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Abstract

Bio-geo-chemical models are useful tools in environmental sciences that can guide management and policy-making. Consequently, significant time and resources are spent developing these models in system-specific contexts. The optimization of model parameters to maximize precision, including transferability of these models to different systems, are fundamental concerns in the development and application of these tools. This study describes quantitative limitations of coupled hydrodynamic-ecological modelling by contrasting numeric and ecological certainty with a systematic framework for characterizing parameter sensitivity and identifability. We evaluate a simple bio-geo-chemical model that is the one-dimensional (1-D) unit of a larger spatio-temporal model of hypoxia on the Louisiana continental shelf of Gulf of Mexico as an example. Results from analysis of the 1-D model are used to infer larger trends in dissolved oxygen dynamics over time, having implications for understanding factors that contribute to environmental conditions that are detrimental to aquatic resources. In particular, we focus on issues of parameter identifiability using local sensitivity analyses to provide quantitative descriptions of numerical constraints on model precision. We argue that quantitative and ecological certainty in model calibration are often at odds and the practitioner must explicitly choose model components to optimize given tradeoffs between the two. We further conclude that numerically optimal parameter sets for models of hypoxia are often small subsets of the complete parameter set because of redundancies in the unique effects of paramater perturbations on model output. As a result, we demonstrate that use of a model for inference into ecological mechanisms of observed or predicted changes in hypoxic condition can be potentially misguided in the absence of quantitative descriptions of identifiability. Although these concerns have been expressed in the literature, they are rarely explicitly addressed or included in model evaluations. In addition to immediate implications for regional models, we provide a framework for describing the effects of parameter uncertainty and identifiability that can be applied to similar models to better inform environmental management.

1   Introduction

1. Simulation/biogeochemical/process-based models overview, contrast with statistical models

2. What models seek to provide - generality, precision, realism Levins (1966), there is a

tradeoff so models are 1) developed in partial independence and dependence on the world and theory, 2) function autonomously from both, or 3) represent both at the same time, from Morrison and Morgan (1999), cited in Ganju et al. (2016). This is similar to the bias-variance tradeoff for statistical models, e.g., overparameterization of a model makes it very biased as it fits the data (the world) exactly, tradeoff between sensitity and error with changes in model complexity (more complexity is less error but increasing sensitivity) described in Snowling and Kramer (2001)

3. How is model performance/uncertainty evaluated regarding what they should provide - structural, observational, parameter Beck (1987)?

4. Parameter uncertainy as low-hanging fruit - can do post-hoc and from inner to outer level of complexity, parameter uncertainty is the most common, e.g., marine ecological model Mateus and Franz (2015), but stopped short, global sensitivity analysis of eutrophication model Estrada and Diaz (2010)

5. Challenges related to uncertainty - similar to degrees of freedom, identifiability definition from Brun et al. (2001) and need to evaluate identifiability Fasham et al. (2006), Omlin et al. (2001) did a similar analysis with freshwater biogeochem model. Identifiability describes the ability to estimate a parameter in relation to variation among the remaining parameters. A parameter is identifiable if all parameters within the set can be uniquely estimated based on the observed data. Parameters that are unidentifiable typically produce similar model outputs for a given relative perturbation, i.e., the effect of altering one parameter can be undone by altering one or more other parameters. Model calibration will not converge for parameters sets that are unidentifiable.

This study describes a parameter sensitivity analysis to evaluate identifiability for a bio-geo-chemical model of hypoxia for the northern Gulf of Mexico (GOM). We evaluate a simple one-dimensional (1-D) unit of a larger spatial-temporal model to explore relationships between multiple parameter sets and hypoxia dynamics on the Louisiana continental shelf (LCS). The study also provides a general framework for sensitivity analysis and parameter identifiability that can be used on similar mechanistic models. Specifically, an assumption is that models are

generally over-parameterized and only a finite and smaller subset of the larger parameter set can be optimized for a given research question or dataset. We provide explicit guidance for choosing such subsets of the parameter space given constraints on identifiability as directly related to sensitivity analyses. The specific objectives are to 1) identify the parameters that have the greatest influence on dissolved oxygen (O_2) using local sensitivity analysis, 2) quantify the identifiability of subsets of the total parameter space based on sensitivity, 3) provide a set of heuristics for choosing parameters based on sensitivity and parameter categories with the larger mechanistic model, including extension to other state variables, and 4) discuss implications for hypoxia formation in coastal regions, including management strategies for nutrient reduction and use of mechanistic models to inform decision-making. The 'optimum' parameter space is defined as the chosen subset that represents the maximum number of identifiable parameters. Here, 'optimum' is both a qualitative description based on a research question or management goal and a quantitative objective based on numerical optimization criteria for fitting model output to a calibration dataset. These results can be used to refine existing models or guide application of models to novel contexts, such as downscaling or application to new environments.

2 Methods

2.1 Model description

Low concentrations of dissolved oxygen occur seasonally on the LCS in the northern GOM. These hypoxic events, defined as <2 mg L^{-1} (< 64 mmol m$^{-}3$ of O_2), occur in bottom waters and are caused by nutrient inputs from the Mississippi-Atchafalaya River Basin (MARB) that drains a significant portion of the continental United States. Nutrient-stimulated primary production in surface waters increases biological oxygen demand in bottom waters as sinking organic matter is decomposed. The hypoxic area averages 15,540 km^2 annually (1993-2015) with minimum concentrations observed from late spring to early fall. Seasonal variation is strongly related to carbon and nutrient export from the MARB (Lohrenz et al. 2008, Bianchi et al. 2010), whereas factors related to hydrologic variation and wind patterns can affect vertical salinity gradients that contribute to the formation of hypoxia (Wiseman et al. 1997).

Three-dimensional numerical simulation models have been developed to describe factors contributing to hypoxia and to predict the effects of management actions or climate scenarios on

future patterns (Fennel et al. 2013, Pauer et al. 2016, Lehrter et al. in review). This study evaluates a recently developed hydrodynamic and ecological model that describes horizontal and vertical transport and mixing of state variables relevant for hypoxia. The Coastal General Ecosystem Model (CGEM) includes elements from the Navy Coastal Ocean Model (Martin 2000) to describe hydrodynamics on the LCS and a biogeochemical model with multiple plankton groups, water-column metabolism, and sediment diagenesis (Eldridge and Roelke 2010). The hydrodynamic component of CGEM provides a spatially-explicit description of hypoxia dynamics using an orthogonal grid with an approximate horizontal resolution of 1.9 km^2 and twenty equally-spaced vertical sigma layers on the shelf (depth $\leq$ 100 m, with additional hybrid layers at deeper depths). The biogeochemical component includes equations for 36 state variables including six phytoplankton groups (with nitrogen and phosophorus quotas for each), two zooplankton groups, nitrate, ammonium, phosphate, dissolved inorganic carbon, oxygen, silica, and multiple variables for dissolved and particulate organic matter from different sources. The model can be run for a set period of time at a given time step using atmospheric and hydrological boundary conditions described in Hodur (1997) and Lehrter et al. (2013).

The core unit of CGEM is a 1-D model called FishTank that implements the biogeochemical equations in Eldridge and Roelke (2010). This model acts as a standalone operational unit from the 3-D model that does not include any form of transport (i.e., advection, mixing, or surface flux) such that it can easily be applied to other hydrodynamic grids. Accordingly, the sensitivity and identifiability analysis described below are informative for both the LCS gridded model as well as potential applications to different systems. The FishTank model provides estimates for the 36 state variables described above using a 1-D parcel that is uniformly mixed. A set of initial conditions is provided as input to the model that was based on observations of relevant variables obtained from research cruises in April, June, and September 2006 (Table 1, Murrell et al. (2014)). The FishTank model was executed from January 1st to December st, 2006 at a timestep of five minutes.

Results from FishTank are based on time-dependent differential equations that describe energy flow between phytoplankton (up to six groups) and zooplankton (two groups) as affected by nutrient uptake rates, organic matter inputs and losses, inherent optical properties, sediment diagenesis, and temperature (Penta et al. 2008, Eldridge and Roelke 2010, see appendix in Lehrter

et al. in review). A total of 108 equations are estimated at each time step to return a value for each of the 36 state variables described by the model. In addition to the initial conditions, a set of parameter values for each of the equations is also supplied at model execution. These parameters define relationships among fixed effects in the equations and represent ecological properties described by the model that influence hypoxia formation. Values for each of the parameters were based on estimates from the literature, field or laboratory-based measurements, or expert-based knowledge in absence of the former. The sensitivity of O_2 was estimated at each timestep from FishTank in relation to 249 parameters that are included in the 108 equations. For simplicity in the discussion below, the parameters were grouped into one of six categories in relation to applicable equations: optics, phytoplankton, zooplankton, temperature, and organic matter. A full description of the equations and parameters is available as an appendix in (Lehrter et al. in review).

2.2 Local sensitivity analysis

The analysis focused on sensitivity of O_2 in the 1-D FishTank model to identify parameters that may affect spatial and temporal variation of hypoxia in the larger model. A local sensitivity analysis was performed for each of the 249 parameters using a simple perturbation approach to evaluate the change in O_2 from the original parameter values. The analyses relied exlusively on concepts used in the FME package developed for the R statistical programming language (Soetaert and Petzoldt 2010). Each parameter was perturbed by 50% of its original value and the model was executed to obtain an estimate of the effect on O_2. For each perturbation, a sensitivity value S was estimated for each time step i given a set value for parameter j as:

$$S_{ij} = \frac{\partial y_i}{\partial \Theta_j} \cdot \frac{w_{\Theta_j}}{w_{y_i}} \tag{1}$$

where the estimate depended on the change in the predicted value for response variable y divided by the change in the parameter Θ_j multiplied by the quotient of scaling factors w for each. The scaling factors, w_{Θ_j} for the parameter Θ_j and w_{y_i} for response variable y_i, were set as the default value of the unperturbed parameter and the predicted value of y_i after perturbation (Soetaert and Petzoldt 2010). The scaling ensures the estimates are unitless such that the relative magnitudes provide a comparison for model sensitivity to parameter changes that may vary in scale.

147 Estimates for S_{ij} were summarized as $L1$ and $L2$ across the time series to obtain individual

148 sensitivity values of O_2 in response to a change in parameter j:

$$L1 = \sum |S_{ij}|/n \tag{2}$$

149

$$L2 = \sqrt{\sum \left(S_{ij}^2\right)|/n} \tag{3}$$

150 In general, positive sensitivity estimates suggested a parameter had a positive effect on O_2

151 for a given increase in the parameter, whereas the converse was true for negative sensitivity

152 estimates. However, the effect of a parameter change may not be uniform over time such that S_{ij}

153 can change in magnitude and sign depending on the location. Time series of O_2 estimates before

154 and after perturbation were also evaluated to identify patterns not captured by the summary

155 statistics. All parameters for each of the six equation categories (optics, phytoplankton,

156 zooplankton, temperature, and organic matter) that had non-zero $L1$ or $L2$ were retained for

157 identifiability analysis.

2.3 Identifiability and selecting parameter subsets

159 Identifiability of parameter subsets was estimated from the minimum eigenvector of the

160 cross-product of a selected sensitivity matrix (Brun et al. 2001, Omlin et al. 2001):

$$\gamma = \frac{1}{\sqrt{\min\left(\mathrm{EV}[\hat{S}^\top \hat{S}]\right)}} \tag{4}$$

161 where γ ranges from one to infinity for perfectly identifiable (orthogonal) or unidentifiable

162 (perfectly collinear) results for a set of parameters in a chosen sensitivity matrix S. The

163 sensitivity functions were supplied as a matrix $\hat{S}$ with rows i and columns j (eq. (1)) that

164 describes deviations of predicted O_2 from the default parameter values. The matrix $\hat{S}$ was first

165 normalized by dividing by the square root of the summed residuals(Omlin et al. 2001, Soetaert

166 and Petzoldt 2010).

167 The collinearity index γ provides a measure of the linear dependence between sensitivity

168 functions described above for subsets of parameters. Estimates of γ greater than 10-15 suggest

169 parameter sets are poorly identifiable (Brun et al. 2001, Omlin et al. 2001), meaning optimal

170 values are inestimable given similar effects of the selected parameters on O_2. Greater sensitivity

171 of a state variable to parameters within a subset does not imply identifiability if the individual

172 effects are similar. An intuitive interpretation of γ is provided by Brun et al. (2001) such that a

173 change in a state variable caused by a change in one parameter can be offset by the fraction

174 $1 - 1/\gamma$ by the remaining parameters. That is, $\gamma = 10$ suggests the relative change in O_2 for a

175 selected parameter can be compensated for by 90% with changes in the other parameters.

176 Initial analyses suggested that considerably limited subsets of parameters were identifiable

177 of the 249 included in the FishTank model. Given this limitation, parameter selection must

178 consider the competing objectives of increased precision with parameter inclusion and

179 identifability as it relates to optimization. An additional challenge is the excessively high number

180 of combinations of parameter sets, which complicates selection given differences in parameter

181 sensitivity and desired ecological categories of each parameter as they relate to the

182 biogeochemical equations. For example, Fig. 1 provides a simple graphic of the unique number of

183 combinations that are possible for different subsets of 'complete' parameter sets of different sizes

184 (i.e., based on n choose k combinations equal to $n!/\left(k!\left(n-k\right)!\right)$). The number of unique

185 combinations increases with the total parameters in the set and is also maximized for moderate

186 selections (e.g., selecting half the total). For example, over $10^{1}4$ combinations are possible by

187 selecting 25 parameters from a set of 50. Accordingly, parameter selection is complicated by

188 differing sensitivity, identifiability, and the difficulty of choosing from many combinations.

189 A set of heuristics was developed to balance the tradeoff in model complexity and

190 identifiability given the challenges described above. These rulesets were developed with the

191 assumption that parameters will be selected given preference for those with high sensitivity and

192 identifability based on $\gamma < 15$ was an acceptable threshold for subsets (e.g., 93% accountability

193 between parameters). Selection heurestics also recognized that parameter categories (i.e., optics,

194 phytoplankton, zooplankton, temperature, organic matter) may have unequal preferences given

195 questions of interest. In all selection scenarios, parameters were selected by decreasing sensitivity

196 starting with the most sensitive until identifiability did not exceed $\gamma = 15$ where selections were

197 1) independent of parameter category, 2) blocked within parameter category, 3) or considering all

198 categories equally . The selection rules produced seven subsets of parameters that could further

199 be used to optimize model calibration for O_2.

200 Finally, the above analyses were repeated for additional state variables estimated by

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FishTank to provide further descriptions of ecological dynamics that are relevant for hypoxia. In addition to O_2, other state variables included chlorophyll *a* (chl-*a*), photosynthetically active radiation (PAR), nitrate, ammonium, particulate organic matter, dissolved organic matter, and phosphorus. Particulate and dissolved organic matter were estimated as the summation of the respective outputs for organic matter from phytoplankon (*OM1_A*, *OM2_A*), fecal pellets (*OM1_fp*, *OM2_fp*), river sources *OM1_rp*, *OM2_rp*), and boundary conditions (*OM1_bc*, *OM2_bc*, see Lehrter et al. in review).

3   Results

3.1   Local sensitivity analysis

The parameters that have the greatest effect on the model by category (optics, organics, phytoplankton, zooplankton) are as follows.

Plotting the raw values from the sensitivity analysis provides a visual assessment of changes.

The identifiability functions evaluate the ability to identify all subsets from pairwise to all parameters in the subset. As an example, the identifiability of pairwise combinations for each of the categories are shown below.

Pairwise identifiability of the top two most sensitive parameters in each category is shown, first as a table showing all unique combinations from two to all parameters and second as a figure showing pairwise combinations.

Reading each plot from left to right can be interpreted as including additional parameters, where each parameter is ranked by relative sensitivity. The inset in each plot shows the identifiability of including parameters, up to a maximum where additional inclusion exceeds the identifability threshold of fifteen. The scenarios for including parameters all begin with the parameters that have the greatest effect on the model output. The inclusion of additional parameters depends on the scenario. The first scenario selected parameters by decreasing sensitivity within each category (i.e., four separate models calibrated for optics, organics, phytoplankton, or zooplankton), the second scenario selected parameters by sensitivity regardless of category, and the third scenario selects parameters by sensitivity with equal representation between categories.

4 Discussion

Questions specific to GOM - what initial conditions are important? How many phytoplankton groups do we need (e.g., related to structural uncertainty)?

How does the assimilation of additional parameters (e.g., other state variables) during calibration influence the conclusions?

How does uncertainty translate to what a model should provide (generality v precision)? The first step - find out what can be optimized but then do not overfit....

What about structural uncertainty - does sensitivity of a model to variation in a parameter imply parameter uncertainty and/or structural uncertainty?

A final point about optimization with identifiable parameter sets - optimization to fit the data still does not ensure a correct model. Failing in one way can be over-compensated by another feature, e.g., the parameter set that is optimized (see Flynn (2005), p. 1207, third paragraph)

Omlin et al. (2001) state that the sensitivity, identifiability, estimation process is iterative (p. 113), need to rinse and repeat for proper calibration.

How to improve identifiability - get more/better observed data, include obs from other state variables in RSS minimization (eqn q in Omlin et al. (2001))

Alternative methods for uncertainty analysis - bayesian, MCMC, nonlinear calibration-constrained optimization (Gallagher and Doherty 2007)

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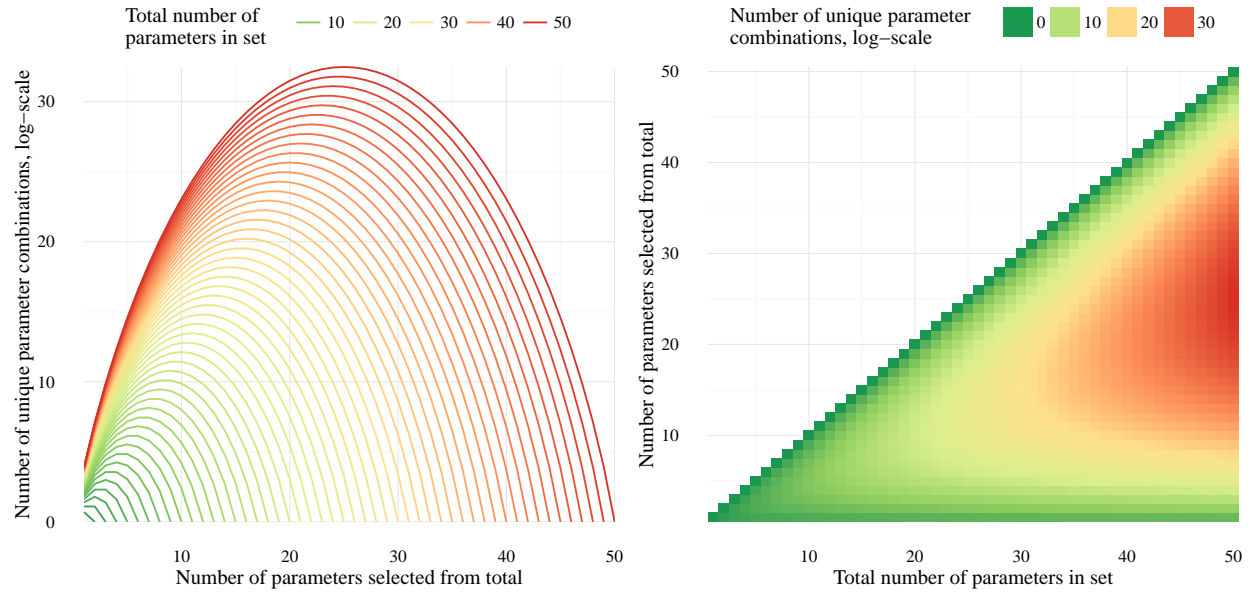
Fig. 1: Number of unique combinations that can occur by selecting parameters for optimization from different parameter sets. The number of combinations are shown for increasing numbers of selected parameters from the total in the set, where 100 parameter sets are shown each with one through 100 total parameters. For example, there are six unique parameter combinations that result from choosing two parameters from a set. Note that the number of unique combinations is shown as the natural-log. The same information is viewed differently in each plot.

Table 1: Test

Parameter	Description	Value	L1	L2
astar490	Chla specific absorption at 490 nm	0.0375	1.64	8.64
astarOMA	OM_A specific absorption at 490 nm	0.1000	2.29×10^{-2}	9.52×10^{-2}
astarOMZ	OM_Z specific absorption at 490 nm	0.1000	5.65×10^{-3}	1.42×10^{-2}
Kcdom	AOP, light attenuation due to CDOM	0.0010	3.18×10^{-6}	1.09×10^{-5}