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A near-optimal sampling strategy for sparse recovery of polynomial chaos expansions

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ABSTRACT

Compressive sampling has become a widely used approach to construct polynomial chaos surrogates when the number of available simulation samples is limited. Originally, these expensive simulation samples would be obtained at random locations in the parameter space. It was later shown that the choice of sample locations could significantly impact the accuracy of resulting surrogates. This motivated new sampling strategies or design-of-experiment approaches, such as coherence-optimal sampling, which aim at improving the coherence property. In this paper, we propose a sampling strategy that can identify near-optimal sample locations that lead to improvement in local-coherence property and also enhancement of cross-correlation properties of measurement matrices. We provide theoretical motivations for the proposed sampling strategy along with several numerical examples that show that our near-optimal sampling strategy produces substantially more accurate results, compared to other sampling strategies.

1. Introduction

In order to facilitate stochastic computation in analysis and design of complex systems, analytical surrogates that approximate and replace full-scale simulation models have been increasingly studied. One of the most widely adopted surrogates is the polynomial chaos expansion (PCE), which approximates the quantity of interest (QoI) by a spectral representation using polynomial functions of random parameters [1–4]. In estimating these spectral surrogates, non-intrusive stochastic techniques, based on either spectral projection or linear regression, are widely used especially because they don't require modifying deterministic solvers or legacy codes, which is an otherwise cumbersome task [5]. These non-intrusive techniques are still the subject of ongoing research as the number of required samples for accurate surrogate estimation rapidly grows with the number of random parameters, even when efficient techniques such as sparse grid are used [6–9].

More recently, researchers have developed techniques, based on compressive sampling (CS), that are particularly advantageous when surrogate expansions are expected to be sparse, i.e. the QoI can be accurately represented with a few polynomial chaos (PC) basis functions. Compressive sampling was first introduced in the field of signal processing to recover sparse signals using a number of samples significantly smaller that the conventionally used Shannon–Nyquist sampling rate [10–12]. Motivated by the fact that the solution of many high dimensional problems of interest, such as high dimensional PDEs, can be represented by sparse, or at least approximately sparse, PCEs, CS was proposed in [13–15] to estimate PC coefficients in underdetermined cases. As CS theorems suggest, the success of sparse estimation of PCE depends not only upon

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the sparsity of the solution of stochastic system, but also on the coherence property of the Vandermonde-like measurement matrix, formed by evaluations of orthogonal polynomials at sample locations [10], as will be elaborated later.

Several efforts have been made in order to improve the two mentioned conditions for successful recovery. For instance in [16], for Hermite expansions with Gaussian input variables, the original inputs are rotated such that a few of the new coordinates, i.e. linear combinations of original inputs, have significant impact on QoI, thereby increasing the sparsity of solution and, in turn, the accuracy of recovery. The second condition, i.e. coherence of the measurement matrix, can be poor especially when trial expansions are high-order and/or high-dimensional. To remedy this, the iterative approaches in [17,18] can be used to optimally include only the "important" basis functions into the trial expansion and its associated measurement matrix. Focusing on this second condition, another class of methods have proposed sampling strategies that produce less coherent measurement matrices [19–21]. Among these approaches, the sampling strategy proposed in [21] was designed to be optimal in achieving the lowest local-coherence.

In this work, we introduce a near-optimal sampling strategy by further improving the local-coherence-based sampling of [21] and filtering sample locations based on cross-correlation properties of the resulting measurement matrix. Specifically, we establish quantitative measures to capture these cross-correlation properties between measurement matrix columns, and use these measures as the criteria for near-optimal identification of sample locations. It will be demonstrated that a sampling strategy that seeks to optimize these measures will lead to CS results that on average outperforms all other CS sampling strategies. This paper is organized as follows. Section 2 presents general concepts in compressive sampling and its theoretical background. In Section 3, we introduce our sampling algorithm along with relevant theoretical supports. Finally, Section 4 includes numerical examples and discussions about the advantages of the proposed approach.

2. Setup and background

2.1. Polynomial chaos expansion

Let $I_{\boldsymbol{\Xi}} \subseteq \mathbb{R}^d$ be a tensor-product domain that is the support of $\boldsymbol{\Xi}$, where $\boldsymbol{\Xi} = (\Xi_1, \ldots, \Xi_d)$ is the vector of independent random variables, i.e. $\Xi_i \in I_{\Xi_i}$ and $I_{\boldsymbol{\Xi}} = \times_{i=1}^{d} I_{\Xi_i}$. Also, let $\rho_i : I_{\Xi_i} \to \mathbb{R}^+$ be the probability measure for variable Ξ_i and let $\rho(\boldsymbol{\Xi}) = \prod_{i=1}^{d} \rho_i(\Xi_i)$. Given this setting, the set of univariate orthonormal polynomials, $\{\psi_{\alpha,i}\}_{\alpha\in\mathbb{N}_0}$, satisfies

$$\int\limits_{I_{\Xi_i}} \psi_{\alpha,i}(\xi_i)\psi_{\beta,i}(\xi_i)\rho_i(\xi_i)\,\mathrm{d}\xi_i = \delta_{\alpha\beta}, \quad \alpha, \beta \in \mathbb{N}_0, \tag{1}$$

where $\mathbb{N}_0 = \mathbb{N} \cup \{0\}$, and δ_{mn} is the delta function. Therefore, the density function of Ξ_i, $\rho_i(\Xi_i)$, determines the type of polynomial. For example, Gaussian and uniform probability distributions enforce Hermite and Legendre polynomials, respectively. The d-dimensional orthonormal polynomials are then derived from the multiplication of one dimensional polynomials in all dimensions. For example,

$$\psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi}) = \psi_{\alpha_1,1}(\xi_1)\psi_{\alpha_2,2}(\xi_2)\ldots\psi_{\alpha_d,d}(\xi_d), \quad \boldsymbol{\alpha} = (\alpha_1, \alpha_2, \ldots, \alpha_d). \tag{2}$$

Consequently, we have

$$\int\limits_{I_{\boldsymbol{\Xi}}} \psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi})\psi_{\boldsymbol{\beta}}(\boldsymbol{\xi})\rho(\boldsymbol{\xi})\,\mathrm{d}\boldsymbol{\xi} = \delta_{\boldsymbol{\alpha}\boldsymbol{\beta}}, \quad \boldsymbol{\alpha}, \boldsymbol{\beta} \in \mathbb{N}_0^d. \tag{3}$$

Using this construction, any function $u(\boldsymbol{\Xi}) : I_{\boldsymbol{\Xi}} \to \mathbb{R}$ that is square-integrable can be represented as

$$u(\boldsymbol{\Xi}) = \sum_{\boldsymbol{\alpha}\in\mathbb{N}_0^d} c_{\boldsymbol{\alpha}}\psi_{\boldsymbol{\alpha}}(\boldsymbol{\Xi}), \tag{4}$$

where $\{\psi_{\boldsymbol{\alpha}}\}_{\boldsymbol{\alpha}\in\mathbb{N}_0^d}$ is the set of orthonormal basis functions satisfying Equation (3). However, for computation's sake, $u(\boldsymbol{\Xi})$ is approximated by a finite order truncation of PC expansion given by

$$u_k(\boldsymbol{\Xi}) := \sum_{\boldsymbol{\alpha}\in\Lambda_{d,k}} c_{\boldsymbol{\alpha}}\psi_{\boldsymbol{\alpha}}(\boldsymbol{\Xi}), \tag{5}$$

where k is the total order of the polynomial expansion and $\Lambda_{d,k}$ is the set of multi-indices defined as

$$\Lambda_{d,k} := \{\boldsymbol{\alpha} \in \mathbb{N}_0^d : \|\boldsymbol{\alpha}\|_1 \le k\}. \tag{6}$$

The cardinality of $\Lambda_{d,k}$, i.e. the number of expansion terms, here denoted by K, is a function of d and k according to

$$K := |\Lambda_{d,k}| = \frac{(k+d)!}{k!d!}. \tag{7}$$