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Review

Least squares polynomial chaos expansion: A review of sampling strategies

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Abstract

As non-intrusive polynomial chaos expansion (PCE) techniques have gained growing popularity among researchers, we here provide a comprehensive review of major sampling strategies for the least squares based PCE. Traditional sampling methods, such as Monte Carlo, Latin hypercube, quasi-Monte Carlo, optimal design of experiments (ODE), Gaussian quadratures, as well as more recent techniques, such as coherence-optimal and randomized quadratures are discussed. We also propose a hybrid sampling method, dubbed *alphabetic-coherence-optimal*, that employs the so-called alphabetic optimality criteria used in the context of ODE in conjunction with coherence-optimal samples. A comparison between the empirical performance of the selected sampling methods applied to three numerical examples, including high-order PCE's, high-dimensional problems, and low oversampling ratios, is presented to provide a road map for practitioners seeking the most suitable sampling technique for a problem at hand. We observed that the alphabetic-coherence-optimal technique outperforms other sampling methods, specially when high-order ODE are employed and/or the oversampling ratio is low.
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Keywords: Polynomial chaos; Least squares approximation; Optimal sampling; Optimal design of experiments; Coherence-optimal

Contents

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1. Introduction

Reliable and rigorous simulations of real world engineering problems involve characterization of the often uncertain system inputs, e.g., material properties, initial, or boundary conditions, and quantification of their impact on the output quantities of interest (QoI's). This is the subject of uncertainty quantification (UQ), an emerging field in computational engineering and science, which aims at providing tools for assessing the credibility of model predictions and facilitating decision making under uncertainty.

A major class of UQ techniques are probabilistic where uncertain parameters are represented by random variables or processes. Among the probabilistic UQ approaches, stochastic spectral methods based on polynomial chaos (PC) expansions [1–4] have received special attention due to their advantages over traditional UQ techniques; see, e.g., [3,5–12]. Let $(\Omega, \mathcal{T}, \mathcal{P})$ be a complete probability space where Ω is the sample set (or design space in the context of design of experiments) and $\mathcal{P}$ is a probability measure on the $\sigma-$field $\mathcal{T}$. Also assume that the system input uncertainty is described by the random vector $\boldsymbol{\Xi} = (\Xi_1, \dots, \Xi_d) : \Omega \to \mathbb{R}^d$, $d \in \mathbb{N}$, consisting of d independent identically distributed (i.i.d.) random variables Ξ_k with realizations $\boldsymbol{\xi} = (\xi_1, \dots, \xi_d)$. The marginal probability density function (pdf) of Ξ_k and the joint pdf of $\boldsymbol{\Xi}$ are denoted by $f(\xi_k)$ and $f(\boldsymbol{\xi}) = \prod_{k=1}^{d} f(\xi_k)$, respectively. The PC representation of $u(\boldsymbol{\Xi})$, a scalar QoI with finite variance, is given by

$$u(\boldsymbol{\Xi}) = \sum_{j=1}^{\infty} c_j \psi_j(\boldsymbol{\Xi}), \tag{1}$$

where $\{\psi_j(\boldsymbol{\Xi})\}$ is a set of multivariate polynomials orthonormal with respect to $f(\boldsymbol{\xi})$ and c_j are the deterministic PC coefficients to be determined. For computational purpose, the infinite series in (1) may be truncated by retaining the first P terms as

$$u(\boldsymbol{\Xi}) = \sum_{j=1}^{P} c_j \psi_j(\boldsymbol{\Xi}) + \epsilon(\boldsymbol{\Xi}), \tag{2}$$

where $\epsilon(\boldsymbol{\Xi})$ represents the random truncation error. A detailed description of the construction of the PC basis $\{\psi_j(\boldsymbol{\Xi})\}$ and the truncated expansion in (2) will be discussed in Section 2.2.

The main task in PC-based methods is to compute the PC coefficients either intrusively or non-intrusively [3,13–15]. In an intrusive approach, the governing equations are projected onto the subspace spanned by the PC basis via the Galerkin formulation [3], often requiring some modifications to the existing deterministic solvers that may not be desirable. On the other hand, non-intrusive methods are based on sampling and treat existing deterministic solvers as a black box. Sampling-based techniques such as least squares approximation (LSA) [16–19],