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Higher-order probabilistic sensitivity calculations using the multicomplex score function method

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ABSTRACT

The score function method used to compute first order probabilistic sensitivities is extended in this work to arbitrary-order derivatives included mixed partial derivatives through the use of multicomplex mathematics. Multicomplex mathematics provides an effective and convenient numerical means to compute the high-order kernel functions with respect to natural parameters or moments (mean and standard deviation) obviating the need to analytically determine the kernel functions. Using these numerical kernel functions, high-order derivatives of the response moments or the probability-of-failure with respect to the parameters of the input distributions can be obtained. Numerical results indicate that the high-order probabilistic sensitivities converge with respect to the number of samples at the same rate as standard Monte Carlo estimates. Implementation of multicomplex mathematics is facilitated through the use of the Cauchy–Riemann matrices; therefore, the extension of common engineering probability distributions to matrix form is presented.

1. Introduction

The score function (SF) method is an effective method for computing the sensitivity of a probability estimate with respect to the parameters of the input random variables. That is, one can obtain the partial derivative of an expected value estimate with respect to the parameters of the distribution, e.g., mean, standard deviation, shape, or scale, of the input random variables.

The SF method has some attractive features for sensitivity analysis as outlined below.

1.1. Partial derivative based

Since SF provides partial derivatives, this information is useful for design modifications. The partial derivatives are computed with respect to the natural parameters or mean and standard deviation of the random variable. Hence, one can project the change in a response with respect to a change in the mean or standard deviation separately. These partial derivatives are global in the sense that the results depend upon the full variation of the random variable. That is, they are local to the random variable parameters but not any particular random variable value. This is analogous to global sensitivity analysis [23] whose results depend up the parameters of the distribution but not on any particular value of the random variable.

1.2. Indifferent to the limit state form

SF is insensitive to the form of the limit state. That is, there is no requirement that the limit state be smooth, differentiable, continuous, etc. Sensitivities for system reliability or component reliability problems can be obtained in an analogous manner.

1.3. Inexpensive to compute

A significant attraction of SF is that the partial derivatives can be computed for negligle computational cost. The calculation of the partial derivatives is formulated as an expected value with respect to the same joint density function as the original problem. Hence SF uses the same random variable realizations and functional responses that were used during original analysis, e.g., to compute the probability-of-failure or response moments.

1.4. Post-processing operation

As outlined in the previous paragraph, since the existing samples and functional responses are already available, SF merely processes the values within auxilary equations that are simple to compute. Hence it is entirely a post-processing operation. This is beneficial in that SF results can be obtained after the original analysis if the samples and responses are available.

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Nomenclature

h	perturbation size
f	scalar function
N	number of samples
$\mathbf{x}$	vector of random variables
z	response function
P_f	probability-of-failure
$[P_f]$	multicomplex probability-of-failure
μ_Z	response mean
$[\mu_Z]$	multicomplex response mean
V_Z	response variance
$[V_Z]$	multicomplex response variance
σ_Z	response standard deviation
$[\sigma_Z]$	multicomplex response standard deviation
$f_X(x)$	probability density function
$[f_X(x)]$	multicomplex probability density function
σ_{RS}	residual strength
σ_{EVD}	maximum applied stress
a_0	initial crack size
K_C	fracture toughness
Y	geometry correction factor
K_I	mode I stress intensity factor
sqrt$M$	matrix square root
log$M$	matrix logarithm
exp$M$	matrix exponential
ΓM	matrix gamma
ψM	matrix digamma

1.5. Variance estimates are available

The partial derivatives, if computed using random sampling, are themselves random variables. However, high quality variance estimates exist and can be used to construct confidence bounds [12].

The development of the SF method has progressed steadily over the past few decades. Much of the foundation of the Score Function method has been conducted by Rubinstein and published in a series of papers. The fundamental methodology is described in [19,20,22] with applications to discrete event static and dynamic systems. Derivatives up to second order are discussed. Rubinstein and Shapiro [21] discuss the basic formulation in the context of discrete event systems and demonstrate the use of the Score Function method in stochastic optimization. Wu [28] applied SF to system reliability analysis and used importance sampling for the probability calculations. Kleijnen and Rubinstein [7] discuss how SF can be combined with experimental design to reduce the factors to be considered. Rubinstein discusses the optimization of computer models with rare events (1997).

Sues and Cesare [25] developed the sensitivity of the response mean and standard deviation with respect to the input probability density function (PDF) parameters. Wu and Mohanty [29] proposed using the methodology as a screening method for problems with a large number of random variables. Millwater and Osborn [12] applied SF to the probabilistic fatigue analysis of a gas turbine disk and developed variance estimates such that confidence bounds can be computed for each probabilistic sensitivity. Millwater demonstrated that the kernel functions must satisfy certain properties regardless of distribution type. These properties were then used to develop distribution-free analytical expressions of the partial derivatives of the response moments (mean and standard deviation) with respect to the PDF parameters for linear and quadratic response functions [11]. Rahman [18] provides an application of dimensional reduction and the SF method for calculating stochastic sensitivities. Millwater et al. [14] extended the kernel functions to the multivariate normal distribution, including derivatives with respect to the correlation coefficient. Millwater and Feng [15] extended the method to the case of derivatives with respect to the bounds of truncated distributions by including a flux term of the PDF across the boundary of the truncated distribution. Lee et al. [9] use copulas with the SF method to consider correlation between random variables. Millwater et al. [13] used the SF method to develop a localized sensitivity method that can identify the important region of a probability distribution. Garza and Millwater [4] applied concepts of the SF to compute the sensitivity of the probability-of-failure with respect to the parameters of a probability-of-detection curve. Wang et al. [27] developed a methodology using the SF method to compute the derivatives (i.e., first and second-order, including mixed) of the first-order variance contribution of a response with respect to parameters of the random variables.

The extension of SF to high order sensitivities is straightforward in concept but has not been extended to high-order sensitivities primarily due to the complexity of generating high-order kernel functions analytically. Although simple in concept, the calculation of the high-order kernel functions is cumbesome and error prone to compute analytically. A significant complicating factor for high dimensional derivatives is that Jacobian transformations are required to map derivatives with respect to the natural parameters into derivatives with respect to the mean and standard deviation. The Jacobian transformations are needed since most PDFs are defined in terms of natural parameters rather than the mean and standard deviation.

In contrast to the complexities involved using analytical methods, numerical methods using multicomplex mathematics to compute the high-order kernel functions are straightforward to implement, remove the need for Jacobian transformations, and are extendable to arbitrary order derivatives. As a result, the high-order kernel functions are computed here numerically using multicomplex mathematics. Since multicomplex numbers can be represented using matrices, the PDFs must be defined in terms of matrices and matrix functions must be used during their evaluation.

2. Multicomplex mathematics

This section introduces the basic concepts of multicomplex mathematics. More details can be found in Price [17], Lantoine et al. [8], Millwater and Shirinkam [24].

2.1. The multicomplex pace $\mathbb{C}_n$

The set of all numbers in the nth dimensional multicomplex space is denoted by $\mathbb{C}_n$. The first case, $n = 0$, is defined as the set of all real numbers (i.e., $\mathbb{C}_0 := \mathbb{R}$). The second case, $n = 1$, is defined as the set of all complex numbers (i.e., $\mathbb{C}_1 := \mathbb{C}$). These two number systems should be very familiar, in that the rules of algebraic operation for numbers and functions defined on these spaces are well known.

Multicomplex numbers are a multi-dimensional generalization