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Sensitivity analysis of correlated outputs and its application to a dynamic model

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ABSTRACT

Risk assessment and decision making in ecology, hydrology and biology often employ dynamic models with multiple calibrations. The global sensitivity analysis of models is usually completed at each time step of a single output. However, due to the enormous volume of data and model complexity, a single index cannot give a full-scale analysis of such models. The purposes of this paper are: (1) to apply T-pooling for analysing multiple outputs at a lower computational cost; (2) to consider the influence of the correlations among the outputs and the output dimensions on sensitivity analysis; and (3) to propose a procedure that combines the Sobol' index for a single output and the generalised sensitivity method and T-pooling index for multiple outputs to analyse dynamic models comprehensively. The proposed procedure and index are applied to a Hydrologiska Byråns Vattenbalansavdelning (HBV) model with three calibrations to provide an uncertainty analysis across time periods ranging from a single time step to the entire time period.

1. Introduction

Computer simulation models are essential components in the research, design, development and decision making for science and engineering applications. With continuous advances in the physical understanding of the processes to be modelled and also computing capabilities, such models continue to evolve with increasing complexity and more user-defined factors (e.g., increased model parameters and boundary conditions). To obtain a better understanding of the role and importance of different model factors on the output model responses, the procedure known as "Sensitivity Analysis" (SA) can be very helpful for developing, evaluating and improving complex modelling studies (Ratto et al., 2012; Fonseca et al., 2014; Tang et al. 2015, 2018; Pianosi et al., 2016; Xia and Tang, 2017).

Traditional methods for SA, including the variance-based method (Homma and Saltelli, 1996; Sobol', 2001), elementary effect method (Campolongo et al. 2007, 2011), derivative-based method (Sobol' and Kucherenko, 2009, Sobol' and Kucherenko, 2010) and safety systems-based method (Tang et al. 2016, 2017), were designed for a scalar output. These methods can be applied to dynamic models, which give information on how the global sensitivity changes over time. They are effective in identifying which inputs affect the uncertainty of a given output at a given time step in the model. However, as indicated by Lamboni et al. (2011), these methods contain considerable redundancy when identifying strong correlations among multiple outputs from different time steps in a given model.

A simple and useful approach, the output decomposition method, was proposed by Campbell et al. (2006) for SA of models with multiple outputs. Lamboni et al. (2011) applied it to mathematical models of crop growth with dynamic outputs. The output decomposition method consists of first performing an orthogonal decomposition of the multivariate outputs, and then applying individual SA to only the most informative components. This method devotes more attention to a few components rather than the entire dynamic process. A new set of sensitivity indices, which is based on the decomposition of the covariance of the model outputs (Gamboa et al. (2013), is both equivalent to the Sobol' indices in the scalar case, and also more computationally efficient since it does not require spectral decomposition, in contrast to the output

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decomposition method (Lamboni et al., 2011). Details on the comparison and equivalence between the output and covariance decomposition approaches can be found in Garcia-Cabrejo and Valocchi (2014). Marrel et al. (2009) have mapped the Sobol' indices over the grid associated to the model outputs, and Rosolem et al. (2012) have presented the rank-based multiple-criteria implementation of the Sobol' variance-based SA approach.

Despite their advantages, these multivariate SA methods are based on the variances of the multivariate outputs. These methods can be used for analysing a single response model or a model with multiple uncorrelated outputs, but they are no longer appropriate for analysing multiple correlated responses. Developing a novel methodology to address this latter case is thus the motivation of the research presented here. There are three key situations where multiple correlated outputs are of interest: (1) a computational model that generates multiple measurements, calibrations or outputs that share similar underlying physics (Hills, 2006; van Werkhoven et al., 2009; Kollat et al., 2012); (2) the collection of model responses from the same experiment that is a function of spatial and/or temporal variables (Oberkampf and Barone, 2006; Dowding et al., 2008, Young and Ratto, 2011); and (3) the dynamic model combines disparate responses or calibrations at multiple time steps (Pianosi and Soncini-Sessa, 2009, Pianosi and Raso, 2012). In each of these cases, there is a strong correlation between any pair of outputs from the same experiment. Therefore, a sensitivity index that refers to the entire distribution of the multivariate outputs should be used if one wants to assess which input influences the decision-maker state of knowledge.

Cui et al. (2010) extended the moment-independent SA method for scalar outputs (Borgonovo, 2007) to the multivariate case, and defined a sensitivity index based on the joint probability density function (PDF) of the multivariate outputs. This method takes both the entire uncertainty and correlation of the multivariate output into account. However, it suffers severely from the “curse of dimensionality” due to the computational costs required for the high dimensional integration in the sensitivity index, as well as the difficulty in estimating the joint PDF of the high dimensional variables. The advantages of using the distance between cumulative distribution functions (CDFs) as a measure of the input importance in the case of a scalar output have been manifested in many papers (Baucells and Borgonovo, 2013; Borgonovo et al. 2013, 2015; Borgonovo et al., 2013, Pianosi and Wagener, 2015), but it has not been extended to the case of multivariate outputs. As pointed output in Liu and Homma (2009), the CDF-based method is easier to implement than the PDF-based method, and the computational efficiency of the CDF-based method can be improved as compared with the PDF-based method. The multivariate probability integral transformation (PIT) is recognised for containing valuable information about the correlation structure of the joint CDF of the outputs, with numerous applications in various fields, including a few examples mentioned here. A paper by Imlahi and Chakak (2007) examined the application of PIT to obtain the maximum likelihood estimation of dependence parameters. Genest et al. (2006) applied PIT to test the goodness of fit of copula function, while Ishida (2005) evaluated the application of PIT in estimating the conditional density forecast in the econometric mainstream. The PIT has also been employed to represent correlated random variables from multivariate outputs by Luyi et al. (2016).

Moreover, the present methods for multivariate outputs are more suitable to the dynamic models with a single calibration rather than the dynamic models with multiple calibrations. It is often difficult to interpret and simultaneously aggregate various data from different time steps and different calibrations, because they are influenced by the dimensions of the model outputs. A sensitivity index that refers to the entire distribution of the multivariate outputs in a dynamic process should thus be used to assess which input influences the decision-maker state of knowledge. The U-pooling metric is used to compare the marginal distributions of simulations and the physical measurements for model validation (Ferson et al., 2008). Physical observations collected at multiple validation sites can be incorporated into a single metric to assess the global predictive capability of a model by applying the U-pooling metric (You and Mahadevan, 2013). Li et al. (2014) extended the U-pooling metric and proposed the T-pooling metric for observations at validation settings of interest. The main advantage of the T-pooling metric is the ability to integrate the evidence from all the relevant data of multi-response quantities over an intended validation domain into a single measure to estimate the overall disagreement. However, this has not been extended to SA for the case of multiple outputs over the time domain. Li et al. (2014) indicated that the CDFs of the model outputs and time points can be transformed twice, first as a multivariate PIT and then as a univariate PIT, to yield a comprehensive and comparable distribution. Furthermore, each of these SA methods has their own merits and drawbacks, such that it is so inappropriate to analyse the dynamic model with multiple calibrations and a single method. We cannot consider some features, such as correlation, dimension or interaction effect, at the same time in the dynamic process. Therefore, a sensitivity procedure that contains different methods and corresponds to the different kinds of requirements should be performed to analyse such models over a range of time windows.

Based on this literature review, we believe that there is a lack of guidance to support global sensitivity analysis (GSA) users attempting to address a problem using a dynamic model with correlated outputs, while there is an opportunity for supplementing current approaches with reduced computational costs. Thus, the objectives of the present study are:

(1) A new importance measure is defined that is based on the T-pooling metric, which allows the pooling of information from multiple outputs at different time steps. The importance of the input over the entire time domain and outputs can be measured by determining the area difference between the joint unconditional CDFs and the joint conditional CDFs of the twice transformed PIT distributions.
(2) We implement our proposed method to address the challenges of considering uncertainty, correlations and dimensions by the twice transformed PIT distributions. Due to the univariate nature of the multivariate PIT, the proposed methods are evaluated through univariate integrations, regardless of the number of simulations, which reduces the computational cost compared to other methods.
(3) A new sensitivity procedure is introduced for a time-dependent model with multivariate outputs, which analyses the global sensitivity from the microcosm (a single time step and a single output) to the macrocosm (the entire time domain and multiple outputs).

The remainder of this paper is presented as follows. A brief introduction of the Hydrologiska Byråns Vattenbalansavdelning (HBV) model, model data and the multi-objective calibrations is provided in Section 2. In Section 3, a brief introduction of the covariance decomposition approach, the probability integral transformation theorem and SA based on PIT are provided, and the new sensitivity index based on T-pooling is defined. The proposed procedure for a time-dependent model with multiple outputs is presented at the end of Section 3. Three numerical examples are