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Practical identifiability analysis of environmental models

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Abstract: Identifiability of a system model can be considered as the extent to which one can capture its parameter values from observational data and other prior knowledge of the system. Identifiability must be considered in context so that the objectives of the modelling must also be taken into account in its interpretation. A model may be identifiable for certain objective functions but not others; its identifiability may depend not just on the model structure but also on the level and type of noise, and may even not be identifiable when there is no noise on the observational data. Context also means that non-identifiability might not matter in some contexts, such as when representing pluralistic values among stakeholders, and may be very important in others, such as where it leads to intolerable uncertainties in model predictions. Uncertainty quantification of environmental systems is receiving increasing attention especially through the development of sophisticated methods, often statistically-based. This is partly driven by the desire of society and its decision makers to make more informed judgments as to how systems are better managed and associated resources efficiently allocated. Less attention seems to be given by modellers to understand the imperfections in their models and their implications. Practical methods of identifiability analysis can assist greatly here to assess if there is an identifiability problem so that one can proceed to decide if it matters, and if so how to go about modifying the model (transforming parameters, selecting specific data periods, changing model structure, using a more sophisticated objective function). A suite of relevant methods is available and the major useful ones are discussed here including sensitivity analysis, response surface methods, model emulation and the quantification of uncertainty. The paper also addresses various perspectives and concepts that warrant further development and use.

Keywords: Identifiability; Environmental models; Model analysis

1. INTRODUCTION

Environmental models are widely used for management and scenario analysis, increasingly for social learning among stakeholders, and in environmental decision support systems (Kelly et al., 2013). Given the expanding importance of models the mission of this paper is to persuade environmental scientists to understand their models better. Understanding model limitations contextually, that is given the purpose and assumptions of the model and the data available to calibrate it, is fundamental. There are two prime

considerations in this exercise: the predictive accuracy of the model (solving the forward problem) relevant to its purpose as treated by Bennett et al. (2013); and the identifiability of the model (also viewed as the well-posedness of the inverse problem of identifying a model structure and parameters from observational data on the system of interest). This paper critically reviews practical problems in assessing model identifiability, groups different perspectives on the validity of estimates and concludes with a discussion of open research issues. It could be regarded as a sequel to Bennett et al. (2013), exploring the behaviour of environmental models and how their usefulness should be assessed. A valuable reference on identifiability is Walter and Pronzato (1997). While Beck (1987) considered identifiability in terms of water quality models, much of the discussion there is also of more generic value. Identifiability can be viewed as a key concept and step to be explored in the development and evaluation of environmental models (see Jakeman et al., 2006).

The paper first considers the concept of identifiability and then focusses on practical methods of identification. The two issues were originally quite separate; with the former providing a clear cut (yes or no) answer to achieving unique parameter estimates, and the second assessing the numerical values of the unknown parameters and the extent of the identification accuracy. These two approaches have progressively converged into a single concept of "reliable" identifiability moving from the purely structural aspects of absolute identifiability, concerning the structural properties of the model, to the joint consideration of the various ingredients leading to a successful identification, including efficient model structure (parameter parsimony), data quality (informative data sets, good signal-to-noise ratio), and efficiency of the identification method (robustness, uniqueness, speed of convergence, versatility).

The paper then proceeds to address the perspectives and techniques that have been used to assess practical identifiability for different application fields, including the use of sensitivity analysis, quadratic and higher degree response surface methods, dynamic identifiability analysis, pseudo Monte Carlo methods (Bayesian and non-Bayesian). This approach allows the reader to infer the relevance of the various identifiability perspectives across environmental fields.

2. A BRIEF HISTORY OF IDENTIFIABILITY AND SOME BASIC METHODS

Sometimes the structure of the model prevents the identification of some or all of its parameters. For this reason identifiability was initially considered a *structural* model property. Early theoretical identifiability tests heavily depended on calculus (Bellman and Astrom, 1970; Glover and Willems, 1974; Pohjanpalo, 1978; Cobelli and DiStefano III, 1980; Norton, 1980; Godfrey et al, 1982; Walter and Lecourtier, 1982) and gave a go/no-go response. They were followed later by more flexible (and practical) methods based on sensitivity analysis. The rationale behind this approach was that a parameter is (more or less) identifiable depending on the relative extent to which they influence the model output. In the paper we would like to stress the converging trend between the theoretical and the practical approaches pointing toward Sensitivity Theory (ST) and its central role in assessing the practical identifiability of a model, not only as a structural property but also in relation to the quality of the data and in some cases the experimental design (Fedorov, 1972; Dochain and Vanrolleghem, 2001; Keesman and Stigter, 2002; Stigter and Keesman, 2004). Sensitivity Theory (ST) from a statistical standpoint includes use of the Fisher Information Matrix (FIM). Briefly the Sensitivity of the model output *y* with respect to a parameter ϑ is defined as $S_\vartheta^y = \frac{\partial y}{\partial \vartheta}$, therefore the larger is S_ϑ^y the better ϑ is identifiable from the output measurement. Since the definition of FIM involves the use of S_ϑ^y which in turn can be used to design optimal experimental conditions, there are considerable degrees of freedom in defining the experimental conditions that maximize S_ϑ^y (optimal experimental design).As we shall see, sensitivity analysis generates other identifiability methods, such as the response surface method (see section 2,2) and one- and two-dimensional projections (e.g. Wagener and Kollat, 2007). These methods analyse the shape of the objective error function in the parameter space to reveal possible numerical difficulties such as local minima, "narrow valley" or parallel troughs, all preventing the optimum to be reached. As an example two different model structures were tested as approximations to a horizontal subsurface constructed wetland (Checchi and Marsili-Libelli, 2005). Though apparently similar, their identifiability greatly differs, as shown in Figure 1, where parameters V_1 and V_2 refer to model A, and b and V_3 are additional parameters introduced in model B. The added complexity of model B is reflected in a partial lack of identifiability (local

minima and horizontal trough). The response surface of model A has a single (global) minimum and is therefore easily identifiable, whereas model B shows local minima and a horizontal valley meaning that the sensitivity to parameter V_2 is nil.

In a recent paper by Anguelova *et al.* (2012) the local structural identifiability problem was solved for a model with 31 states and 49 parameters (including the initial conditions) using computer algebra software (that, incidentally, was not used to compute *any* sensitivity of states or outputs to the parameters). Solution of this very hard problem required approximately a day of computation time. Although this is quite an impressing result that shifts the bounds on what currently can be achieved, the propagation of measurement uncertainty on the parameter estimates was not a part of this study, while this is certainly an important topic for environmental engineering. Yet, the computational result hallmarks the current possibilities in testing for local structural identifiability. In addition, these kinds of results are certainly useful in assisting, for example, with the problem of finding *a minimal sensor set* that allows identification of *all* model parameters in the model.

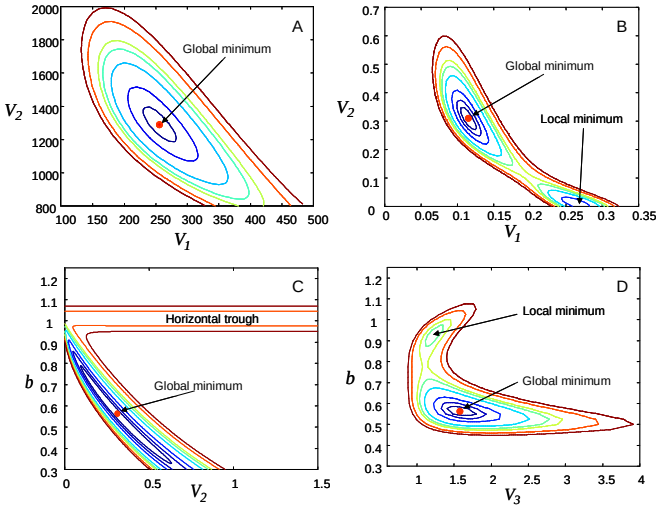

Figure 1. Response surface plots of the two models (graph A: model A; graphs B, C, D: model B).

Another interesting problem in system identification is to address the question of which parameters (from a large set of unknowns) can be reliably identified given the current model and experimental setup (inputs and outputs to the system). Brun and Reichert (2001), for example, consider this problem for a model with 3 states and 13 parameters. Through comparison of collinearities (dependencies between parametric output sensitivities) and magnitudes of relative sensitivities, a ranking can be calculated that indicates which of the parameters can be identified and which ones can be fixed to a realistic but arbitrary value without influencing the model prediction substantially. Of course their analysis depends on the particular values of the parameters involved, but this does not hamper Brun and Reichert in concluding which parameters are the most relevant in explaining, for example, the dominant behaviour of a modest size bio-reactor model.

2.1 Correlation between parameters and structural identifiability

Another (and by now classical) example of the issues encountered in an identifiability analysis involves correlation between parameters, and is presented in Dochain *et al.* (1995). In this example, analysis of a simple 4 parameter model describing the oxygen uptake rate of a population of micro-organisms shows a strong correlation between the parameters. Analysis of the Jacobi matrix can identify such issues, as well as yielding a reduced parameterization (in this example, a reduction to 3 parameters). While the search for a re-parameterisation may be very rewarding in terms of gaining considerable reliability in the parameter estimates, the possible price that may have to be paid for a re-parameterisation is a loss of insight in the model's structural relations. However, the question is: 'how should we re-parameterise?' Some feasible solutions to the model re-parameterisation problem have been presented in Keesman (2011), Section 5.2.5.

2.2 Quadratic response surfaces

Graphical methods using surface response plots, as in Figure 1, are typically limited to cases with less than three parameters. Response surface-based identifiability analysis of models with more than three parameters is possible if the response surface can be locally approximated by a quadratic surface (see

e.g. Box and Draper, 1987; Abusam *et al*. 2001). For the two-parameter case, as presented in Figure 1, this reads as

$$y = a_0 + a_1\vartheta_1 + a_2\vartheta_2 + a_{11}\vartheta_{12} + a_{12}\vartheta_1\vartheta_2 + a_{22}\vartheta_{22} \quad (1)$$

with y the model response, ϑ_1:=V_2, ϑ_2:=b and second-order polynomial parameters a_0, ..., a_{22}.

In general, for the p-dimensional parameter case, we can write

$$y = a_0 + A\vartheta + \vartheta^T B\vartheta \quad (2)$$

with ϑ:=$[\vartheta_1, \vartheta_2, ..., \vartheta_p]^T$, A:= $[a_1, a_2, ..., a_p]$, and B a symmetric $p \times p$ matrix with diagonal elements $a_{11}, a_{22}, ..., a_{pp}$ and off-diagonal elements $a_{ij}/2$. Eigenvalue decomposition of B gives eigenvectors that represent the direction of the main axes of the quadratic surface, and corresponding eigenvalues that represent the length of the semi-axes of the ellipsoidal contours. If both eigenvalues have the same sign then ellipsoidal contours appear. Different signs lead to a saddle plane. Non-identifiability of two parameters is shown by a valley or ridge in the response surface. Equal eigenvalues give a circular contour plot, an ideal identifiability case, as both parameters are fully uncorrelated.

Hence, when one or more of the eigenvalues are close to zero, nearly non-identifiable parameters are present in the model. The corresponding eigenvectors show the directions in the parameter space of a valley or trough, and thus the nearly non-identifiable parameter combinations.

2.3 Role of Data

In parallel, extensions of these techniques have been used to investigate the dependence of identifiability on the dataset used for parameter estimation. Analytical methods can be used to identify the data characteristics necessary to achieve 'persistence of excitation' (Norton, 1986). This is related to the notion of 'observability' of parameters. For example, parameters of some hydrological models may only be active in rare conditions (Sorooshian & Gupta, 1983). For black-box models, Dynamic Identifiability Analysis (DYNIA) identifies a time-varying measure of information in data with respect to parameters (Wagener et al., 2003). This can also be approached by investigating time-variation of sensitivity (e.g. Herman et al 2013).

In a numerical study on data worth in the context of unsaturated zone models, Brunner et al. (2012) observed that certain observations can significantly reduce predictive uncertainty without informing any specific parameters. Therefore, the reduction of uncertainty must be related to information concerning combinations of parameters. This raises questions concerning the adequate level of complexity because in this case the ability of the model to reduce the uncertainty of predictions does not rely on the precise estimation of all model parameters. Instead it relies on good estimations of only combinations. This information can be used to simplify the model as suggested through the calibration process.

As identifiability relates to the inability to estimate unique parameters, it has naturally been extended to the idea of uncertainty in parameter estimation more generally. As a result of mismatch between model structure and error characteristics relative to the data available, parameter values identified may vary depending on the dataset and objective function used. Calculating cross-validated performance can give a measure of the significance of the problem. This broader understanding of identifiability has been approached through the concept of 'non-stationarity,' multi-objective optimisation and trade-offs between objectives (e.g. Madsen, 2000, Oudin et al. 2006), equifinality (e.g. Beven, 2006), uncertainty analysis (e.g. Beck and Halfon, 1991) and uncertainty quantification generally (e.g. Vrugt et al., 2008).

2.4 Regularisation

Regularisation is often used to enhance the identifiability of a model. In principle, two approaches to regularization exist (Doherty 2010). Tikhonov regularization stabilizes an ill-posed inverse problem (i.e.

enhances identifiablilty) by providing information directly relating to the calibrated parameters (Aster et al. 2005). An alternative to this method is through subspace approaches such as Singular Value Decomposition (SVD). In this approach, the parameter space is decomposed into a solution and a null-space. These subspaces are orthogonal and spanned by orthogonal unit vectors. Unit vectors which span the calibration solution space are the combinations of parameters that can be estimated with a given calibration dataset. The null space is spanned by parameter combinations that cannot be estimated. This decomposition allows identifying super-parameters (Tonkin and Doherty 2005) that represent combinations of orthogonal base parameters. The calibration of super parameters rather than all individual parameters represents a reduction of the dimensionality to the inverse problem.

3. PRACTICAL PROBLEMS ENCOUNTERED IN THE PARAMETER ESTIMATION OF ENVIRONMENTAL SYSTEMS

3.1 Numerical techniques for practical parameter estimation

The parameter estimation problem, for a state-space model, can be stated in the following terms: given a model and a set of N experimental measurements

$$\begin{cases} \frac{d\boldsymbol{x}}{dt} = \boldsymbol{f}(\boldsymbol{x}, \boldsymbol{u}_{exp}, \boldsymbol{P}) & \boldsymbol{x} \in \mathbb{R}^n \\ \boldsymbol{y} = \boldsymbol{g}(\boldsymbol{x}, \boldsymbol{u}_{exp}, \boldsymbol{P}) & \boldsymbol{y} \in \mathbb{R}^q \\ & \boldsymbol{P} \in \mathbb{R}^{n_p} \end{cases} \quad with\ experimental\ data\ y_k^{exp} = \begin{bmatrix} y_1^{exp} \\ y_2^{exp} \\ \vdots \\ y_q^{exp} \end{bmatrix}_k \in \mathbb{R}^q, k = 1, \dots, N \quad (3)$$

where $\boldsymbol{x}$ is the system state, $\boldsymbol{y}$ its input, u_{exp} the experimental input and $\boldsymbol{P}$ the vector of parameters; then a set of optimal model parameters can be found by solving

$$\hat{P} = arg\ min\, E(P),\ E(P) = \sum_{k=1}^{N} \left(y_k(P) - y_k^{exp}\right)^T Q_k \left(y_k(P) - y_k^{exp}\right), \quad (4)$$

where Q_k represents the accuracy of the k-th measurement. Usually this is expressed as a diagonal matrix with the reciprocal of the measurement variances $Q_k = diag\left(\frac{1}{\sigma_1^2}, \frac{1}{\sigma_2^2}, \dots, \frac{1}{\sigma_q^2}\right)$. Since parameters generally appear non-linearly in the output of model Eq. (3), numerical search methods must be used, the most popular being based on the Nelder and Mead flexible polyhedron algorithm and variations thereof, such as optimized search step, multi-start, etc. The main pitfall of this method is the possibility of being trapped in local minima. For this reason it is advisable to have a preliminary exploration of the error functional surface (see Section 2) or use a robust global optimizer, e.g. based on a genetic algorithm. This is especially recommended with data-driven models involving many parameters with little or no physical significance.

3.2 Insensitivity of output to parameter changes

Lack of identifiability of parameters commonly manifests itself in two key forms: insensitivity of the output to change in a single parameter change, and to changes in correlated parameters (Sorooshian & Gupta, 1983). In the first case, if varying a parameter while keeping others fixed has no effect on the output, this suggests a problem with persistence of excitation or observability. The parameter needs to either be omitted, along with the processes it was meant to capture, or be estimated with a different forcing dataset in which its effect can be observed.

The correlation of parameters results in lack of identifiability because a change in one parameter is compensated by a change in another, such that multiple parameter sets give the same output according to some quantity of interest. This effect can in some cases be addressed by removing or reducing correlation between the parameters (e.g. Gupta and Sorooshian 1983).

3.3 Failure of optimisation algorithms

Even if an objective function response surface has a unique optimal point, optimisation algorithms may not be able to consistently identify it due to multiple regions of attraction, minor local optima, roughness, poor sensitivity and non-convex shape (Duan et al. 1992). A number of advances in optimisation methods (e.g. Duan et al. 1992; Vrugt et al. 2008) mean that a number of these can be overcome. They are however generally symptomatic of underlying issues with the data and model structure, and it may be desirable to instead improve properties of the response surface (e.g. Gupta and Sorooshian 1983, Kavetski et al 2006).

3.4 Noise and estimation accuracy

When a model structure has been selected, reliable identification also depends on the quality and richness of information in the data. In environmental problems, the available data were often collected for other purposes than modelling, so they are far from the "optimal experiment" conditions and yet in many instances they are the only available ones and the modeller has to make do with them. Noisy data can be filtered, for example by smoothing splines or by wavelets, in order to remove part of the noise without significantly affecting the information contained in the data (Torrence and Compo, 1998; Marsili-Libelli and Tabani, 2002; Marsili-Libelli et al., 2003, Marsili-Libelli, 2004; Marsili-Libelli and Arrigucci, 2004.

Consider the estimation of Monod kinetics from noisy observations of substrate and biomass, as shown in Figure 2. The μ_{max} sensitivity – and estimation accuracy - in the noise-free case is compared to the results obtained with increasing levels of noise. If the noise is moderate (σ = 0.0147) the estimated value is still the exact one, but as the noise level increases the estimation accuracy is affected as the estimated value (red dots) is displaced from the correct value (μ_{max} = 0.5). In all cases the noisy estimation is more sensitive.

The presence of noise raises the potential for overfitting when using automated parameter estimation. Parameters need to be unique despite error, which relies on capacity to account for error, typically in objective/likelihood function. It may be necessary to accept that there is no unique solution, and instead use an approach to quantify uncertainty or to explore its effects.

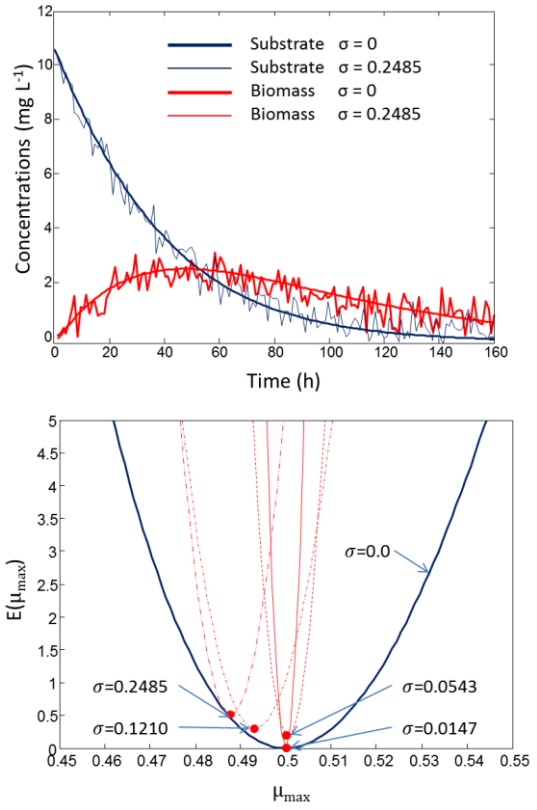

Figure 2. Estimation of μ_{max} with noisy observations.

3.5 Transparency of improvements to identifiability

Issues of identifiability are by their very nature hidden from the modeller's view. If the issues were obvious, the modeller would have addressed them, and no identifiability issue would be experienced. Therefore addressing identifiability generally requires changes that the modeller would not generally have considered, e.g. transforming parameters, selecting specific data periods, changing model structure, using a more sophisticated objective function. It is important that these changes do not undermine the

ability to understand the concepts that went into creating the model in the first place. This relates to the debate on appropriate model complexity (e.g. Simmons and Hunt, 2012).

3.6 Time required to analyse identifiability

Ability to address identifiability is limited by skills, resources and available time, both of the modeller and computational time. Response surface methods also known as surrogate or model emulation methods are often essential for identifiability analysis. When evaluating a model is computationally expensive, the number of times the model can be run is limited. In such situations many of the methods mentioned in this paper are infeasible, especially Monte Carlo based algorithms. Surrogate models can be used to alleviate the computational burden, by using techniques such as Polynomial Chaos Expansions (PCE) or Gaussian Processes (GP) (Rasmussen and Williams, 2005; Xiu and Westhaven, 2005), to efficiently approximate the model response surface. Once built, these surrogates can be sampled repeatedly at a negligible cost relative to that of running the true model. Provided a surrogate of sufficient accuracy (problem dependent) can be constructed with fewer samples than required by the identifiability analysis, response surface methods are extremely effective at enabling the application of more computationally-demanding methods.

4. PERSPECTIVES ON VALIDITY OF THE ESTIMATES

A modeller's experience of identifiability differs depending on the problem, model and data characteristics, as indicated in the case of model structure issues (e.g. Gupta et al., 2012; Lin and Beck, 2012). Perspectives therefore vary on what constitutes valid parameter estimates (and whether such even exist), and what should be done when no valid estimate can be identified. This depends on the type of identifiability considered and the assumptions that can be justified in the problem domain. While perspectives on identifiability have not been rigorously surveyed, we can at least distinguish between identifying an identifiability problem, elimination of the problem, quantification of uncertainty, and evaluating risk (impact of uncertainty).

4.1 Identifying an identifiability problem

Identifying limitations involves determining whether or not estimated parameters are 'valid', whether an identifiability problem exists, and perhaps identifying the cause of the issue. It considers that 'a problem well-stated is a problem half-solved', and suggests that future work may need to address the identifiability issued identified.

Once a set of optimal parameters, in the sense defined in Eq. (4) has been obtained, the credibility of these estimates should be challenged. Possible statistical approaches are:

- Non parametric methods, in which the agreement between data and model response is considered, irrespective of the parameter values. These methods rely on regression analysis and F-statistics to decide whether the null hypothesis (correct model) should be accepted or rejected.
- Parametric methods, which consider confidence regions, based on the parameter covariance matrix, in which acceptable parameters should fall. These methods are mainly based on the Fisher Information Matrix and may involve a feedback path whereby an unsatisfactory estimation can be improved by changing the experimental conditions (Optimal Experimental Design, see e.g. Fedorov, 1972; Seeber and Wild, 1989; Dochain and Vanrolleghem, 2001).
- A number of analytical techniques can evaluate structural identifiability, including some supported by computer algebra (e.g. Bellu et al., 2007).
- Calculation of degree of interaction can be obtained by a number of means: Sobol indices for specific parameter interactions obtained by PCE for example, eigenvalues of quadratic response surface, indices of concentricity and interaction, sensitivity ratio (Sorooshian & Gupta, 1985).
- Certain surrogate methods provide additional benefits other than reduction in the computational cost. For example, the structure of Polynomial Chaos Expansions (PCE) allows the derivation of analytical

expressions for the mean, variance, and Sobol sensitivity indices. If the model samples used to build the PCE are chosen carefully the estimates of these statistics converge much faster than Monte Carlo estimates. This typically allows one to obtain high-order interaction Sobol indices which are often not computed using Monte Carlo-based Sobol methods (Sudret, 2008).

4.2 Eliminating an identifiability problem

Some symptoms of identifiability may be considered intolerable, such as non-uniqueness of automated parameters estimated, lack of observability of a parameter or lack of transferability of a model to specific conditions, e.g. to drought in hydrological applications. Eliminating these symptoms typically requires invasive changes to the model or model identification procedure. Correlation of parameters can be eliminated by principal component analysis, factor analysis, reparameterisation and rescaling of variables to achieve an elliptical response surface (Gupta and Sorooshian, 1983). Selection of a data record, typically approached simply in hydrology by selecting a long enough period, but may not have the right information (see Sorooshian and Gupta 1983).

4.3 Quantification of uncertainty

In some cases, an identifiability problem is not a priori intolerable. Instead, the identifiability problem is transformed into an uncertainty problem, and the resulting uncertainty is quantified. The emphasis is on providing information so that its users have an understanding of the effect of identifiability. In general, no value judgement is made as to whether the uncertainty is *a posteriori* tolerable.

An ellipsoidal parameter confidence region can be defined as the parameter set $\boldsymbol{P}$ that satisfies the following inequality

$$\left\{ \boldsymbol{P} : \left(\boldsymbol{P} - \hat{\boldsymbol{P}} \right)^T \boldsymbol{C}^{-1} \left(\boldsymbol{P} - \hat{\boldsymbol{P}} \right)^T \le n_p F_{n_p, N-n_p}^{1-\alpha} \right\} \tag{5}$$

where n_p is the number of parameter, N the experimental data and α is the selected confidence level of the *F* statistics. In Eq. (5) the weighing matric $\boldsymbol{C}$ is an approximation of the parameter covariance matrix and can obtained as the inverse of the FIM, i.e. $C = FIM^{-1}$. Alternatively, uncertainty regions, without using statistics and not necessarily ellipsoidal, can be obtained via Monte Carlo simulation.

As pointed out earlier regarding Optimal Experimental Design, the following tutorial example shows how trajectory sensitivity, FIM and estimation accuracy are related. Consider a simple Streeter and Phelps model describing the dynamics of organic pollution in rivers

$$\begin{cases} \dfrac{dB}{dt} = -K_b \cdot B \\ \dfrac{dC}{dt} = K_c \left(C_{sat} - C \right) - K_b \cdot B \end{cases} \tag{6}$$

where B is the Biological Oxygen Demand (BOD) and C is the Dissolved Oxygen (DO), with C_{sat} representing its saturation concentration. Consider the estimation of kinetic constants K_b and K_c in the simple situation of **Error! Reference source not found.** with two pollution point sources, assuming that only Dissolved Oxygen measurements are available.

It is interesting to compare the estimation accuracy in the two cases. It can be seen in Table 1 that by concentrating the samples in the highly sensitive points of the system evolution a higher accuracy can be obtained. In fact the FIM in the concentrated samples case is much larger than in the evenly spaced samples. As a consequence, the parameter uncertainty brackets in the latter case are almost half those of the even case.

As pointed out in Marsili-Libelli et al. (2003) the actual agreement or disagreement between confidence ellipsoids computed with differing methods can be diagnostic in questioning the accuracy of the estimated parameters.

The concept of an indifference region can also be useful in this respect. Indifference is the "approximate region in the parameter space around a parameter estimate for which the model output sequences are considered to be indistinguishable." (Sorooshian and Gupta, 1985).

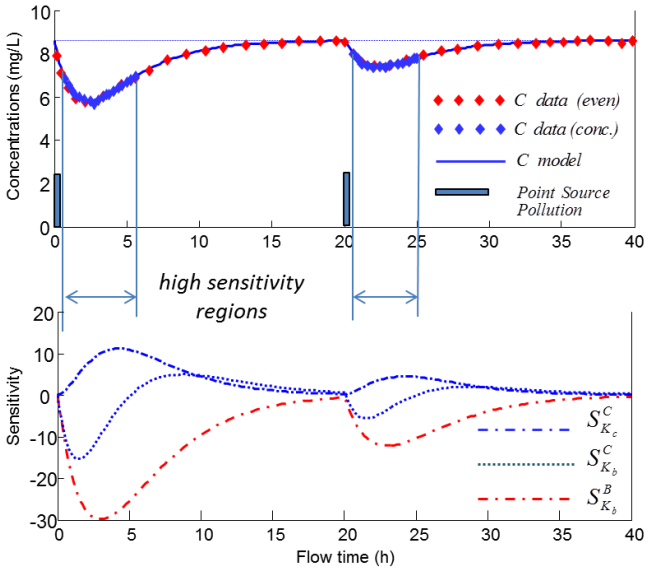

Figure 3. A simple Streeter and Phelps model with two point sources. The trajectory sensitivities are shown in the lower graph. In the first case evenly spaced measurements are taken along the entire reach (red diamonds) whereas in the second case the samples are restricted to the highly sensitivity zones (blue diamonds).

Table 1. Comparison of estimation accuracies.

Evenly spaced samples	Concentrated samples
$\sigma_{DO} = 0.042475$	$\sigma_{DO} = 0.046638$
$FIM = \begin{bmatrix} 1150.30 & -314.90 \\ -314.90 & 867.50 \end{bmatrix}$	$FIM = \begin{bmatrix} 3360.70 & -1537.00 \\ -1537.00 & 2740.60 \end{bmatrix}$
$C = \begin{bmatrix} 0.1741\times10^{-5} & 0.0632\times10^{-5} \\ 0.0632\times10^{-5} & 0.2309\times10^{-5} \end{bmatrix}$	$C = \begin{bmatrix} 0.0871\times10^{-5} & 0.0488\times10^{-5} \\ 0.0488\times10^{-5} & 0.1067\times10^{-5} \end{bmatrix}$
$\delta K_b = \pm 2.2264\times10^{-3}$ $\delta K_c = \pm 2.5637\times10^{-3}$	$\delta K_b = \pm 1.5544\times10^{-3}$ $\delta K_c = \pm 1.7213\times10^{-3}$

4.4 Evaluating risk (impact of uncertainty)

Uncertainty due to identifiability issues (whether explicitly quantified or not) can also be assessed in terms of its risk, i.e. effect on the final product of the analysis, such as for decision making. If it does not change the result, perhaps there is not a need to worry about it. This is typically the default approach if modellers are aware of identifiability issues. By professional judgment, modellers often assert that a given issue is not significant, in order to be able to provide results efficiently rather than futilely trying to tie up every loose end. For example, uncertainty in parameter estimates may not be significant compared to many other issues in complex modelling.

Identifiability issues may also be beneficial in some cases. This is particularly the case with models where parameter values are manually-defined, e.g. cost benefit analysis, expert opinion in Bayesian networks. There may be multiple/pluralistic ways of expressing the situation in order to enhance and share understanding. Not only may identifiability not matter because the emphasis is on promoting discussion, it may be useful to have multiple equivalent models that emphasise different aspects of a situation, e.g. gross margins $/ML and $/ha to emphasise value of water or viability of farm land.

5. OPEN RESEARCH ISSUES

- Many methods for investigating uncertainty are dependent on the type of model. Some model types are therefore under-served, e.g. those that have no explicit mathematical formulation (Sorooshian & Gupta 1983), or have non-smooth derivatives.
- Making techniques accessible to modellers and results accessible to end-users limits the techniques that can be used, e.g. re-parameterisation needs to maintain interpretable parameters.
- Need for teaching re identifiability issues to non-mathematical model users, particularly when optimisation and uncertainty quantification tools are used as black boxes.
- Need for development of general techniques for identifying how correlation of parameters can be removed. Outside of a small set of specific cases, this is currently an ad-hoc exercise.
- Estimating parameters that are expected to become important in the future but do not have a significant effect presently. When parameters are poorly observable with existing data more advanced parameter estimation techniques are required. Parameters can also be non-identifiable (less identifiable) on some parts of a data set when (more) identifiable on others, so guidance is need in this respect (Shin et al., 2013).
- Design of data collection to improve identifiability. Even in modelling of environmental systems where experiments are not possible, it is possible to design monitoring processes. Existing literature takes an uncertainty-focussed approach (often emphasising return on investment). This could be extended to identifying how additional parameters can be identified, rather than reducing uncertainty on existing parameters.
- There are many open questions related to generating response surfaces, however the overarching theme of these questions is how can the number of model runs used to build a surrogate be reduced. Most research to date has focused on approximating smooth response surfaces, but very little has been done to approximate discontinuous response surfaces. One approach that has shown initial promise is enriching surrogates of computationally expensive high-fidelity models with information from lower-fidelity models.
- To address the curse of dimensionality better adaptive sampling strategies are needed that focus on dimensions and/or regions of interest, and variable transformations that identify important directions in the input space.

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