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Adaptive Locally Weighted Projection Regression Method for Uncertainty Quantification

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Abstract. We develop an efficient, adaptive locally weighted projection regression (ALWPR) framework for uncertainty quantification (UQ) of systems governed by ordinary and partial differential equations. The algorithm adaptively selects the new input points with the largest predictive variance and decides when and where to add new local models. It effectively learns the local features and accurately quantifies the uncertainty in the prediction of the statistics. The developed methodology provides predictions and confidence intervals at any query input and can deal with multi-output cases. Numerical examples are presented to show the accuracy and efficiency of the ALWPR framework including problems with non-smooth local features such as discontinuities in the stochastic space.

AMS subject classifications: 65C30, 65C05, 60-08, 62J05

Key words: Locally weighted projection regression, multi-output, adaptivity, uncertainty quantification.

1 Introduction

Uncertainty Quantification (UQ) is critical in all engineering and scientific fields. UQ is a broad topic involving many aspects, for example, representation of uncertainty, propagation of uncertainty across scales, validation and verification for predictive computational science, visualization of uncertainty in high-dimensional spaces and so on [1–5]. The aim of this paper is to present a methodology for investigating the propagation of uncertainty from the input space to the response space using a deterministic code. The Monte Carlo (MC) is the traditional method for addressing such UQ tasks. Its wide acceptance is due to the fact that it can compute the complete statistics of the solution, while having

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a convergence rate that is independent of the input dimension. Nevertheless, it quickly becomes inefficient in high dimensional and computationally intensive problems, where only a few samples are available.

Another well-known approach for uncertainty quantification is the spectral finite element method [6]. It involves the projection of the response on a space spanned by orthogonal polynomials of the random variables and the solution of a system of coupled deterministic equations involving the coefficients of the expansion in these polynomials. The scheme was originally developed for Gaussian random variables which correspond to Hermite polynomials (polynomial chaos (PC)). It was later generalized to include other types of random variables (generalized PC (gPC)) [7] and then expanded to the multi-element case. The multi-element generalized polynomial chaos (ME-gPC) method [8, 9] decomposes the stochastic space in disjoint elements and then employs gPC on each element. The coupled nature of the resulting equations that determine the coefficients of the polynomials make the application of the method to high input dimensions rather difficult [10].

Another commonly used UQ method is stochastic collocation. The response is represented as an interpolative polynomial of the system response (output) in the random input space constructed by calls to the computer code at specific input points. In [11, 12], a Galerkin based approximation was introduced alongside a collocation scheme based on a tensor product rule using one-dimensional Gauss quadrature points. These methods do not scale well with the number of random input dimensions. To address high dimensionality problems, various sparse grid collocation (SGC) methodologies were developed based on the Smolyak algorithm [13]. In [14], the authors developed an adaptive hierarchical sparse grid collocation algorithm and considered a number of applications with non-smooth behavior in the stochastic space. However, the piecewise local linear nature of the scheme performed poorly when only a few data points were used while interpolation of adverse functions was shown that it can trick the adaptive algorithm into stopping prior to convergence.

While it is evident that a local approach to uncertainty propagation is required to capture localized features in the stochastic space, it is essential to select within each local model the most informative input to maximize predictive capability. In [15, 16], the authors developed such kind of method, specifically, a treed Gaussian process model where on each leaf of the tree, Bayesian Experimental Design techniques were used to learn a multi-output Gaussian process. The active learning aspects of these Bayesian approaches was shown to lead to better convergence than interpolation-based methods such as adaptive sparse grids [15].

Locally weighted projection regression (LWPR) is an algorithm for incremental nonlinear function approximation in high-dimensional spaces [17–19]. At its core, it employs nonparametric partial least squares regression to locally approximate the relationship between input and output. This methodology has several merits including no need to memorize the training data, adjusting the local models only by the local information, an ability to deal with high dimensional correlated data and providing a confidence interval