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Non-intrusive low-rank separated approximation of high-dimensional stochastic models

Alireza Doostan [a,*], AbdoulAhad Validi [b], Gianluca Iaccarino [c]

[a] Aerospace Engineering Science Department, University of Colorado, Boulder, CO 80309, USA
[b] Mechanical Engineering Department, University of Colorado, Boulder, CO 80309, USA
[c] Department of Mechanical Engineering, Stanford University, Stanford, CA 94305, USA

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ABSTRACT

This work proposes a sampling-based (non-intrusive) approach within the context of *low-rank separated representations* to tackle the issue of curse-of-dimensionality associated with the solution of models, e.g., PDEs/ODEs, with high-dimensional random inputs. Under some conditions discussed in details, the number of random realizations of the solution, required for a successful approximation, grows linearly with respect to the number of random inputs. The construction of the separated representation is achieved via a regularized alternating least-squares regression, together with an error indicator to estimate model parameters. The computational complexity of such a construction is quadratic in the number of random inputs. The performance of the method is investigated through its application to three numerical examples including two ODE problems with high-dimensional random inputs.

1. Introduction

In most practical situations, the behavior and evolution of complex systems are known only with limited certainty. This is mainly due to the lack of knowledge about the governing physical laws or limited information regarding their operating conditions and input parameters, e.g., fuel or material properties. A reliable computer simulation of such systems, therefore, requires a systematic representation of uncertainties and quantification of their impact on quantities of interest.

In the probabilistic framework, uncertainties are represented using random variables and processes characterized by, for instance, the available experimental data or expert opinion. A major task is then to quantify the dependence of quantities of interest – also random variables or processes – on these random inputs. Development of efficient numerical tools for the computation of such mappings has been a research subject over the past few decades and has become an emerging field of study more recently.

Statistical tools such as Monte Carlo sampling and its variations have been widely used for this purpose. To address the low convergence rate of these methods, stochastic basis expansions, for instance, in chaos polynomials [32,31,77] and multivariate numerical integration/interpolation, such as those based on the sparse grid collocation [70,52,76], have been recently proposed. While proven efficient both numerically and analytically on numerous problems in engineering and science, these techniques may face difficulties when input uncertainties are characterized by a large number of independent random variables (i.e., high-dimensional random inputs) [76,75]. Specifically, the computational complexity of these methods, in their original forms, grows exponentially fast with respect to the number of input random variables: an issue known as the *curse-of-dimensionality*. The reason for such a fast growth is the tensor product construction of multi-dimensional bases (in polynomial chaos methods) or quadrature rules (in sparse grid collocation approaches) from one-dimensional bases or quadrature rules, respectively. Such tensorizations, therefore, impose an explicit dependence on the input dimensionality. Instead, a number of recent techniques have been proposed that exploit, for instance, *low-rank* or *sparsity* structures of quantities of interest in order to reduce this exponential complexity growth, see, e.g. [23,71,58,11,49,10,12,27,59,25]. However, effective treatment of the curse-of-dimensionality still remains an open problem.

Alternatively, in the present study, we propose an approach that constructs a *separated representation* of the solution of interest. Specifically, let $u(\boldsymbol{y})$ with $\boldsymbol{y}(\omega) = (y_1(\omega), \ldots, y_d(\omega)) : \Omega \to \mathbb{R}^d$, $\omega \in \Omega$ and $d \in \mathbb{N}$, be a stochastic function defined on a suitable probability space $(\Omega, \mathcal{F}, \mathcal{P})$. Then $u(\boldsymbol{y})$ admits a separated representation if, for some (small) $r \in \mathbb{N}$ and accuracy $\epsilon \geqslant 0$

* Corresponding author.
E-mail addresses: doostan@colorado.edu (A. Doostan), AbdoulAhad.Validi@colorado.edu (A. Validi), jops@stanford.edu (G. Iaccarino).

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$$u(\boldsymbol{y}) = \sum_{l=1}^{r} s_l u_1^l(y_1)\cdots u_d^l(y_d) + \mathcal{O}(\epsilon), \tag{1}$$

where the univariate functions $\{u_k^l(y_k)\}_{k=1}^d$, $l = 1,\ldots,r$, are unknown and $\{s_l\}$, $l = 1,\ldots,r$, are some normalization constants. When the *separation rank* r is independent of d, the approximation (1) may be obtained with a computational complexity that is linear in d [8,9,7,25], hence drastically reducing the curse-of-dimensionality. When the approximation (1) is achieved by a small r, then $u(\boldsymbol{y})$ is said to admit a *low-rank separated representation*.

Separated representations, also known as canonical decompositions (CANDECOMP) or parallel factor analysis (PARAFAC), have been first introduced by Hitchcock [39] to represent a multi-way tensor as a finite sum of rank-one tensors. Consequently, they have been extensively applied to several areas including image compression and classification [67,30], telecommunication [69,68,48], neuroscience [55,29,6], chemometrics [14], and data mining [8,9,44,42,72,35,1,7,2,43].

Separated representations have been recently used for the reduced order solution of deterministic PDEs in solid and fluid mechanics, where they are often called proper generalized decompositions (PGDs), see, e.g. [45,46,4,5,16,57,15,47,18,17] and the references therein.

In the context of stochastic problems, an expansion based on the separation of spatial and random variables has been proposed in [59,60]. While this approach significantly reduces the computational complexity of full-order polynomial chaos (PC) approximations, it suffers from the curse-of-dimensionality for high-dimensional random inputs. A separated representation of the form (1) for the solution of PDEs and ODEs with high-dimensional random inputs has been first studied in [26,24,25]. Similar representations, although with different solution strategies, have been later investigated in [61,41,28].

The current separated approximation of models with high-dimensional random inputs are *intrusive*, that is, one has to rewrite deterministic solvers in order to propagate the uncertainty. However, for many large-scale complex systems, it is desirable to develop *non-intrusive* solvers, where deterministic codes are treated as black box. Such a construction is the purpose of the present study. Specifically, we here extend the alternating least-squares regression approach of [7] to problems with high-dimensional random inputs. To enhance the stability and accuracy of this technique, we propose a Tikhonov regularization of the regression problem along with an error indicator for the selection of two main parameters of the separated representation. Under some conditions to be discussed in Section 3.4, the number of random realizations of the solution, required for a successful approximation, grows linearly with respect to d. Furthermore, the computational complexity of the alternating least-squares regression approach is quadratic in d.

The rest of this paper is structured as follows. In Section 2, we introduce the problem of interest in an abstract form. Following that, in Section 3, we discuss the separated representations in more details and describe their non-intrusive construction using an alternating least-squares regression. Additionally, we discuss the computational complexity of this non-intrusive method. In Section 4, we propose a regularization approach together with an error indicator to derive a stopping criterion and, hence, avoid over-fitting the solution realizations. Finally, in Section 5, we demonstrate the performance and efficiency of the proposed approach on a manufactured function as well as two ODE problems with high-dimensional random inputs. The first ODE problem is a linear elliptic equation with random diffusion coefficient. The second one is concerned with a hydrogen oxidation problem where reaction rate constants and species thermodynamics are uncertain.

2. Problem setup

Let $(\Omega, \mathcal{F}, \mathcal{P})$ be a complete probability space on which the random inputs are defined. Here Ω is the set of elementary events, $\mathcal{F} \subset 2^\Omega$ is the σ-algebra of events, and $\mathcal{P} : \mathcal{F} \to [0,1]$ is a probability measure. For the sake of demonstration, we consider a generic stochastic ordinary differential equation (ODE)

$$\mathcal{A}(t, \boldsymbol{y}(\omega); u) = 0, \quad (t,\omega) \in [0,T] \times \Omega, \tag{2}$$

that holds $\mathcal{P}$-*a.s.* for $\omega \in \Omega$. Appropriate initial condition and forcing function are also considered. Here, $\mathcal{A}$ denotes the ordinary differential operator, $t \in [0,T]$, $T > 0$, is the time variable, and $\boldsymbol{y}(\omega) = (y_1(\omega),\ldots,y_d(\omega)) : \Omega \to \mathbb{R}^d$, $d \in \mathbb{N}$, represents the vector of random variables defining the input uncertainty. We further assume that the components of the random vector $\boldsymbol{y}(\omega)$ are statistically independent and identically distributed (i.i.d.) according to a probability density function $\rho(y_k) : \Gamma \subseteq \mathbb{R} \to \mathbb{R}_{\geqslant 0}$, $k = 1,\ldots,d$.

Our goal is to estimate the possibly non-linear solution

$$u(t,\boldsymbol{y}) := u(t,\boldsymbol{y}(\omega)) = u(t,y_1(\omega),\ldots,y_d(\omega)) : [0,T] \times \Gamma^d \to \mathbb{R} \tag{3}$$

of (2) in a non-intrusive fashion, i.e., with the assumption that the deterministic solver of (2) is a black box. This entails the evaluation of $u(t,\boldsymbol{y})$ at a set of random or deterministic realizations of $\boldsymbol{y}$ and subsequently the construction of an approximation $\hat{u}(t,\boldsymbol{y})$ based on an interpolation, a regression, or a discrete projection scheme.

In the present study, we consider the random sampling of $\boldsymbol{y}$, similar to the standard Monte Carlo simulation. We denote by D a set of N independent realizations $\boldsymbol{y}^{(j)}$, $j = 1,\ldots,N$, drawn according to the probability density function $\rho(\boldsymbol{y}) = \prod_{k=1}^d \rho(y_k)$, and the corresponding solution realizations $u(t,\boldsymbol{y}^{(j)})$,

$$D = \left\{ \left(\boldsymbol{y}^{(j)}; u(t,\boldsymbol{y}^{(j)})\right) \right\}_{j=1}^N. \tag{4}$$

Using the *data* set D, we then extend the regression approach of [7] to stably construct $\hat{u}(t,\boldsymbol{y})$ in the separated form (1).

For the interest of description and without loss of generality, we henceforth restrict our analyses to a fixed instance of t and adopt the short notation $u(\boldsymbol{y})$ for the solution of interest. We next introduce the separated representation (1) in more details and subsequently discuss our non-intrusive approach to construct and regularize such an approximation.

3. Separated representations

To motivate the separated representation of $u(\boldsymbol{y})$, we first briefly describe the standard multivariate approximation of $u(\boldsymbol{y})$ using polynomial chaos (PC) expansions [32,77].

Let $\{\psi_{\alpha_k}(y_k)\}_{k=1}^d$ be the set of univariate polynomials of degree $\alpha_k \in \mathbb{N}_0 := \mathbb{N} \cup \{0\}$ orthonormal with respect to the probability density function $\rho(y_k)$, i.e.,

$$\int_\Gamma \psi_{\alpha_k}(y_k)\psi_{\beta_k}(y_k)\rho(y_k)dy_k = \delta_{\alpha_k\beta_k}.$$

A tensorization of the univariate basis $\{\psi_{\alpha_k}(y_k)\}_{k=1}^d$, i.e.,

$$\psi_{\boldsymbol{\alpha}}(\boldsymbol{y}) = \psi_{\alpha_1}(y_1)\psi_{\alpha_2}(y_2)\ldots\psi_{\alpha_d}(y_d), \quad \boldsymbol{\alpha} \in \mathbb{N}_0^d, \tag{5}$$

with $\mathbb{N}_0^d = \{(\alpha_1,\ldots,\alpha_d) : \alpha_k \in \mathbb{N}_0\}$, forms an orthonormal basis in $L_2(\Gamma^d,\rho)$. Then, for $u(\boldsymbol{y}) \in L_2(\Gamma^d,\rho)$, the infinite series

$$u(\boldsymbol{y}) = \sum_{\boldsymbol{\alpha}\in\mathbb{N}_0^d} s_{\boldsymbol{\alpha}}\psi_{\boldsymbol{\alpha}}(\boldsymbol{y}) \tag{6}$$

with coefficients

$$s_{\boldsymbol{\alpha}} = \int_{\Gamma^d} u(\boldsymbol{y})\psi_{\boldsymbol{\alpha}}(\boldsymbol{y})\rho(\boldsymbol{y})d\boldsymbol{y} \tag{7}$$