57$. By contrast, the corresponding logistic differential system is never chaotic. In this case, the chaos is thought to be an artifact of the formulation and not representative of the dynamics of simple populations.

We primarily focus here on systems for which no governing theory for the dynamics exists to enable modelers to distinguish between a differential or discrete model based on first principles. For example, the classical problem of planetary motion (discussed in depth in [3]) starts with Newton's laws of motion. Hence, in this case, there is a theoretical basis for choosing a set of differential equations to model planets' motion. The mechanics of planetary motion are inherently differential, and the quantities of interest are continuous and meaningfully represented as real numbers.

By contrast, when modeling a system in ecology, it is often difficult or impossible to reduce the system's behavior down to a set of core interactions that are well-understood. The models themselves are often entirely hypothetical because the underlying behaviors are difficult or impossible to resolve in a complex system. In ecology, therefore, unlike in classical physics, modelers often present discrete formulations instead of differential equations to explain observed phenomena.

In many cases, the choice to use discrete equations is motivated by the problem itself, which may have discrete variables (e.g., the population of wolves is a whole number). In this work, we

question specifically whether such a choice is made of necessity or for greater simplicity, elegance, or other subjective criteria. We will discuss the feasibility of formulating population models in differential form and how to handle fractional parts of variables representing discrete quantities.

We will hypothesize here that differential equations involving real-valued variables are to be preferred for modeling ecological (and similar) systems of all varieties, even ones involving apparently discrete quantities. We do not attempt to prove such a statement robustly but rather present the chief mathematical arguments favoring dynamical analyses starting with differential formulations. The goal is to provide high-level modeling guidelines for avoiding the potentially serious pitfalls of discrete mathematics.

Discrete-Time Systems

Researchers have posed dynamical problems in finite-differenced form at the outset to describe systems such as populations that have inherently discrete variables. Numerical solutions to dynamical systems' models are always approximations but are nevertheless of tremendous practical value. Hence, computational science has received a continual stream of research funding, and techniques for numerically approximating differential equations have steadily improved.

For problems with continously varying quantities, differential equations provide a natural mathematical framework with which to express dynamical interactions. The theory of differential equations is well-developed, as well as computational tools for solving them numerically. The literature is replete with discussions of time-discretization of differential equations. For the most general problems, adaptive methods achieve a good balance between performance and accuracy for a broad range of applications. For smooth functions, extrapolation methods such as Burlisch-Stoer provides rapid convergence [5, p. 707-52].

The need for such sophisticated methods points to a serious difficulty with discrete-time representations of dynamical systems. First, in a coupled system, the meaningful timescales for each species can be very different. This makes choosing an appropriate single value for every timestep problematic. The finite-differenced form thus builds in a dubious assumption from the outset. Second, without adaptive time-step control, finite-differenced approximations to non-linear differential equations (of any order) diverge exponentially from the real solution [2]. Thus, forecasting capability with computers is inherently limited.

Consider a simple predator-prey model in which the predators are wolves and the function $W(t)$ represents the time-varying number of wolves in the ecosystem under study. We furthermore define a related variable $w(t)$, whose fractional part is $W(t)$; that is, $W = frac(w)$. Furthermore, we denote the whole-number prey populations as $P_i(t)$ and corresponding real values as $p_i(t)$. A fully discrete representation of the dynamics (i.e., discrete in both time and space) of the wolf population in this system would have the form

$$W_{i+1} = F(W_i, P_i), \tag{10}$$

where F is an arbitrary function of the populations of all species. In this system, each iteration of the map advances the solution by a fixed quantity of time whose magnitude is built into F. Notice

in Equation 10, F cannot be a real-valued function, as its inputs and outputs are only defined for a discrete set of values (the non-negative natural numbers).

We note that for every discrete-time formulation (Equation 10), there exists an analogous ordinary differential equation:

$$dw/dt = f(w, p), \tag{11}$$

where $f(w, p)$, unlike $F(W_i, P_i)$ in Equation 10, spans the set of real numbers.

The existence of a differential representation can be seen by recognizing that all models formulated using Equation 10 can be rewritten as a differential equation whose first-order approximation is the map. We hypothesize that the second formulation is preferable in all cases to the discrete map as a starting point in modeling such systems. Then, solutions of any order of accuracy can be obtained and compared.

Integer Variables

Problems with inherently discrete (integer-valued) variables represent the most interesting modeling dilemmas. On the one hand, the use of discrete mathematics for these problems seems natural. On the other hand, discrete representations are prone to instabilities not seen in differential formulations. Furthermore, the multiplicative constants (parameters) are normally not required to be integer-valued, which leads to fractional parts when the equations are solved. Enforcing integer intervals for the parameters precludes mixing continuous and discrete variables and would thus severely limit the richness with which discrete dynamical systems can be captured in models.

In practice, what is often done is to take (at every time step) integer parts of solutions for discrete dynamical variables (e.g., number of organisms in an ecosystem) represented as real numbers in the model. It is not clear this is conceptually sound, and if so, whether the discrete formulation itself builds instability into the solution. Is truncation (or rounding) a problem mathematically consistent? We argue it is in general problematic to allow variables only defined as discrete quantities to have intermediate real-valued solutions.

Hence, we suggest a different approach: do not allow any variables in the problem to be discrete. For example, present the number of wolves in a population as a real number in which the fractional part has a viable interpretation in the model. We advocate starting with a continuous formulation, which can be a more tractable way of looking at the problem. Then solutions of the differential equations at the end of each time step can be rounded at any step to the nearest integer (if required). We argue that the drawbacks of representing quantities in ecology with real-valued variables can be overcome without serious difficulties.

Discussion and Conclusions

In this work, we have presented a mathematically concrete way to think about "unknown unknowns" for a given application. Our framework involves recasting (or encapsulating) abstract uncertainties about the impact of an external effect in the form of a new parameterized term (that is, a new "known unknown"). This new term is applied to the original model (whether additive, multiplicative, functional, etc.) in order to assess its importance. For any particular application, the procedure we have described must be applied iteratively to search the complete space of potential structural additions.

By measuring the sensitivity of a model's output to the presence of new effects, one can begin to quantify its predictive power for a given scenario. For example, one might with these ideas be able to exclude car-sized meteor impacts as a meaningful contributor to global climate change. However, the potential climatological perturbation caused by the Earth colliding with a 100 km asteroid cannot be discounted in a (statistically complete) forecast, since the probability of such a drastic event occurring is known.

The core result of the analysis presented is pessimistic (from a theoretical standpoint) about uncertainties in model results projected into an unknown region of the problem domain. When the collection of functional elements playing the role of $g(x)$ is completely unrestricted, then it is always possible to find a $\mathbf{c}g(x)$ that is within the ε-error bound for a given sample domain, while also yielding arbitrarily large errors outside it (Equation 8). The unbounded error for the simple function chosen, $g(x) = e^{kx}$, underlines the result that nothing can be said about potential errors in the unrestricted case.

The fact that models cannot in general be predictive outside a control region without also imposing constraints on external forcing underscores a related point about the activity of modeling itself. Fitting data or measurements is a necessary but insufficient condition for a model to be useful because fits only reflect back to us what we already understand about a system and its behavior. Furthermore, data fits (or models that achieve good agreement with data) are in general not unique. In many cases, multiple functional compositions or algorithms can be used to reproduce the results of experiments or observations. Usefulness of models derives from elucidating the governing processes and dynamics that underly a system's behavior, with which we can expect to achieve some level of predictive power outside domains that have been well-measured.

We conclude with two caveats about these results. First, we have left out structural alterations that involve a multiplication $\mathbf{c}g(x) \cdot f(x)$ or other compositional $\mathbf{c}g(f(x))$ function of the unknown functional factor. For external effects that cannot be represented as simple additive functions, it is impossible to capture the behavior of a new structural feature in isolation of base model characteristics. That is, the error will itself be a function of the model. We note also that this framework does not treat (or attempt to treat) completely unforseen events whose perturbative effects cannot even be estimated without analysis that is likely to be highly speculative.

Finally, with respect to discrete systems, we stipulate that providing meaning for real-valued extensions of integer-valued variables solves multiple problems simultaneously. First, it avoids the

instability of discrete maps and other issues with integer computations (e.g., overflow). Second, integration and analysis tools can be borrowed from the realm of differential equations, for which decades of theory exist. Finally, the scale of the problem becomes unimportant in formulating models. Whether there are tens or millions of organisms, the semi-discrete modeling approach we are advocating is applicable.

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