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Calibration of computer models with multivariate output

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ABSTRACT

The problem of calibrating computer models that produce multivariate output is considered, with a particular emphasis on the situation where the model is computationally demanding. The proposed methodology builds on Gaussian process-based response-surface approximations to each of the components of the output of the computer model to produce an emulator of the multivariate output. This emulator is then combined in a statistical model involving field observations, which is then used to produce calibration strategies for the parameters of the computer model. The results of applying this methodology to a simulated example and to a real application are presented.

1. Introduction

Computer models are implementations of sophisticated mathematical models that aim at reproducing a particular real process. Before we can run these computer models, we have to specify a vector of inputs which typically includes calibration parameters. Scientists are thus often interested in combining data obtained in computer model runs and in physical experiments to determine estimates of these calibration parameters which make the output of the model "match" in some sense the real process. This is what is meant by calibration of a computer model.

When a physical experiment is conducted to obtain field data, it is sometimes the case that several (presumably correlated) measurements are taken. In the realm of the computer model, it is also not uncommon that the output contains in fact a wealth of information, some of which can even be considered irrelevant for the actual calibration problem at hand. Clearly, the evaluation of a model depends on how one intends to use it and, as part of the calibration process, one must specify which particular aspect(s) of the output are of main interest. In practice, the spirit underlying the specification of these aspects is often a mix of genuine practical interest and the need to keep the analysis feasible. This paper proposes methodology to address the following situation: one is simultaneously interested in several univariate aspects of the output, but the joint calibration of the computer model against these aspects is perceived as too difficult to tackle. In this situation, a simplistic strategy would consider separate calibration exercises, one per univariate component of the output. Besides being formally incorrect, the main drawback associated with this approach is that it potentially produces one calibration strategy for each of the components considered. This may result in an illusory perception of the quality of the computer model as a representation of reality, as there may be calibration strategies which accommodate the individual discrepancies very well, but not one that does so globally. Also, there may be too much variability – or several sensible calibration strategies – associated with calibrating each univariate output separately, which may render the analyses inconclusive. By combining

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all sources of information, one may be able to substantially reduce the uncertainty and pin down a particular calibration strategy. Section 2 illustrates these ideas with a motivating example.

Specifically, this paper makes contributions to two aspects of the statistical analysis of computer models producing multivariate output, namely, emulation and calibration. On the emulation aspect, we propose a method that is computationally much simpler and easier to implement than currently available techniques. It builds on the univariate emulators independently produced for each of the components, thus avoiding the use of multivariate Gaussian processes. Also, the emulator we propose is presented as a closed-form expression, and hence does not require a full-Bayesian estimation of unknown parameters. In spite of this simplicity, the results we have obtained through this method have been very similar to the ones we get using more sophisticated approaches; cf. Section 4.4.

On the calibration aspect, our contribution is to produce a method that incorporates the emulator we propose into a statistical model involving experimental observations that allows for the estimation of the uncertain parameters in the computer model. The novelty here includes the fact that the priors on the parameters of this statistical model are all non-informative (with the exception of the calibration parameters), and hence do not require any additional input from the user. Although the emulator we propose is valid in complete generality, the calibration methodology that we develop in this paper is restricted to the case where only one configuration of the vector of controllable inputs is exercised to obtain the field data. Possible extensions of this setup are discussed in Section 8.

1.1. Background

The approach to computer model calibration that we espouse is Bayesian and has roots in Craig et al. (1996), Kennedy and O'Hagan (2001), Kennedy et al. (2002) and Higdon et al. (2004), and most directly in Bayarri et al. (2007b). It hinges on modeling the relationship between reality and computer model output in a Bayesian fashion introducing the notion of bias, effectively combining model and field data to produce estimates of the calibration parameters. A key ingredient of the methodology is the use of Gaussian processes as priors for unknown functions. This technique dates back at least to O'Hagan (1978) although its use in the realm of the computer model world is more recent: Sacks et al. (1989) and Currin et al. (1991). The end result is a Gaussian process response-surface approximation to the output of the computer model, and its associated measure of uncertainty, which is sometimes called the 'emulator'. This is a key component of the analysis, as frequently the models are computationally very demanding and this precludes their direct evaluation within Markov chain Monte Carlo algorithms. The construction of this emulator and its subsequent integration in the calibration process clearly depends on the characteristics of the output. To give a few examples, Bayarri et al. (2007b) and Higdon et al. (2004) deal with scalar output, Bayarri et al. (2009) with functional output that is very smooth, Bayarri et al. (2007a) with very irregular functional output. Higdon et al. (2008) utilizes a related approach to deal with high-dimensional output like images. The issue of emulating a computer model that exhibits nonstationary behavior is dealt with by means of partitioning in Gramacy and Lee (2008a,b). Reichert et al. (2011) have recently proposed an emulator for dynamic models with application in hydrology.

Methodological developments to directly model multivariate aspects of a computer model's output have been addressed in several papers, including Habib et al. (2007), Rougier (2008), McFarland et al. (2008), Higdon et al. (2008), Higdon et al. (2010), Conti and O'Hagan (2010), Fricker et al. (2010), Bhat et al. (2010) and Wilkinson (2010). In Section 4 we describe some of these approaches in the common framework of the linear model of coregionalization (Gelfand et al., 2004).

1.2. Overview

The remainder of this paper is organized as follows: in Section 2 we use a simple example to illustrate the drawbacks of the simplistic strategy of independent calibration analyses, one per dimension of the multivariate output. Section 3 precisely describes the problem we want to address and sets up the necessary notation. In Section 4 we describe previous contributions in the literature to produce a multivariate emulator, highlighting the fact that they can all be seen as special cases of the linear model of coregionalization. We also describe the approach that we propose in this paper. The problem of embedding this emulator in a calibration setting is addressed in Section 5. Section 6 describes how we propose to go about implementing our calibration methodology in practice, and Section 7 presents the results of applying it to a real application.

2. A motivating example

In order to highlight the drawbacks that may result from performing separate analyses to handle responses that are multivariate in nature, we introduce the following example. Additionally, we suggest how these problems can be addressed under the combined approach we propose. We skip technical details and formal definitions, since these will be accurately presented in the remainder of the paper in more general scenarios.

Suppose that the real process, depending on a scalar u, is the bivariate function $\boldsymbol{y}^R(u) = (y_1^R(u), y_2^R(u))'$, $u \in (0, 0.5)$, where $y_1^R(u) = \exp(-1.4u - 0.05/u)\ \cos(7\pi u/2)$ and

$$y_2^R(u) = 0.1\ \exp(-1.4u - 0.05/u)\left[-1.4 + \frac{0.05}{u^2}\cos(7\pi u/2) - \frac{7\pi}{2}\sin(7\pi u/2)\right].$$