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An estimation algorithm for fast kriging surrogates of computer models with unstructured multiple outputs

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Abstract

Computationally intensive computer models are used in many areas of engineering. In order to speed up the investigations, fast statistical surrogates have been developed in the literature. The surrogates addressed in this paper incorporate a general and unstructured covariance, best suited for modeling nonlinear and nonstationary multiple outputs. We propose an efficient algorithm to cope with the estimation of a large number of parameters. Then multivariate kriging is used to construct the fast surrogate. This algorithm can be embedded in both maximum likelihood and cross-validation estimation methods. We compare the proposed method with a current method based on principal components. The methodology is illustrated with a mechanical engineering application involving a vehicle suspension system.

Keywords: Computer experiments; Emulators; Multidimensional data; Prediction

1. Introduction

Computational modeling and simulation have become increasingly important in engineering. Physical laws characterizing engineering systems are translated into mathematical relationships, which are then implemented in computer programs, also known as computer (or simulation) models. A computer model can be schematically represented as

$$input \rightarrow \boxed{\text{computer model}} \rightarrow output.$$

Varying the inputs within plausible ranges and assessing the resulting changes in the outputs is called computer experimentation and gives engineers a first-hand insight into *what if* scenarios. For example, if a vehicle mass (*input*) will be increased by 10%, how will the force (*output*) exerted on its suspension system change? While the computer models are useful exploratory tools, one of the major drawbacks may be their computational inefficiency. Only a few computer model runs can be executed (at a small number of inputs), therefore limiting the model's exploratory capability.

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In order to speed-up the engineering investigations, fast statistical approximations (also known as surrogates, metamodels or emulators) of computationally intensive computer models have been developed over the past twenty five years, both for scalar output (e.g., [1–5]) and multiple outputs, such as time-dependent curves (e.g. [6–10] among others). These statistical surrogates are output predictions from kriging-based regression models with correlated errors at new inputs, trained on output data at a set of inputs. When dealing with multiple outputs, their ideal covariance matrix should be unstructured, as general as possible, in order to capture their possibly nonlinear and non-stationary behavior. Here, unstructured covariance matrix means that all its elements are estimable parameters, thus not amenable to simple parametric modeling. The number of parameters in an unstructured covariance matrix, however, quickly becomes large even for a moderate number of multiple outputs. In this paper we propose an iterative algorithm to estimate these parameters.

The motivating engineering application for our algorithm aims at improving the design of vehicle suspension systems. It involves computer model outputs as the time history of forces acting on the shock towers of a suspension system. These forces will have local sharp maxima at the times the vehicle runs over potholes. The focus in this engineering application is on several local maxima of the time-dependent output force since a vehicle may run over multiple potholes on a road. These maxima will be used as multiple outputs in our example.

In Section 2 we outline the methodology, including the development of the statistical model, estimation and prediction. We discuss the engineering application in Section 3 and conclude with some remarks in Section 4.

2. Fast surrogates for multiple outputs

2.1. Statistical model

Denote by $\alpha = (\alpha_1, \ldots, \alpha_r)$ a generic input vector, and by $\mathbf{E}(\alpha) = [E_1(\alpha), E_2(\alpha), \ldots, E_K(\alpha)]'$ the output vector of length K. Here $\mathbf{E}(\alpha)$ represents the multiple output at input α. We denote it by $\mathbf{E}$ because our application deals with vectors of extremes, but the method presented in this paper is very general and applicable to any problem involving vectorial outputs. The goal is to create a fast surrogate (or approximation) for $\mathbf{E}(\alpha)$ at any α in an input space. One of the challenges here is that $\mathbf{E}(\alpha)$ is a vector, so we need surrogates for vectors with correlated components, instead of surrogates for scalars.

Let $\alpha^{(1)}, \ldots, \alpha^{(D)}$ be the input vectors where the computer model is run and the output vectors $\mathbf{E}(\alpha^{(1)}), \ldots, \mathbf{E}(\alpha^{(D)})$ are obtained. Here we assume that the inputs are selected in an input space according to some space-filling design, such as the maximin Latin Hypercube Design. Johnson et al. [11] and Morris et al. (1993), among others, discuss the topic of design for computer experiments. To facilitate an easier formulation of the surrogate, we will stack these output vectors on top of each other and denote by $\mathbf{E}$ the new vector of length KD. The Kronecker product helps expressing a statistical model for data defined in two (or several) dimensions. The proposed statistical model in this paper is

$$\mathbf{E} = (\mathbf{U} \otimes \mathbf{1}_K)\eta + (\mathbf{1}_D \otimes \mathbf{X})\nu + \epsilon \tag{1}$$

where ϵ is a vector of errors with zero mean vector and covariance matrix $\mathbf{\Sigma}$. Each of the terms in model (1) are explained next.

The matrix $\mathbf{U}$ has rows given by input coordinates $\mathbf{U}_{i,.} = [\alpha_1^{(i)}, \ldots, \alpha_r^{(i)}]$, $i = 1, \ldots, D$. This is a parsimonious choice of $\mathbf{U}$, but higher order polynomials in the columns of $\mathbf{U}$ can also be incorporated at the expense of increasing the overall number of statistical parameters in the model. However, since the number of covariance statistical parameters in the proposed model will be large, higher order polynomials in the mean should be included only if needed. Note that $\mathbf{U} \otimes \mathbf{1}_K$ is obtained by replicating K times each row of $\mathbf{U}$. The second term of the mean suggests that these output vectors have similar shapes (e.g. have a common trend, as in Fig. 3 left panel), modeled by $\mathbf{X}\nu$. Note that $\mathbf{1}_D \otimes \mathbf{X}$ is obtained by replicating D times the matrix $\mathbf{X}$. In order to obtain a more general fit, we allow the mean $\mathbf{X}\nu$ to be unstructured, i.e. $\mathbf{X} = \mathbf{I}_K$. In a more compact form, the general model (1) can be written as

$$\mathbf{E} = \mathbf{M}\beta + \epsilon, \tag{2}$$

where the two regression matrices above have been combined into a larger matrix

$$\mathbf{M} = \begin{bmatrix} \mathbf{U} \otimes \mathbf{1}_K & \mathbf{1}_D \otimes \mathbf{X} \end{bmatrix} \tag{3}$$

and $\beta = (\eta, \nu)$.