Mechanical Systems and Signal Processing 34 (2013) 57–75

Contents lists available at SciVerse ScienceDirect

Mechanical Systems and Signal Processing

journal homepage: www.elsevier.com/locate/ymssp

Bayesian sensitivity analysis of bifurcating nonlinear models

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ARTICLE INFO

Article history:
Received 30 June 2011
Received in revised form
21 May 2012
Accepted 25 May 2012
Available online 23 June 2012

Keywords:
Sensitivity analysis
Gaussian process
CART
Metamodel
Bifurcation

ABSTRACT

Sensitivity analysis allows one to investigate how changes in input parameters to a system affect the output. When computational expense is a concern, metamodels such as Gaussian processes can offer considerable computational savings over Monte Carlo methods, albeit at the expense of introducing a data modelling problem. In particular, Gaussian processes assume a smooth, non-bifurcating response surface. This work highlights a recent extension to Gaussian processes which uses a decision tree to partition the input space into homogeneous regions, and then fits separate Gaussian processes to each region. In this way, bifurcations can be modelled at region boundaries and different regions can have different covariance properties. To test this method, both the treed and standard methods were applied to the bifurcating response of a Duffing oscillator and a bifurcating FE model of a heart valve. It was found that the treed Gaussian process provides a practical way of performing uncertainty and sensitivity analysis on large, potentially-bifurcating models, which cannot be dealt with by using a single GP, although an open problem remains how to manage bifurcation boundaries that are not parallel to coordinate axes.

1. Introduction

Uncertainty analysis (UA) is a field of increasing interest in computer modelling, both within and beyond the realm of engineering. Advances in the theory of numerical simulation (such as the continuing advances in finite element (FE) analysis and computational fluid dynamics), coupled with a steady increase in available processing power, have enabled the use of increasingly sophisticated simulations to model complicated real-world processes. However, the increased complexity of these models tends to require a greater amount of information to be specified at the input. Examples of input variables within the context of engineering models could include material properties, loads, dimensions and temperatures. Any of these inputs can be subject to some uncertainty; for example, the operating temperature of a structure could be within a wide range, or the material properties could vary naturally (a good example of this is in modelling biomaterials—see [1]). The question, central to UA, then arises: what is the uncertainty in the model output, given the input uncertainty?

A furtherance of UA is Sensitivity Analysis (SA), which evaluates the contribution of inputs (and sets of inputs) to the output uncertainty, and the effects of varying parameters within specified ranges. The motivations of SA are various (Saltelli provides an extensive list [2]), including the identification of particularly influential parameters to see whether their uncertainty can be reduced somehow (thereby reducing output uncertainty), and gaining deeper understanding of a

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http://dx.doi.org/10.1016/j.ymssp.2012.05.010

model's response to its inputs. In general, SA is seen as a useful tool to increase the robustness and overall quality of computer simulations, and often goes hand in hand with UA.

Introducing some notation, let the model to be investigated be denoted as $f(\boldsymbol{x})$, where $\boldsymbol{x}$ is a d-dimensional vector of uncertain inputs (there may also be a number of model inputs that are regarded as known, which will not be considered here). The model may indeed be a very complex system of nonlinear equations, but from a "black box" point of view it can simply be regarded as a function of inputs. The model could yield any number of outputs, but attention here will be restricted to a scalar output $y=f(\boldsymbol{x})$.

In order to perform an uncertainty analysis, it is necessary to somehow quantify the uncertainty on the inputs. Although there are many ways of doing this – see the recent book by Klir for a summary [3] – this article will consider the probabilistic framework. It is therefore assumed from here on that the inputs are random variables $\{X_i\}_{i=1}^{d}$, and that a joint probability density function (pdf) $p(\boldsymbol{x})$ can be defined over them. This lightly skips over the often-troublesome problem of eliciting the pdf, though an extensive discussion on this matter can be found in [4].

From the probabilistic perspective, the aim of UA is to estimate the pdf of the output random variable Y, given the $p(\boldsymbol{x})$ assigned to the inputs. In practice, this is often simplified to the estimation of the expected value $E(Y)$, and the variance $\mathrm{var}(Y)$. SA, on the other hand, requires a quantification of the sensitivity of y to changes in the inputs. Saltelli discusses a great number of ways to do this [5]. Two simple types of SA are simply ranking variables in order of importance (screening); and taking partial derivatives of y with respect to individual inputs (local SA). Screening is usually done as a precursor to a more sophisticated SA, to filter out unimportant variables. Local SA is also useful, but only considers small perturbations about the nominal values of input parameters. In the case of complex nonlinear models with wide uncertainties, this approach is unsatisfactory.

The most informative approach is known as *global SA*, in which the variation of y is examined over the whole of the input space. By far the most widely used method of doing this, proposed by Sobol' [6], involves decomposing $\mathrm{var}(Y)$ into portions attributable to inputs and subsets of inputs. Specifically, a variance decomposition is used (under an assumption of independence between inputs) such that

$$\mathrm{var}(Y)=\sum_i V_i+\sum_i\sum_{j>i}V_{ij}+\cdots+V_{12\ldots d} \tag{1}$$

$$V_i=\mathrm{var}(E(Y|X_i))$$

$$V_{ij}=\mathrm{var}\{E(Y|X_i,X_j)\}-\mathrm{var}\{E(Y|X_i)\}-\mathrm{var}\{E(Y|X_j)\}$$

$$\vdots$$

The quantity V_i represents the amount that $\mathrm{var}(Y)$ would be reduced, if X_i were to become known, therefore giving a global measure of importance of that variable. The higher order terms V_{ij} represent variance due to interactions between variables, additional to the variance caused by the inputs acting alone. There are 2^d-1 terms in this decomposition, with interactions up to the final d-way interaction between all variables (the last term in Eq. (1)). Typically these quantities are standardised by dividing by $\mathrm{var}(Y)$, giving, e.g. $S_i=V_i/\mathrm{var}(Y)$, where S_i is known as the main effect index (MEI), and the S_{ij}, S_{ijk}, etc. follow from similar definitions. Note that this implies that

$$\sum_i S_i+\sum_i\sum_{j>i}S_{ij}+\cdots+S_{12\ldots k}=1 \tag{2}$$

Since there may be a great number of terms in Eq. (2), Homma and Saltelli proposed a further quantity S_{Ti}, known as the total sensitivity index (TSI) [7], which is defined as

$$S_{Ti}=\frac{E\{\mathrm{var}(Y|X_{-i})\}}{\mathrm{var}(Y)}=1-\frac{\mathrm{var}\{E(Y|X_{-i})\}}{\mathrm{var}(Y)} \tag{3}$$

This measure is therefore the sum of the variance caused by X_i and all its interactions with other variables. Finally, another useful (but qualitative) indicator of sensitivity is to plot the *main effect* $E(Y|X_i)$against X_i, which illustrates how the output varies with respect to variations in a single variable.

All the quantities addressed here can be expressed as integrals, e.g.

$$E(Y|X_i)=\int_{\mathcal{X}_{-i}} f(\boldsymbol{x})p(\boldsymbol{x}_{-i}|x_i)d\boldsymbol{x}_{-i} \tag{4}$$

where X_{-i} denotes the sample space (support) of the variables X_{-i}, where $-i$ denotes all variables except i. If the function $f(\boldsymbol{x})$ were tractable, this could be done analytically, however in the majority of practical cases it is not (consider a large FE model, for instance). In such cases, the usual approach is to use the Monte Carlo (MC) method [8], using specific estimators built for the purpose [9,10]. To achieve an acceptable level of accuracy, this requires sampling the model a large number N_{MC} of times across the input space (at least several hundred, often thousands) for every quantity to be calculated—i.e. $d\times N_{\mathrm{MC}}$ samples for the MEIs, plus the same number again for the TSIs. The key problem with this approach is that many