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Assessment of structural simulation models by estimating uncertainties due to model selection and model simplification

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ABSTRACT

In this paper several methods for model assessment considering uncertainties are discussed. Sensitivity analysis is performed to quantify the influence of the individual model input parameters. In addition to the well-known analysis of a single model, a new procedure for quantifying the influence of the model choice on the uncertainty of the model prediction is proposed. Furthermore, a procedure is presented which can be used to estimate the model framework uncertainty and which enables the selection of the optimal model with the best compromise between model input and framework uncertainty. Finally Bayesian methods for model selection are extended for model assessment without measurements using model averaging as reference.

1. Introduction

In structural design the prediction of the structural response is estimated often by using numerical or analytical models. Every prediction underlies a certain uncertainty which could be interpreted as a measure of the quality of the prediction. Following [1], uncertainty is the term to describe incomplete knowledge about models, parameters, constants, data, and beliefs. There are many sources of uncertainty, including the science underlying a model, uncertainty in model parameters and input data, observation error, and code uncertainty. Generally, uncertainties that affect model quality are categorised as:

- Model framework uncertainty: the uncertainty in the underlying science and algorithms of a model. Model framework uncertainty is the result of incomplete scientific data or lack of knowledge about the factors that control the behaviour of the system being modelled. Model framework uncertainty can also be the result of simplifications necessary to translate the conceptual model into mathematical terms.
- Model niche uncertainty: resulting from the use of a model outside the system for which it was originally developed and/or developing a larger model from several existing models with different spatial or temporal scales.
- Model input uncertainty: resulting from data measurement errors, inconsistencies between measured values and those used by the model (e.g., in their level of aggregation/averaging), and parameter value uncertainty. We can distinguish between data uncertainty caused by measurement errors, analytical imprecision, and limited sample sizes during the collection and the treatment of data, and the stochasticity, which are fluctuations in ecological processes that are due to natural variability and inherent randomness.

As an additional indicator of model quality the model complexity can be utilised. Model complexity is the degree of complexity desired for the model. Models become more complex in order to treat more physical processes, their performance tends to degrade because they require more input variables, leading to greater data uncertainty [1]. Model complexity influences uncertainty. Models tend to uncertainty as they become increasingly simple or increasingly complex. Thus complexity is an important parameter to consider when choosing among competing model frameworks or determining the suitability of the existing model framework to the problem of concern. The optimal choice generally is a model that is no more complicated than necessary to guide the regulatory decision. The types of model uncertainty have a reciprocal relationship, with one increases as the other decreases. Thus an optimal level of complexity (the "point of minimum uncertainty") exists for every task that shall be solved by a given set of engineering simulation models.

Generally models are assessed concerning how they can reproduce a certain structural or system behaviour already observed e.g. in experiments. By inverse strategies the unknown input parameters are identified and the model is fitted to optimally reproduce a set of measurements. This is state of the art in engineering modeling. If we think a step further, the engineer or user wants to know, what is the most appropriate model out of a set of given models (different simplification levels, etc.) for the analysis or

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prediction of an unknown, new situation, e.g. the design of a new building. An example: the engineer may use in his analysis simple analytical or highly complex numerical models to represent the behaviour of a certain structural part (e.g. linear elastic beam formulation vs. linear elastic Finite Element calculation vs. Finite Element calculation considering nonlinear material behaviour). Now he wants to know if a simpler model is sufficient enough or if a more complex model is necessary. For this decision, we are interested if possible nonlinear effects play a significant role and if we can improve our prediction by considering such effects while introducing additional uncertainties in our prediction due to the additional model parameters. Thus we want to find the optimal model for a certain task with minimum total uncertainty in its prediction. For a possible task a simple linear model may be absolute sufficient since nonlinear effects are not activated, while for an experimental verification generally more complex models may give a better reproduction of the measurements. The intention of the paper is to find methods to decide which model is optimal with respect to the prediction uncertainty for an unknown situation, without having measurements of the final structure or system.

In the recent years some more or less empirical estimates of model uncertainty have been proposed [3,4,2], which were motivated to find the best model out of a given set of plausible models, which is more appropriate for the prediction of an unknown response. For model selection based on a known response in terms of measurements, Bayesian methods have become very popular in the recent years [5,6]. In these procedures the model with the best compromise in representing the data and the remaining uncertainty in the identified parameters is indicated with higher probability.

Furthermore, sensitivity analysis has become an important tool for model assessment. Sensitivity analysis is the study of how the uncertainty in the output of a model can be apportioned, qualitatively or quantitatively, to different sources of variation in the input of a model [7]. Although sensitivity and uncertainty analysis are closely related, sensitivity analysis assesses the "sensitivity" of the model to specific parameters and uncertainty analysis assesses the "uncertainty" associated with parameter values [1]. Sensitivity analysis can be used to simplify models and is applied without using measurements. The analysis is based only on the output of a numerical or analytical model.

In this study the contribution of variance based sensitivity analysis to the assessment of numerical models is discussed and extended by proposing a procedure to estimate the sensitivity of the model choice on the prediction. In the next step model framework uncertainty of single models is estimated based either on model averaging or on the selection of a reference model. With this information the best compromise between model input and model framework uncertainty is found. As a third assessment procedure, Bayesian methods are extended in order to use reference values instead of measurements. All methods are finally used to evaluate the quality of four cohesive crack models for the simulation of concrete cracking.

2. Methods for model assessment and model selection

2.1. Sensitivity analysis of the model output

Assuming a single model $\mathcal{M}$ with a scalar output Y as a function of a given set of m random input parameters X_i

$$Y = f(X_1, X_2, \ldots, X_m), \tag{1}$$

the first order sensitivity measure was introduced as [8]

$$S_i = \frac{V_{X_i}(E_{\mathbf{X}_{\sim i}}(Y|X_i))}{V(Y)}, \tag{2}$$

where $V(Y)$ is the unconditional variance of the output of model $\mathcal{M}$ and $V_{X_i}(E_{\mathbf{X}_{\sim i}}(Y|X_i))$ is named the *variance of conditional expectation* with $\mathbf{X}_{\sim i}$ denoting the matrix of all factors but X_i.$V_{X_i}(E_{\mathbf{X}_{\sim i}}(Y|X_i))$ measures the first order effect of X_i on the model output Y. According to [9] first order indices should be used for factor prioritisation: "If the cost of discovering factors were the same for all input factors, which factor should I try to discover first?"

Since complex engineering models contain not only a first order (decoupled) influence of the input variables but also coupled, which are called higher order effects on the model output, total sensitivity indices have been introduced [10]

$$S_{Ti} = 1 - \frac{V_{\mathbf{X}_{\sim i}}(E_{X_i}(Y|\mathbf{X}_{\sim i}))}{V(Y)}, \tag{3}$$

where $V_{\mathbf{X}_{\sim i}}(E_{X_i}(Y|\mathbf{X}_{\sim i}))$ measures the first order effect of $\mathbf{X}_{\sim i}$ on the model output Y which does not contain any effect corresponding to X_i. Total effect indices are suitable for factor fixing [9]: "Can I fix a factor or a subset of input factors at any given value over their range of uncertainty without reducing significantly the output?" According to [9] factor fixing is useful to achieve model simplification and relevance. "We cannot use S_i to fix a factor since $S_i = 0$ is a necessary condition for X_i to be non-influential but not a sufficient one. X_i could be influent at the second order."

According to Zadeh's incompatibility principle [11] model simplification supported by factor fixing is useful. "As the complexity of a system increases ... precision and significance (or relevance) become almost mutually exclusive characteristics."

By means of the calculated sensitivity indices, the designer may judge if a certain phenomenon considered in the model has a significant influence on the model output variation. By defining a threshold for a minimum sensitivity index, the model "relevance" can be formulated

$$R = \frac{\text{Number of inputs that induce variations in the output}}{\text{Total number of inputs in the model}}, \tag{4}$$

where low R could flag a model meant to intimidate.

In the general case, first order and total effect sensitivity indices can not be calculated analytically. Thus, numerical procedures have been developed to estimate these indices by using stochastic sampling strategies, e.g. see [9] or [12]. In our study we use the estimation procedure presented in [9] in combination with Latin Hypercube Sampling [13].

2.2. Sensitivity of the model choice

In contrast to the previous section where a single model is assessed by means of the sensitivity indices, in this section we discuss how to quantify the influence of the model choice on the uncertainty of the predicted response. For a set of given models $\boldsymbol{\mathcal{M}} = \mathcal{M}_1, \mathcal{M}_2, \ldots, \mathcal{M}_k$ the standard first order and total effect sensitivity indices $S_i^{\mathcal{M}_j}$ and $S_{T_i}^{\mathcal{M}_j}$ can be calculated for each model individually.

These indices are shown exemplary in Fig. 1 for three one-dimensional polynomials with increasing order

$$\begin{aligned}
&Y^{\mathcal{M}_1}(l) = X_1 + X_2 \cdot l,\\
&Y^{\mathcal{M}_2}(l) = X_1 + X_2 \cdot l + X_3 \cdot l^2,\\
&Y^{\mathcal{M}_3}(l) = X_1 + X_2 \cdot l + X_3 \cdot l^2 + X_4 \cdot l^3,\\
&l = 0.0, 1.0, 2.0, \ldots, 10,\\
&X_1 \sim \mathcal{N}(0.00, 0.50), \quad X_2 \sim \mathcal{N}(1.00, 0.10),\\
&X_3 \sim \mathcal{N}(0.02, 0.01), \quad X_4 \sim \mathcal{N}(0.001, 0.0025).
\end{aligned} \tag{5}$$

Since the models are purely additive their first order and total effect sensitivity indices coincide. Due to the independent input parameters the sensitivity indices can be calculated analytically.