Journal of Computational Physics 371 (2018) 20–49

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

Basis adaptive sample efficient polynomial chaos (BASE-PC)

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ARTICLE INFO

Article history:
Received 2 February 2017
Received in revised form 14 March 2018
Accepted 22 March 2018
Available online 4 April 2018

Keywords:
Polynomial chaos
Orthogonal polynomials
Uncertainty quantification
Compressive sensing
Basis adaptation
Importance sampling

ABSTRACT

For a large class of orthogonal basis functions, there has been a recent identification of expansion methods for computing accurate, stable approximations of a quantity of interest. This paper presents, within the context of uncertainty quantification, a practical implementation using basis adaptation, and coherence motivated sampling, which under assumptions has satisfying guarantees. This implementation is referred to as Basis Adaptive Sample Efficient Polynomial Chaos (BASE-PC). A key component of this is the use of anisotropic polynomial order which admits evolving global bases for approximation in an efficient manner, leading to consistently stable approximation for a practical class of smooth functionals. This fully adaptive, non-intrusive method, requires no *a priori* information of the solution, and has satisfying theoretical guarantees of recovery. A key contribution to stability is the use of a presented correction sampling for coherence-optimal sampling in order to improve stability and accuracy within the adaptive basis scheme. Theoretically, the method may dramatically reduce the impact of dimensionality in function approximation, and numerically the method is demonstrated to perform well on problems with dimension up to 1000.

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1. Introduction

A reliable approach to analyzing complex engineering systems requires understanding how various Quantities of Interest (QoI) depend upon system inputs that are often uncertain; where a poor understanding will lead to poor executive decisions. Uncertainty Quantification (UQ) [1–3] is a field that aims at addressing these issues in a practical and rigorous manner, giving a meaningful characterization of uncertainties from the available information and admitting efficient propagation of these uncertainties for a quantitative validation of model predictions.

Probability is a natural framework for modeling uncertainty, wherein we assume uncertain inputs are represented by a d-dimensional random vector $\boldsymbol{\Xi} := (\Xi_1, \cdots, \Xi_d)$ with some joint probability density function $f(\boldsymbol{\xi})$ supported on Ω, where we further assume that the coordinates of $\boldsymbol{\Xi}$ are independent. In this manner, the scalar QoI to be approximated, here denoted by $u(\boldsymbol{\Xi})$, is modeled as a fixed but unknown function of the input. In this work we approximate $u(\boldsymbol{\Xi})$, assumed to have finite variance, by a spectral expansion in multivariate basis functions, each of which is denoted by $\psi_k(\boldsymbol{\Xi})$, and are naturally chosen to be orthogonal with respect to the distribution of $\boldsymbol{\Xi}$ [4,5]. We focus here on the case that ψ_k are polynomials, a method referred to as a Polynomial Chaos (PC) expansion [1,4],

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https://doi.org/10.1016/j.jcp.2018.03.035
0021-9991/Published by Elsevier Inc.

$$u(\boldsymbol{\Xi}) = \sum_{k=1}^{\infty} c_k \psi_k(\boldsymbol{\Xi}). \tag{1}$$

We note that the independence assumption for the coordinates of $\boldsymbol{\Xi}$ may be removed if care is taken in prescribing orthogonal basis functions ψ_k, although we do not consider any such examples here.

For computation, we allow an arbitrary number of input dimensions d but assume u can be accurately approximated in some relatively small set of basis functions. Let $\boldsymbol{k} = (k_1, \cdots, k_d)$ be a vector such that $k_i \in \mathbb{N} \cup \{0\}$ represents the order of the polynomial $\psi_{k_i}(\Xi_i)$, which is orthonormal with respect to the distribution of Ξ_i. For instance, when Ξ_i follows a uniform or Gaussian distribution, $\psi_{k_i}(\Xi_i)$ are normalized Legendre or Hermite polynomials, respectively [4,5]. For a d-dimensional vector $\boldsymbol{k}$, the d-dimensional polynomial $\psi_{\boldsymbol{k}}(\boldsymbol{\Xi})$ is then constructed by the tensorization of $\psi_{k_i}(\Xi_i)$, where k_i is the ith coordinate of $\boldsymbol{k}$. Specifically,

$$\psi_{\boldsymbol{k}}(\boldsymbol{\Xi}) = \prod_{i=1}^{d} \psi_{k_i}(\Xi_i).$$

In this work we select basis functions in a manner that iteratively adjusts parameters that define a basis. Specifically, we consider a definition of anisotropic total order [6] using one parameter, p_i, per dimension. We combine these into a vector, $\boldsymbol{p} := (p_1, \cdots, p_d)$, so that an order-$\boldsymbol{p}$ basis is defined by a related set of $\boldsymbol{k} = (k_1, \cdots, k_d)$, specifically

$$\mathcal{B}_{\boldsymbol{p}} := \left\{ \psi_{\boldsymbol{k}} \middle| \sum_{i=1}^{d} \frac{k_i}{p_i} \leq 1 \right\}. \tag{2}$$

This basis definition has a number of parameters that scales with dimension, and which we will repeatedly modify to improve the quality of our polynomial approximation. We note that if all $p_i = p$, then the order-$\boldsymbol{p}$ basis is identical to a total order basis of order p. We also note that this basis can have an additional hyperbolicity parameter associated with it as considered in [7], although we do not consider any such parameter here. Heuristically, we expect most p_i to be low and only a few to be relatively high, allowing a basis that faithfully approximates the QoI with relatively few basis functions compared to a total order basis with an order that is able to achieve the same accuracy in the reconstruction. This definition of order allows us to adjust the working basis functions as a complete set, rather than adding or removing basis functions one at a time. We note that p_i indicates the largest order for basis function that appears in dimension i, while the k_i indexes the order of each potential basis function. Often, the subscript on $\mathcal{B}$ is omitted; replaced with a scalar index related to iterative adjustment; or replaced with a bound on approximation error achieved in that basis; and this should not be confusing in context. For the remainder of this text, we refer to an order-$\boldsymbol{p}$ basis as an anisotropic order basis.

We use $|\mathcal{B}|$ to denote the total number of basis functions in a set $\mathcal{B}$, indexed in an arbitrary manner for $k = \{1, \cdots, |\mathcal{B}|\}$, while the vector $\boldsymbol{k}$ specifically identifies the basis function by determining the order in each dimension. This facilitates a polynomial surrogate approximation to u for any basis set $\mathcal{B}$, given by

$$u(\boldsymbol{\Xi}) \approx \sum_{k=1}^{|\mathcal{B}|} c_k \psi_k(\boldsymbol{\Xi}). \tag{3}$$

The error introduced by this truncation is referred to as *truncation error*, and converges to zero – in the mean squares sense as basis functions are added – when

$$c_k = \mathbb{E}(u(\boldsymbol{\Xi})\psi_k(\boldsymbol{\Xi})). \tag{4}$$

Here, $\mathbb{E}$ denotes the mathematical expectation operator. Without any *a priori* information as to what $\mathcal{B}$ should be, we seek to identify $\mathcal{B}$ based solely on solution characteristics as revealed by computed coefficients, $\{c_k\}$.

Identifying an optimal $\mathcal{B}$ first involves identifying a scalar quantity to optimize. In the present work, this quantity is related to a cross-validated error computed via ℓ_1-minimization using non-intrusive methodology [8,9]. Specifically, for a fixed basis, to identify the PC coefficients $\boldsymbol{c} = (c_1, \cdots, c_{|\mathcal{B}|})^T$ in (3) we consider a sampling-based method. This method does not require changes to deterministic solvers for u as we generate realizations of $\boldsymbol{\Xi}$ to identify $u(\boldsymbol{\Xi})$, or perform a related importance sampling as in [10,11]. We denote the ith such realizations as $\boldsymbol{\xi}^{(i)}$ and $u(\boldsymbol{\xi}^{(i)})$, respectively. We let N denote the number of samples of the QoI which we utilize, and define,

$$\boldsymbol{u} := (u(\boldsymbol{\xi}^{(1)}), \cdots, u(\boldsymbol{\xi}^{(N)}))^T; \tag{5}$$

$$\boldsymbol{\Psi}(i, j) := \psi_j(\boldsymbol{\xi}^{(i)}), \tag{6}$$

where we refer to $\boldsymbol{\Psi}$ as the *measurement matrix* associated with $\mathcal{B}$. These definitions imply the matrix equality $\boldsymbol{\Psi c} = \boldsymbol{u}$, or more generally that this equality holds approximately. We also introduce a diagonal positive-definite matrix $\boldsymbol{W}$ such