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Bayesian calibration of mathematical models: Optimization of model structure and examination of the role of process error covariance

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ABSTRACT

The integration of Bayesian inference techniques with mathematical modeling offers a promising means to improve ecological forecasts and management actions over space and time, while accounting for the uncertainty underlying model predictions. In this study, we address two important questions related to the ramifications of the statistical assumptions typically made about the model structural error and the prospect of Bayesian calibration to guide the optimization of model complexity. Regarding the former issue, we examine statistical formulations that whether postulate conditional independence or explicitly accommodate the covariance among the error terms for various model endpoints. Our analysis evaluates the differences in the posterior parameter patterns and predictive performance of a limiting nutrient (phosphate)–phytoplankton–zooplankton–detritus (particulate phosphorus) model calibrated with three alternative statistical configurations. The lessons learned from this exercise are combined with those from a second comparative analysis that aims to optimize model structure. In particular, we selected three formulas of the zooplankton mortality term (linear, hyperbolic, sigmoidal) and examine their capacity to determine the posterior parameterization as well as the reproduction of the observed ecosystem patterns. Our analysis suggests that the statistical characterization of the model error as well as the mathematical representation of specific ecological processes can be influential to the inference drawn by a modeling exercise. Our findings could be useful when selecting the most suitable statistical framework for model calibration and/or making informative decisions about model structure optimization. In the absence of adequate prior knowledge, we also advocate the use of Bayesian model averaging for obtaining weighted averages of the forecasts from different model structures and/or statistical descriptions of the process error terms.

1. Introduction

The rigorous analysis of decision problems in eutrophication management requires fundamental understanding of the biogeochemical cycles; specification of objective functions for evaluating alternative management strategies; predictive models of ecosystem dynamics formulated in terms of variables relevant to management objectives; a finite set of alternative management plans, including any limitations on their use; and a monitoring program to follow system response to restoration actions (Arhonditsis et al., 2011). An inherently difficult task in practical applications of decision theory is the impartial characterization of an objective function, which specifies the value of alternative management actions and usually accounts for benefits, costs, and conditional constraints (Dorazio and Johnson, 2003). Likewise, the predictive models aim to realistically reproduce the relevant behaviors of aquatic ecosystems that are nonlinear, complex, and are characterized by spatial, temporal, and organizational heterogeneity (Arhonditsis and Brett, 2004). Perhaps even greater challenges are posed by the uncertainty in predictions of management outcomes. This uncertainty may stem from inadequate control of management actions, incomplete knowledge of system behavior, errors in measurement and sampling of aquatic ecosystems, natural variability, and model structural or parametric uncertainty (Arhonditsis et al., 2007; Borsuk et al., 2004; Walters and Holling, 1990). Failure to recognize and account for these sources of uncertainty can severely compromise management performance, and in some cases, has led to catastrophic environmental and economic losses (Williams et al., 1996; Walters, 1986). However, the general lack of uncertainty estimates for most eutrophication models, the arbitrary selection of higher – and often unattainable – threshold values for water quality standards as a hedge against unknown forecast errors, risky model-based management decisions and unanticipated system responses are still the typical management practice (Arhonditsis, 2009; Arhonditsis et al., 2007; 2008a,b).

Given this ominous context, there has been a growing interest in the theory of stochastic decision processes and the development of practical methods that can explicitly accommodate the uncertainty in the response of environmental systems to both controlled and uncontrolled factors (Dorazio and Johnson, 2003). In this regard, particular emphasis has been placed on the implementation of Bayesian inference methods that enable the explicit consideration of model uncertainty, can be engaged with the policy practice of adaptive management, and have the

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ability to update and improve model predictions and management actions in space and time (Kennedy and O'Hagan, 2001; Zhang and Arhonditsis, 2008). The Bayesian inference is consistent with the scientific process of progressive learning and offers a natural mechanism for sequentially updating beliefs (specified in terms of model parameters) every time new data are collected from the system and for predicting the consequences of future management actions, while properly accounting for uncertainty in the updated beliefs (Arhonditsis et al., 2008a). Recent research has also shown that the Bayesian paradigm can effectively alleviate problems of spatiotemporal resolution mismatch among different submodels of integrated environmental modeling systems, overcome the conceptual or scale misalignment between processes of interest and supporting information, exploit disparate sources of information that differ with regard to the measurement error and resolution, and accommodate tightly intertwined environmental processes operating at different spatiotemporal scales (Boone et al., 2012; Hooten et al., 2011; Qian et al., 2010; Wikle, 2003; Wikle et al., 1998; Zhang and Arhonditsis, 2009).

Several recent studies have attempted to demonstrate the benefits of Bayesian inference techniques in the context of model-based water quality management. For example, Arhonditsis et al. (2007; 2008a,b; 2011) introduced a Bayesian calibration scheme using a wide range of complexity mathematical models and statistical formulations that explicitly accommodate measurement error, parameter uncertainty, and model structure imperfection. In particular, the statistical characterization of the calibration framework was based on one of the following assumptions: (*i*) a "perfect" model structure along with additive (or multiplicative) measurement error; (*ii*) a simulator that imperfectly represents the dynamics of the natural system and the process error is invariant with the input conditions, i.e., the difference between model and system dynamics was assumed to be constant over the annual cycle for each state variable; and (*iii*) a model structure that imperfectly represents the dynamics of the environmental system but the corresponding process error varies with the input conditions, i.e., time variant error terms were specified for each state variable. The former formulation postulates that the model misfit is solely caused by the error associated with the data, whereas the latter ones also consider errors in the model structure, e.g., missing key ecological processes, misspecified forcing functions, and erroneous mathematical expressions. It should also be noted that, aside from the analytical/sampling error, the term measurement error also reflects the notion that the observational data are just a "snapshot" of the real system, an instantaneous record of few components from numerous complex and interactive processes that depending on the sampling network used, the ecosystem modeled and the questions addressed, can form a pragmatic basis for evaluating model performance (Arhonditsis and Brett, 2004). The characterization of the uncertainty underlying the model parameters prior to model calibration (prior parameter distributions) was based on field observations from the studied system, laboratory studies, literature information, and expert judgment using the protocol presented by the Steinberg et al. (1997) study. The Bayesian calibration framework can then be used to quantify the information the data contain about model inputs, to offer insights into the covariance structure among parameter estimates, and to obtain predictions along with credible intervals for model outputs.

A common denominator of the aforementioned statistical formulations was the postulation of conditional independence among the error terms for various model endpoints. Striving for simplicity, this strategy offers a convenient statistical description of the "model calibration" problem, but profoundly downplays the observed covariance patterns among interconnected ecosystem variables, e.g., nutrients-phytoplankton–zooplankton. The question arising though is to what extent this pragmatic approach introduces a systematic bias in the model parameterization and may affect the capacity of the modeling exercise to support robust predictive statements. To this end, our analysis evaluates the posterior parameter patterns and predictive performance of a limiting nutrient–phytoplankton–zooplankton–detritus model when the Bayesian calibration framework explicitly accommodates the covariance of the error terms associated with different state variables. We synthesize the lessons learned from this exercise with the findings of a second comparative analysis that aims to optimize model structure. In particular, we selected three formulas of the zooplankton mortality term (linear, hyperbolic, sigmoidal) and examine their capacity to determine the posterior parameterization as well as the reproduction of the observed patterns. Our intent is to illustrate the variety of options along with the critical decisions involved when selecting the most suitable statistical framework for model calibration and/or the optimal model structure. It is our belief that our case study will offer – much needed – prescriptive guidelines for the effective integration of Bayesian inference with process-based models.

2. Methods

2.1. Case study

The study site for our modeling work was the Hamilton Harbour, Ontario, Canada, a large embayment with long history of eutrophication problems primarily manifested as excessive algal blooms, low water transparency, predominance of toxic cyanobacteria, and low hypolimnetic oxygen concentrations during the late summer (Hiriart-Baer et al., 2009; Ramin et al., 2011). Since the mid 80s, when the Harbour was identified as one of the 43 Areas of Concern (*AOC*) in the Great Lakes area, the Hamilton Harbour Remedial Action Plan (*RAP*) was formulated through a variety of government, private sector, and community participants to provide the framework for actions aimed at restoring the Harbour environment (Hall et al., 2006). The foundation of the remedial measures and the setting of water quality goals reflect an ecosystem-type approach that considers the complex interplay between abiotic variables and biotic components pertinent to its beneficial uses (Charlton, 2001). The drastic nutrient loading reduction has historically played a central role in the restoration efforts, although the determination of the critical levels has been a thorny issue as the population growth and increasing urbanization accentuate the pressure for expansion of the local wastewater treatment plants (*WWTP*s) (Charlton, 2001).

Recent modeling work suggests that the water quality goals for TP levels $<20\ \mu g\ L^{-1}$, chlorophyll *a* concentrations between 5–10 $\mu g\ L^{-1}$ and water clarity >3 m will likely be met, if the proposed phosphorus loading reductions at the level of 142 kg day^{-1} are actually achieved (Gudimov et al., 2010; 2011; Ramin et al., 2011). However, it was emphasized that the predictive capacity of any modeling exercise in the Harbour is conditional upon the credibility of the contemporary nutrient loading estimates, which are uncertain and appear to inadequately account for the contribution of non-point sources, episodic meteorological events (e.g., spring thaw, intense summer storms), and short-term variability at the local *WWTP*s (Gudimov et al., 2011). A follow-up analysis considered the fact that there is no true model of an ecological system and used an averaging scheme for obtaining weighted averages of the forecasts from two models of different complexity (Ramin et al., 2012). Two important unknown factors were identified that can potentially modulate the response of the system to the exogenous nutrient loading reduction and may shape the duration of the transient phase as well as the system resilience in the "post-recovery" era. First, the dynamics of phosphorus in the sediment-water column interface are still poorly understood, and thus the historical notion that the internal loading in the Harbour is minimal may be inaccurate. Second, the lack of fundamental knowledge of the regulatory factors of herbivorous zooplankton abundance and composition, even though existing evidence suggests that a thriving zooplankton community can be instrumental for achieving faster recovery rates in the Harbour. The latter prospect highlights a central conclusion drawn from the recent modeling work