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METAMODEL VARIABILITY ANALYSIS COMBINING BOOTSTRAPPING AND VALIDATION TECHNIQUES

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ABSTRACT

Research on metamodel-based optimization has received considerably increasing interest in recent years, and has found successful applications in solving computationally expensive problems. The joint use of computer simulation experiments and metamodels introduces a source of uncertainty that we refer to as metamodel variability. To analyze and quantify this variability, we apply bootstrapping to residuals derived as prediction errors computed from cross-validation. The proposed method can be used with different types of metamodels, especially when limited knowledge on parameters' distribution is available or when a limited computational budget is allowed. Our preliminary experiments based on the robust version of the EOQ model show encouraging results.

1 INTRODUCTION

Nowadays, the use of computer simulation techniques is relatively well established in many practical contexts, ranging from industrial to public-sector applications. For many years, most of research has been focusing on deterministic simulation models, thus neglecting uncertain input factors. More recently, many researchers started to investigate robustness issues arising in simulation and optimization (Bates et al. 2006, Janusevskis and Riche 2012, Marrel et al. 2012). Metamodels may be profitably used to reduce the computational cost of running the simulation model (Barton and Meckesheimer 2006); when uncertainty arises, advantages coming from metamodels become more evident. However, in such a case, randomness affects not only the behaviour of the simulated system but also the whole metamodel construction process. We refer to the resulting phenomenon as *metamodel variability*. This depends on multiple factors, such as the type of simulation model, the design of experiments, the metamodeling technique; different choices might determine alternative metamodels. Furthermore, metamodels are commonly used for further analyses; e.g., for optimization purposes. So, ignoring possible variations in the metamodel may lead to suboptimal or even wrong solutions, being far from the response of the original simulation model. To guarantee reliable results, validating the metamodel may not suffice; this issue, often underestimated, is the focus of the present research. This work mainly refers to deterministic simulation models affected by epistemic uncertainty; i.e., uncertain inputs take values from a prior distribution with given parameters. Nevertheless, it applies to purely stochastic simulation models (i.e., with only aleatory input variables) as well, and can be easily extended to simulation models where both epistemic and aleatory uncertainty emerge.

2 INVESTIGATING METAMODEL VARIABILITY

The use of bootstrap methods in metamodeling is subject to active international research (Cheng 2006, Barton et al. 2010). We use them as a fast way to reproduce the metamodel construction process, accounting for possible sources of variability. The idea behind our approach is to use bootstrapping to obtain several realizations of the metamodel, exploiting the information provided by the metamodel's validation process. More specifically, rather than producing a single point estimate of the unknown response, which might be inaccurate because of metamodel variability, we derive a range of possible responses reflecting the degree of metamodel uncertainty (e.g., through confidence intervals); see Dellino et al. (2012). Our approach aims to provide results close to what one would get in the *ideal* scenario derived from an infinite number of simulations—assuming the computer simulation to be a *perfect* representation of the real system. When applying bootstrapping to metamodeling, we have to decide *how* to resample and *what* to resample. To answer the first question, we may choose between *distribution-free* and *parametric bootstrapping*. As for the second question, three ways of resampling are possible (Cheng 2006); namely, parameter sampling, case sampling and residual sampling. Residual sampling is commonly applied to linear regression models; however, metamodeling techniques providing exact interpolation (such as Kriging) have zero residuals for all the input points used to fit the metamodel; so residual sampling as described before would not be suitable. Inspired by Cheng (2006) and Kleijnen et al. (1998), we propose to bootstrap cross-validation errors, which we consider as some kind of *residuals* of the corresponding *validated* metamodel. More specifically, we fit a metamodel to a set of n design points. During the validation process, we compute the relative error err_i for each design point $\mathbf{x}_i$ $(i = 1,\ldots,n)$. We apply distribution-free bootstrapping to these data, which gives err_i^*. Then, we compute the bootstrapped simulation output as $Y_{s,i}^* = Y_{s,i}\,(1+err_i^*)$. We now fit a metamodel to these bootstrapped I/O data $(\mathbf{x}_i, Y_{s,i}^*)$ $(i = 1,\ldots,n)$, and repeat this sampling B times. So, we analyse the prediction data associated to this bundle of B bootstrapped metamodels, to quantify metamodel variability. Preliminary experiments have been conducted on the EOQ model, based on the assumptions discussed by Dellino et al. (2009). We addressed metamodel variability applying residual sampling to both regression and Kriging metamodels, obtaining promising results: they reveal that our bootstrapping approach based on residual sampling provides good estimation of the metamodel variability. Moreover, we observe that, in general, metamodel variability is not constant over the experimental area of interest; such information can be profitably used to guide a sequential design procedure to improve the overall quality of the metamodel. A number of issues deserve further investigation: the integration of our tool in a simulation-optimization framework; the application of our approach to dependent and heteroscedastic data; a wider experimental campaign on models affected by both aleatory and epistemic uncertainty.

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