



Full-field sensitivity analysis through dimension reduction and probabilistic surrogate models

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ABSTRACT

Computational mechanics models often are compromised by uncertainty in their governing parameters, especially when the operating environment is incompletely known. Computational sensitivity analysis of a spatially distributed process to its governing parameters therefore is an essential, but often costly, step in uncertainty quantification. A sensitivity analysis method is described which features probabilistic surrogate models developed through equitable sampling of the parameter space, proper orthogonal decomposition (POD) for compact representations of the process' variability from an ensemble of realizations, and cluster-weighted models of the joint probability density function of each POD coefficient and the governing parameters. Full-field sensitivities, i.e. sensitivities at every point in the computational grid, are computed by analytically differentiating the conditional expected value function of each POD coefficient and projecting the sensitivities onto the POD basis. Statistics of the full-field sensitivities are estimated by sampling the surrogate model throughout the parameter space. Major benefits of this method are: (1) the sensitivities are computed analytically and efficiently from regularized surrogate models, and (2) the conditional variances of the surrogate models may be used to estimate the statistical uncertainty in the sensitivities, which provides a basis for pursuing more data to improve the model. Synthetic examples and a physical example involving near-ground sound propagation through a refracting atmosphere are presented to illustrate the properties of the surrogate models and how full-field sensitivities and their uncertainties are computed.

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1. Introduction

1.1. Defining the context

Computational models of complex physical systems are unavoidably compromised by assumptions, uncertainties, and errors. A natural consequence is that the analyst's work may lack credibility, both because the problem at hand is complicated and the model building process lacks transparency. The concepts and method presented here support on-going computational modeling efforts to define models of systems and their environments in ways that promote increased confidence in predictions. We pursue this by developing tools that can provide (i) an informed basis for using measurements to support predictions, (ii) insight into the model building process, and (iii) insight into how limited knowledge of model parameters may compromise predictions. This paper describes a sampling-based method for developing probabilistic surrogate models in support of global, full-field sensitivity analysis,

a concept which is defined below. The sensitivity calculations are fast and insensitive to the number of parameters because the sensitivities are computed by analytically differentiating the conditional expected value of the surrogate model rather than fitting a local response surface to samples of the surrogate model. Through the conditional variance of the surrogate model, the method also permits estimating the statistical uncertainty induced in the sensitivities by fitting the surrogate model to a given set of samples.

Constructing and making the best use of parametric models for uncertainty quantification (UQ) requires knowledge of how the parameters may vary throughout the system's lifetime and how these variations can alter the system's state. Sensitivity analysis (SA) has been developed by many researchers and applications specialists to fulfill these needs. To continue enhancing the practicality and benefits of SA, we study what we call global, full-field sensitivity analysis, which we define in the following section. Our goal is to provide a framework that enables the use of SA to support UQ of realistic computational mechanics models. We see this as an essential step toward validating these models and enhancing their utility in decision making. The reader should note before proceeding that we do not consider non-probabilistic or generalized probabilistic methods, which commonly involve the

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Nomenclature

$a_q^{(n)}$	q th generalized Fourier coefficient of n th snapshot.
D_{ζ}	M -dimensional hypercube in the normalized parameter space.
d_{ζ_m}	Range of parameter ζ_m .
$f(\cdot)$	Probability density or mass function.
M	Number of system parameters.
N	Number of Latin hypercube sample vectors.
N_c	Number of parameter clusters in cluster-weighted model.
n_c	Cluster number.
N_g	Number of grid points in a snapshot.
N_r	Number of retained proper orthogonal decomposition modes.
$p(\cdot)$	Response random field.
S	Column-oriented array of snapshots.
s	Snapshot.
S_m^q	Sensitivity of POD coefficient $a^{(q)}$ to normalized parameter ζ_m .
t	Time.
V	Array of eigenvectors of $S^T S$.
x	Position vector.
m	Parameter number.
β_{n_c}	Linear regression parameters in cluster n_c .
$\Delta a^{(q)}$	Uncertainty in forecast of POD coefficient $a^{(q)}$.
Λ	Array of eigenvalues of $S^T S$.
$\langle g \rangle_{n_c}$	Expected value of function g given cluster n_c .
μ_a	Expected value function of POD coefficient a in cluster n_c .
$\mu_{n_c, m}$	Expected value of parameter m in cluster n_c .
Ω	Sample space.
ω	Element in the sample space, i.e. an event.
Φ	Array of proper orthogonal decomposition modes.
σ_{a, n_c}	Standard deviation of POD coefficient a in cluster n_c .
$\sigma_{n_c, m}$	Standard deviation of parameter m in cluster n_c .
$\zeta(\omega)$	Random vector of system parameters.

introduction of fuzzy or non-additive measures; see the handbook edited by Nikolaidis, et al. [1] for authoritative introductions to the various methods and the supporting literature. We also do not pursue the even broader problem of assessing model validity.

In the authors' current field of study, predictions of near-ground sound propagation are compromised by statistical uncertainty and model errors in the atmosphere and terrain characterization. High quality physical and numerical representations are available, but imprecise knowledge of the heterogeneous propagation environment impedes attempts to achieve spatial and temporal accuracy in sound field predictions [2]. Embleton [3] summarizes many of these environmental factors, which include (i) the topography and acoustic impedance of the ground or lower boundary of the propagation domain, (ii) the interaction of turbulent and radiative exchanges with this surface, which alters the velocity and thermal gradients in the atmospheric surface layer (ASL), and (iii) spatio-temporal variability in the atmosphere. After describing the components and products of our SA method, we demonstrate it by studying the sensitivity of a near-ground sound propagation model throughout both the relevant parameter space and the physical domain. However, we emphasize that the method is independent of this application.

1.2. Local, global, and full-field sensitivity analyses

Sensitivity analysis of a computational model is restricted here to the organized assessment of changes in a model's output

due to changes in its parameters. UQ of any complex, multiple parameter model ought to begin with SA to reveal the parameters that can induce the most imprecision and randomness in the response. Doing so helps to determine the relative accuracies required in measurements and probabilistic parameter models. It also provides information for planning measurement programs to support more extensive modeling efforts.

The most direct form of SA is to compute through analysis or finite differences how variations in the neighborhood of baseline parameter values influence an output of interest; this is *local SA* [4]. A parallel, but distinct, concern, especially when SA is used to support UQ, is how to estimate efficiently the range of sensitivities throughout the feasible portion of a multidimensional parameter space; this is *global SA* [4]. The distinction is important when a model exhibits substantial variations in its parameter sensitivities, i.e. nonlinear sensitivities, as various neighborhoods in the parameter space are interrogated [4,5].

The most direct application of SA for a spatially continuous system is to study the response at a limited set of points in the spatial domain. Another common use of SA occurs when the output of interest is a subset or functional of fundamental response variables, e.g. the integrated aerodynamic forces on a wing. In these cases, adjoint SA is a powerful method that has been demonstrated successfully in many applications [6,7]. SA methods appear to have been less widely studied for directly examining the influence of model parameters and initial conditions on the response field throughout the spatial domain. We refer to this as *full-field sensitivity analysis* (FFSA). In the SA method described herein, we compute sensitivities throughout both the parameter space and the spatial grid in which the response field is simulated; hence, we call this *global, full-field sensitivity analysis*, or global FFSA.

2. Full-field surrogate models for sensitivity analysis

2.1. Latin hypercube sampling

The response process is viewed as a random field, $p(x; \zeta(\omega))$, where $x \in \mathbb{R}^3$ is the position vector, $\omega \in \Omega$ is an element of the sample space, and $\zeta(\omega)$ is an M -dimensional random vector of system parameters. Latin hypercube sampling (LHS) [8–10] is used to choose N random realizations of the normalized parameter vector, ζ , distributed throughout the Cartesian product space $\times_{m=1}^M [-0.5, 0.5] \subset \mathbb{R}^M$, the goal being to ensure every portion of each parameter's range is sampled. To simplify the sampling process, the parameters are assumed to be independent. This does not compromise the conclusions of our study because the goal is to compute sensitivity to each parameter; assessing the importance of each sensitivity based on the actual variability of each parameter in a specific application is a related but separate concern.

2.2. Proper orthogonal decomposition of the response field

For the sake of generality, we can write the response as $p(t, x; \zeta(\omega))$, where time is now allowed to be an independent variable; i.e. for a given ω , $p(t, x)$ is a single realization that varies over time and space. Proper orthogonal decomposition (POD) is used herein to compute a mean-square optimal representation of the ensemble of response fields produced by LHS. POD shares its theoretical foundation with a variety of methods from several disciplines, including empirical orthogonal functions and principal component analysis. The underlying approximation theory is embodied by the finite-dimensional Karhunen–Loève decomposition, but these connections will not be discussed much here; consult Holmes, et al. [11], Kirby [12], and Mallat [13] for more background.

POD is not an inherently probabilistic technique. Often it is applied in deterministic applications, e.g. Hall, et al. [14] and Pettit and Beran [15], but its practical implementation requires the computation of many *snapshots* of the process. Snapshots

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