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Basis adaptation in homogeneous chaos spaces

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A B S T R A C T

We present a new method for the characterization of subspaces associated with low-dimensional quantities of interest (QoI). The probability density function of these QoI is found to be concentrated around one-dimensional subspaces for which we develop projection operators. Our approach builds on the properties of Gaussian Hilbert spaces and associated tensor product spaces.

1. Introduction

The curse of dimensionality is a significant challenge that remains at the forefront of scientific computing. We address it in the present paper by recognizing the low-dimensional structure of many quantities of interest (QoI) even in problems that have been embedded, via parameterization, in very high-dimensional settings. We take advantage of the geometric structure associated with the parameterization to discover very low-dimensional structure around which the probabilistic content of the QoI is concentrated. Our methodology is uniquely suited for the limiting situation when the QoI is a scalar functional of a high-dimensional stochastic process, in which case massive reduction is achieved.

Recent advances in sensing technologies have enabled querying the natural world with resolutions that continue to shed new light on many physical processes that underlie phase transformation and other instabilities. The mathematical formulation of these problems typically involves systems of coupled equations parameterized with stochastic processes that attempt to capture the effect of unmodeled features on the state variables. This stochastic parameterization naturally embeds the problem in a high-dimensional parameter space where methods of white-noise calculus have recently been adapted to characterizing and estimating the solution of these equations [1–3]. While this setting served to develop general insight into the significance of the stochastic component on the predictability of associated physical processes, it continues to present challenges when dealing with realistic problems that involve very high-dimensional parameterizations. The difficulty is associated with the observation that, in addition to the fine spatio-temporal discretization required to resolve underlying physical phenomena, resolving the dependence in parameter space increases the number of degrees of freedom exponentially with the number of parameters involved. Some attempts have been made in recent years to address this problem by pursuing sparse [4–6] or multilevel [7] representations that have succeeded in reducing the computational effort by an order of magnitude. Given the exponential growth with dimension, however, the residual effort remains often prohibitive.

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This complexity is inherited from the mathematical construction used to describe the physical processes involved, and often belies the simplicity of many quantities of interest (QoI) upon which decisions are eventually based. These QoI's have typically slow dependence on the parameters and pertain to a small number of functionals of the solution. Thus while describing the full solution field as a high-dimensional mathematical object may seem conceptually reasonable, a similar characterization of inherently low-dimensional quantities seems like an overkill and begs for a rational reduction. The Mori–Zwanzig formalism [9,8], already elucidated by Hertz [10], addresses this issue for general dynamical systems, through suitable Hilbert space projections, yielding a generalized Langevin equation for macroscopic observables. This procedure has provided sound foundation for various upscaling methods [11–13], but is designed for systems whose full-scale model is driven by an external random forcing. A recent adaptation of the Mori–Zwanzig formalism to parametric uncertainty [14] has developed reduced equations for a subset of the full observables considered as coarse scale variables. Cumulants expansions have also been adapted to sifting through high-dimensional parameterizations using rearrangements and cluster expansions [15,16]. These expansions provide expressions of certain averages of random processes in terms of cumulants of the process. They are robust when applied to certain functionals of the random process, but would be unwieldy to generalize to other quantities of interest. Equation-free and projective integration approaches [17] present a useful methodology for tackling these problems when the functional dependence of the QoI on the parameterization of the original problem is not significant to the QoI. Sobol decompositions [18] have also been considered as a mechanism for the reduction of complex maps. They represent functions of several variables into the sum of functions of lower dimensions in the original variables, with the objective of discovering sufficiently accurate low-dimensional representations. These expansions, also known as HDMR and ANOVA-HDMR [19–22] have been used to rank the input variables relative to their contribution to the variance of the output variables. One challenge with such expansions is that nonlinear functions of the input variables are not invariants to linear transformations on these variables. This has limited the scope of parameter ranking to subsets of the initial variables. In this paper we develop a procedure that identifies dominant effects in the form of linear combinations of input variables, and demonstrate the construction of accurate sparse L_2 representations of the output in terms of these new dimensions. By capitalizing on the mathematical structure of Gaussian Hilbert spaces and the associated Homogeneous Chaos space obtained from them through a tensor product construction, we obtain a reduced model that, while capturing the probabilistic content of the QoI, maintains its functional dependence on the original parameterization. This can be important for carrying out deterministic and stochastic sensitivity analyses and worth of information studies. The approach hinges on Gaussian parameterization of the problem. This does not signify that the parameters in the problem are assumed to be Gaussian, but rather that they are functions of some underlying Gaussian variables or processes. In a first step, an isometry is applied to an underlying Gaussian variables to induce a particular desired structure in the representation of the solution. In a second step, a reduction through projection of the resulting representation is carried out that has a probabilistic interpretation, thus providing further justification for the algebraic manipulations. The methodology is demonstrated on an algebraic problem, a problem associated with an elliptic equation from elasticity with stochastic coefficients, and a problem associated with 1-dimensional stochastic diffusion.

2. Polynomial chaos decomposition

Consider an experiment described by the probability triple $(\Omega, \mathcal{F}, P)$ and $\boldsymbol{\xi} = (\xi_1, \ldots, \xi_d)$ a set of independent Gaussian random variables on Ω. Let H denote the Gaussian space spanned by $\boldsymbol{\xi}$ and $\mathcal{F}(H)$ the σ-algebra generated by H. For notational simplicity, let $L_2(\Omega)$ be a shorthand for $L_2(\Omega, \mathcal{F}(H), P)$. Denote by $H^{:n:}$ the space of d-dimensional polynomials in $\boldsymbol{\xi}$ of exact degree n. When generated by Gaussian variables, $H^{:n:}$ is also referred to as the Homogeneous Chaos of order n. Then it can be shown that $L_2(\Omega) = \bigoplus_n H^{:n:}$ [23]. Given this construction, any basis in H induces a corresponding basis in $H^{:n:}$ and $L_2(\Omega)$. The main contribution of this paper is to adapt the Hilbertian basis in $L_2(\Omega)$ by a judicious basis transformation in the underlying Gaussian space H. Introducing the multi-index $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_d)$, then each $H^{:n:}$ is spanned by $\{h_{\boldsymbol{\alpha}},\ |\boldsymbol{\alpha}| = n\}$, the set of multivariate Hermite polynomials of order n. We introduce a normalization of these polynomials

$$\psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi}) = H_{\boldsymbol{\alpha}}(\boldsymbol{\xi})/\sqrt{\boldsymbol{\alpha}!}, \qquad \|H_{\boldsymbol{\alpha}}\|^2_{L_2(\Omega)} = \boldsymbol{\alpha}!, \tag{1}$$

and consider $q : R^d \mapsto R$ such that $\int_{R^d} (q(\boldsymbol{x}))^2 e^{-\frac{1}{2}\boldsymbol{x}^T \boldsymbol{x}}\, d\boldsymbol{x} < \infty$. Then $q \in L_2(\Omega)$ and can be represented in a Polynomial Chaos decomposition of the form [1]

$$q^p(\boldsymbol{\xi}) = \sum_{|\boldsymbol{\alpha}| \leqslant p} q_{\boldsymbol{\alpha}} \psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi}), \tag{2}$$

where $\lim_{p\to\infty} q^p(\boldsymbol{\xi}) = q(\boldsymbol{\xi})$ in the $L_2(\Omega)$ norm. In the above, $|\boldsymbol{\alpha}| = \sum_{i=1}^d \alpha_i$ and $\boldsymbol{\alpha}! = \prod_{i=1}^d \alpha_i!$.

In order to guide our basis adaptation process, we next introduce a few sets of multi-indices. Denote by $\mathcal{I}_p$ the set of all d-dimensional multi-indices of degree less than or equal to p, by $\mathcal{E}_i$ the subset of $\mathcal{I}_p$ corresponding to non-zero indices only at the ith location, and let $\mathcal{E} = \bigcup_{i=1}^d \mathcal{E}_i$. Also let $\mathcal{E}_{ij}$ $(i \neq j)$ denote the subset of $\mathcal{I}_p$ with zeros except at locations i and j. Moreover, let $\boldsymbol{e}_i$ and $\boldsymbol{e}_{ij}$ denote the unit vectors in $\mathcal{E}_i$ and $\mathcal{E}_{ij}$, respectively, where the non-zero entries are equal to 1.