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Sparse polynomial chaos expansions via compressed sensing and D-optimal design

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Abstract

In the field of uncertainty quantification, sparse polynomial chaos (PC) expansions are commonly used by researchers for a variety of purposes, such as surrogate modeling. Ideas from compressed sensing may be employed to exploit this sparsity in order to reduce computational costs. A class of greedy compressed sensing algorithms use least squares minimization to approximate PC coefficients. This least squares problem lends itself to the theory of optimal design of experiments (ODE). Our work focuses on selecting an experimental design that improves the accuracy of sparse PC approximations for a fixed computational budget. We propose a novel sequential design, greedy algorithm for sparse PC approximation. The algorithm sequentially augments an experimental design according to a set of the basis polynomials deemed important by the magnitude of their coefficients, at each iteration. Our algorithm incorporates topics from ODE to estimate the PC coefficients. A variety of numerical simulations are performed on three physical models and manufactured sparse PC expansions to provide a comparative study between our proposed algorithm and other non-adaptive methods. Further, we examine the importance of sampling by comparing different strategies in terms of their ability to generate a candidate pool from which an optimal experimental design is chosen. It is demonstrated that the most accurate PC coefficient approximations, with the least variability, are produced with our design-adaptive greedy algorithm and the use of a studied importance sampling strategy. We provide theoretical and numerical results which show that using an optimal sampling strategy for the candidate pool is key, both in terms of accuracy in the approximation, but also in terms of constructing an optimal design.
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1. Introduction

Our understanding of complex scientific and engineering problems often stems from a general Quantity of Interest (QoI). Practical analysis, design, and optimization of complex engineering systems require modeling physical processes and accounting for how uncertainties impact QoIs. Uncertainties may arise from variations in model inputs,

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measurements and data, or boundary and operating conditions. Much research has been done to quantify how the presence of uncertainty within a model manifests changes in a QoI [1–3]. This problem is often studied in the field of Uncertainty Quantification (UQ).

A common approach in UQ for problems with random inputs involves expanding the QoI in a polynomial basis, referred to as a *polynomial chaos expansion* [1,4]. One way to construct a PC expansion is to formulate a regression problem using Monte Carlo samples of the QoI. Often QoIs in scientific and engineering applications admit *sparse PC expansions*, i.e., the QoI can be approximated by a small subset of the polynomial basis functions which capture important features of the model. This work focuses on QoIs which admit sparse PC expansions as detailed below. Sparsity may be exploited to regularize the regression problem; a concept studied in the context of compressed sensing [5–9]. In UQ, sparse PC expansions have been applied for a variety of different purposes [10–28].

Assume that the input parameters of our model are represented by a d-dimensional random vector $\boldsymbol{\Xi} := (\Xi_1, \ldots, \Xi_d)$ with independent, identically distributed entries, where we denote all realized random vectors by $\boldsymbol{\xi}$. Further, assume that $\boldsymbol{\Xi}$ obeys some joint probability density function $f(\boldsymbol{\xi})$. We wish to approximate an unknown scalar QoI, with finite variance, denoted by $u(\boldsymbol{\Xi})$. Let $\psi_k(\boldsymbol{\Xi})$ represent a multivariate orthogonal polynomial, then we may write our QoI using a PC expansion as

$$u(\boldsymbol{\Xi}) = \sum_{k=0}^{\infty} c_k \psi_k(\boldsymbol{\Xi}). \tag{1}$$

We truncate the expansion in (1) for computation, i.e., let $\mathbf{c} = (c_1, \ldots, c_P)^T$ so that

$$u(\boldsymbol{\Xi}) = \sum_{k=1}^{P} c_k \psi_k(\boldsymbol{\Xi}) + \epsilon(\boldsymbol{\Xi}) \approx \sum_{k=1}^{P} c_k \psi_k(\boldsymbol{\Xi}), \tag{2}$$

where $\epsilon(\boldsymbol{\Xi})$ represents the *truncation error* introduced by truncating the expansion to a finite number of terms. Often, in practice, many of the coefficients c_k are negligible and thus $u(\boldsymbol{\Xi})$ admits a sparse representation of the form

$$u(\boldsymbol{\Xi}) \approx \sum_{k \in \mathcal{C}} c_k \psi_k(\boldsymbol{\Xi}), \tag{3}$$

where the index set $\mathcal{C}$ has few elements, say $s = |\mathcal{C}| \ll P$, and we say that our QoI is *approximately sparse* in the polynomial basis.

The polynomials $\psi_k(\boldsymbol{\Xi})$ are selected with respect to the probability measure $f(\boldsymbol{\xi})$ so that they are orthogonal, e.g., when $\boldsymbol{\Xi}$ obeys a jointly uniform or Gaussian distribution (with independent components), $\psi_k(\boldsymbol{\Xi})$ are multivariate Legendre or Hermite polynomials, respectively [4]. We assume $\psi_k(\boldsymbol{\Xi})$ is obtained by the tensorization of univariate polynomials orthogonal with respect to the probability density function of the coordinates of $\boldsymbol{\Xi}$, and that $\psi_k(\boldsymbol{\Xi})$ is of *total order* less than or equal to p. This total order construction implies that there are $P := \binom{p+d}{d}$ basis polynomials, and facilitates approximations of the form of (3) which favor lower order polynomials. Furthermore, we assume that $\psi_k(\boldsymbol{\Xi})$ are normalized such that $\mathbb{E}\left[\psi_k^2\right] = 1$, where $\mathbb{E}[\cdot]$ denotes the mathematical expectation operator.

For $i = 1, \ldots, N$, where N is the number of independent samples considered, the computational model is evaluated for each realization of $\boldsymbol{\Xi}$, which we denote $\boldsymbol{\xi}_i$, and yields a corresponding value of the QoI $u(\boldsymbol{\xi}_i)$. The coefficients $\mathbf{c}$ are approximated using an experimental design consisting of samples $\left\{\boldsymbol{\xi}_i\right\}_{i=1}^{N}$ and their corresponding QoIs $\left\{u(\boldsymbol{\xi}_i)\right\}_{i=1}^{N}$, which are related by the linear system $\mathbf{u} \approx \boldsymbol{\Psi}\mathbf{c}$, where

$$\boldsymbol{\Psi}(i, j) := \psi_j(\boldsymbol{\xi}_i) \text{ and } \mathbf{u} := \left[u(\boldsymbol{\xi}_1), \ldots, u(\boldsymbol{\xi}_N)\right]^T. \tag{4}$$

Further, let $\boldsymbol{W}$ be a diagonal positive-definite weight matrix such that $\boldsymbol{W}(i, i)$ is a function of $\boldsymbol{\xi}_i$, which depends on the sampling strategy described in Section 2. Let $\boldsymbol{\Phi} := \boldsymbol{W}\boldsymbol{\Psi}$ and $\mathbf{v} := \boldsymbol{W}\mathbf{u}$. Under this sampling strategy, we consider the linear system

$$\mathbf{v} \approx \boldsymbol{\Phi}\mathbf{c}. \tag{5}$$

In compressed sensing, a sparse approximation $\hat{\mathbf{c}}$ of $\mathbf{c}$ is obtained by solving the optimization problem

$$\hat{\mathbf{c}} = \underset{\mathbf{c}}{\operatorname{argmin}} \|\mathbf{c}\|_0 \quad \text{subject to } \|\mathbf{v} - \boldsymbol{\Phi}\mathbf{c}\|_2 \le \delta, \tag{6}$$

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