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Polynomial meta-models with canonical low-rank approximations: Numerical insights and comparison to sparse polynomial chaos expansions

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A B S T R A C T

The growing need for uncertainty analysis of complex computational models has led to an expanding use of meta-models across engineering and sciences. The efficiency of meta-modeling techniques relies on their ability to provide statistically-equivalent analytical representations based on relatively few evaluations of the original model. Polynomial chaos expansions (PCE) have proven a powerful tool for developing meta-models in a wide range of applications; the key idea thereof is to expand the model response onto a basis made of multivariate polynomials obtained as tensor products of appropriate univariate polynomials. The classical PCE approach nevertheless faces the "curse of dimensionality", namely the exponential increase of the basis size with increasing input dimension. To address this limitation, the sparse PCE technique has been proposed, in which the expansion is carried out on only a few relevant basis terms that are automatically selected by a suitable algorithm. An alternative for developing meta-models with polynomial functions in high-dimensional problems is offered by the newly emerged low-rank approximations (LRA) approach. By exploiting the tensor–product structure of the multivariate basis, LRA can provide polynomial representations in highly compressed formats. Through extensive numerical investigations, we herein first shed light on issues relating to the construction of canonical LRA with a particular greedy algorithm involving a sequential updating of the polynomial coefficients along separate dimensions. Specifically, we examine the selection of optimal rank, stopping criteria in the updating of the polynomial coefficients and error estimation. In the sequel, we confront canonical LRA to sparse PCE in structural-mechanics and heat-conduction applications based on finite-element solutions. Canonical LRA exhibit smaller errors than sparse PCE in cases when the number of available model evaluations is small with respect to the input dimension, a situation that is often encountered in real-life problems. By introducing the conditional generalization error, we further demonstrate that canonical LRA tend to outperform sparse PCE in the prediction of extreme model responses, which is critical in reliability analysis.

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1. Introduction

It is nowadays common practice to study the behavior of physical and engineering systems through computer simulation. Proper analysis of the system response must account for the prevailing uncertainties in the system model and the underlying phenomena, which requires repeated simulations under varying scenarios for the input parameters. Modern advances in computer science combined with the improved understanding of physical laws are leading to computational models of increasing complexity. Uncertainty propagation through such models may become intractable in cases when a single simulation is computationally demanding. A remedy is to substitute a complex model with a *meta-model* that possesses similar statistical properties, but has a simple functional form.

The focus of the present work is on meta-models that are built with polynomial functions due to the simplicity and versatility they offer. A popular class of meta-models thereof are the so-called polynomial chaos expansions (PCE) [1,2]. The key idea of PCE is to expand the model response onto an appropriate basis made of orthonormal multivariate polynomials, the latter obtained as tensor products of univariate polynomials in each of the input parameters. In non-intrusive approaches that are of interest herein, the coefficients of the expansion are evaluated in terms of the response of the original model at a set of points in the input space, called the experimental design [3–5]. Although PCE have proven powerful in a wide range of applications, they face limitations in cases with high-dimensional input. This is because the number of the basis terms, and thus of the unknown expansion coefficients, grows exponentially with the number of input parameters, which is commonly referred to as the "curse of dimensionality". As shown in [6,7], the efficiency of the PCE approach can be significantly improved by using a sparse basis.

A promising alternative for developing meta-models with polynomial functions in high-dimensional spaces is provided by canonical decompositions. In canonical decompositions, also known as separated representations, a tensor is expressed as a sum of rank-one components. This type of representation constitutes a special case of tensor decompositions, which are typically used to compress information or extract a few relevant modes of a tensor; a survey on different types of tensor decompositions can be found in [8]. The original idea of canonical decomposition dates back to 1927 [9], but became popular in the second half of the 20th century after its introduction to psychometrics [10,11]. Since then, it has been used in a broad range of fields, including chemometrics [12,13], neuroscience [14,15], fluid mechanics [16,17], signal processing [18,19], image analysis [20,21] and data mining [22,23]. More recently, canonical decompositions are attracting an increasing interest in the field of uncertainty quantification [24–31].

By exploiting the tensor–product structure of the multivariate polynomial basis, canonical decompositions can provide equivalent to PCE representations in highly-compressed formats. It is emphasized that the number of parameters in canonical decompositions grows only linearly with the input dimension, which, in cases of high-dimensional problems, results in a drastic reduction of the number of unknowns compared to PCE. Naturally, canonical decompositions with a few rank-one components are of interest, thus leading to the name low-rank approximations (LRA). We note that although the present study is constrained to the use of polynomial bases, different basis functions may be considered for the construction of LRA in a general case (see, e.g. [31]).

Recently proposed methods for building canonical LRA meta-models in a non-intrusive manner rely on the sequential updating of the polynomial coefficients along separate dimensions. The underlying algorithms require solving a series of minimization problems of small size, independent of the input dimension, which can be easily handled using standard techniques. However, the LRA construction involves open questions that call for further investigations. In particular, stopping criteria in the sequential updating of the polynomial coefficients as well as criteria for selection of the optimal rank and polynomial degree are not yet well established. Considering a particular greedy algorithm for building canonical LRA meta-models, we herein shed light on the aforementioned issues through extensive numerical investigations. In the sequel, we assess the comparative accuracy of canonical LRA and sparse PCE in applications involving finite-element models pertinent to structural mechanics and heat conduction. In these applications, sparse PCE are built with a state-of-art method, where a candidate basis is defined by means of a hyperbolic truncation scheme and the final sparse basis is determined using least angle regression. Comparisons between the meta-model errors are carried out for experimental designs of varying sizes drawn with Sobol sequences and Latin hypercube sampling.

The organization of the paper is as follows: In Section 2, we present the mathematical setup of non-intrusive meta-modeling and describe corresponding error measures. Sections 3 and 4 respectively describe the sparse PCE and canonical LRA approaches. After investigating open questions in the construction of LRA in Section 5, we confront the two types of polynomial meta-models in Section 6. The paper concludes with a summary of the main findings and respective outlooks in Section 7.

2. Non-intrusive meta-modeling

2.1. Mathematical setup

We consider a physical or engineering system whose behavior is represented by a computational model $\mathcal{M}$. Let $\boldsymbol{X} = \{X_1, \ldots, X_M\}$ and $\boldsymbol{Y} = \{Y_1, \ldots, Y_N\}$ respectively denote the M-dimensional input vector and the N-dimensional response vector of the model. In order to account for the uncertainty in the input and the resulting uncertainty in the response, the elements of $\boldsymbol{X}$ and $\boldsymbol{Y}$ are described by random variables. For the sake of simplicity, we hereafter restrain our analysis to the