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SPARSE POLYNOMIAL SURROGATES FOR UNCERTAINTY QUANTIFICATION IN COMPUTATIONAL FLUID DYNAMICS

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Abstract. This paper is concerned with the construction of polynomial surrogates of complex models typically arising in computational fluid dynamics for the purpose of propagating uncertainties pertaining to geometrical and/or operational parameters. Polynomial chaos expansions are considered and different techniques for the intrusive and non intrusive reconstruction of the polynomial expansion coefficients are outlined. A sparsity-based reconstruction approach is more particularly emphasized since it benefits from the "sparsity-of-effects" trend commonly observed on global quantities of interest such as the aerodynamic coefficients of a profile.

Keywords: Computational fluid dynamics, polynomial chaos, stochastic Galerkin method, stochastic collocation method, compressed sensing.

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§1. Introduction

The polynomial chaos or Wiener-Hermite expansion consists in the decomposition of a second-order random variable in a series of multivariate Hermite polynomials in a countable sequence of independent Gaussian random variables [3, 22]. Specifically, truncations of such an expansion are considered as approximations of random vectors, tensors or fields for the purpose of quantifying uncertainties in complex models. They have been intensively used in recent years in computational methods for solving ordinary or partial differential equations with poorly known, indeed random data or parameterized by Gaussian random parameters. As the solutions of these equations are stochastic processes indexed by spatial and/or time coordinates, which are typically second-order random fields from physical considerations (they have finite energy), polynomial chaos expansions are used to approximate them along the stochastic dimension. Mean-square convergence is guaranteed by the Cameron-Martin theorem [3] and is optimal (*i.e.* exponential) for Gaussian probability measures. For random fields parameterized by non Gaussian, arbitrary random variables the numerical study in [24] has shown that the convergence rates of Hermite polynomial chaos are not optimal. This observation has prompted the development of generalized polynomial chaos expansions involving other families of polynomials which are orthogonal with respect to the probability measures of the random parameters [9, 24]. Optimal convergence rates can be achieved once this substitution has been done.

The earlier approach of using polynomial chaos to numerically solve differential equations proposed truncated expansions as trial functions in a Galerkin formulation, resulting

in the spectral stochastic finite element method, or stochastic Galerkin method [20] subsequently developed in [10, 13]. More precisely, the chaos expansions of the sought solutions are substituted in the model equations, which in turn yield evolution equations for their expansion coefficients from Galerkin projections using the orthogonal polynomials as test functions. The stochastic Galerkin method is intrusive in that it may require significant alterations of the existing deterministic codes utilized for solving the differential equations of interest. Generally it also yields coupled equations for the expansion coefficients. This situation has prompted the development of non intrusive approaches, which require only repetitive executions of existing deterministic codes. Stochastic collocation and regression methods [2, 14, 23] have become widely popular in computational fluid dynamics (CFD), for the applicability and precision of these uncertainty quantification techniques is not affected by the complexity and high nonlinearity of the existing flow solvers so long as they achieve a reasonable accuracy. Complex aerodynamic analysis and design of aircraft make use of such high-fidelity CFD tools for shape optimization for example, whereby some robustness is achieved by considering uncertain operational, environmental, or manufacturing parameters represented by random variables.

Both the intrusive and non intrusive approaches yield polynomial representations of the solution processes, known as surrogate models or response surfaces in the space of random parameters. They approximate the original stochastic processes solving the differential equations of interest accurately (in the mean-square sense), while being many orders faster to evaluate. One can thus consider these surrogates to compute the probability measures, moments, and/or sensitivities of the solutions or output quantities of interest related to them such as integrals, supremum norms, *etc*. The robust and most popular way to quantify uncertainties is Monte-Carlo estimation, but it may become intractable for complex models in which a simulation for one single value of the parameters may take several hours or days and a large number of model outputs have to be evaluated. Polynomial chaos is essentially a spectral representation in the random space, which typically exhibits fast convergence when the expended processes depend smoothly on the random parameters. Exponentially fast convergence can even be achieved under certain circumstances [24]. This rest of the paper is organized as follows. In section 2 we formulate our problem and introduce the probabilistic framework, focusing on the polynomial chaos expansion methodology. The actual methods for computing the polynomial chaos expansion coefficients are outlined in section 3. Here we also briefly review how these polynomial surrogates are used for uncertainty quantification. In the last section 4 we discuss the different approaches for their implementation in computational fluid dynamics with applications in aerodynamics and aeroelasticity, where complex configurations have been considered in recent works. We more particularly stress the "sparsity-of-effects" trend observed there that favors regression techniques benefitting from the sparsity of the output quantities of interest, such as compressed sensing.

§2. Problem setup

2.1. Model equations

Let $\mathcal{D} \subset \mathbb{R}^3$ be a fixed domain with a boundary $\partial\mathcal{D}$ and $\mathbf{x} \in \mathcal{D}$ the physical coordinates. Let $(\Omega, \mathcal{A}, \mathcal{P})$ be a probability space where Ω is the abstract set of elementary events, $\mathcal{A}$ is a σ-

algebra of subsets of Ω, and $\mathcal{P}$ is a probability measure on $\mathcal{A}$. Our aim is to approximate the random field $u(\mathbf{x};\boldsymbol{\xi}) : \mathcal{D}\times\Gamma \to \mathbb{R}^m$ satisfying the parameterized partial differential equations:

$$\begin{aligned} \mathcal{L}(\mathbf{x},\boldsymbol{\xi};u) &= 0 \quad \text{in } \mathcal{D}\,, \\ \mathcal{B}(\mathbf{x},\boldsymbol{\xi};u) &= 0 \quad \text{on } \partial\mathcal{D}\,, \end{aligned} \tag{1}$$

where $\mathcal{L}$ is a linear or non linear differential operator and $\mathcal{B}$ is a boundary operator. Here $\boldsymbol{\xi}(\omega) = (\xi_1(\omega), \xi_2(\omega), \ldots, \xi_d(\omega)) : \Omega \to \Gamma \subseteq \mathbb{R}^d$ is a vector of d random parameters defined on $(\Omega, \mathcal{A}, \mathcal{P})$ with probability distribution $\mathcal{P}_{\boldsymbol{\Xi}}$, of which components $\xi_1, \xi_2, \ldots, \xi_d$ are mutually independent random variables with values in subsets of $\mathbb{R}$, $\Gamma_1, \Gamma_2, \ldots \Gamma_d$ respectively. We consider without loss of generality that the random field u has scalar values, *i.e.* $m = 1$. In practice one may also be interested in quantities:

$$y = F(u(\cdot;\boldsymbol{\xi}))\,, \tag{2}$$

that are functions of the solution u of the boundary value problem (1), in addition to the solution itself. In CFD for instance, u may be the pressure field satisfying the compressible Navier-Stokes equations about a fixed profile, and y may be the aerodynamic forces (*e.g.* drag, lift) exerted by the flow on that profile. In this latter case, the differential operator $\mathcal{L}$ may also depend on time t, and the boundary value problem (1) needs be supplemented with initial conditions. We do not consider that more general situation in the following discussion, for its main features basically extend to time-dependent problems.

2.2. Probabilistic framework

The vector of random parameters $\boldsymbol{\xi}$ is representative of variable geometrical characteristics, boundary conditions, loads, physical or mechanical properties, or combinations of them. It can be discrete, continuous, or a combination of both. In the continuous case, it is understood that its probability distribution $\mathcal{P}_{\boldsymbol{\Xi}}$ admits a probability density function $\boldsymbol{\xi} \mapsto W_{\boldsymbol{\Xi}}(\boldsymbol{\xi})$ with values in $\mathbb{R}_+ = [0, +\infty[$ such that $\mathcal{P}_{\boldsymbol{\Xi}}(B) = \int_B W_{\boldsymbol{\Xi}}(\boldsymbol{\xi}) d\boldsymbol{\xi}$ for any subset B of $\mathbb{R}^d$. In addition, $\mathcal{P}_{\boldsymbol{\Xi}}(d\boldsymbol{\xi}) = \mathcal{P}_1(d\xi_1)\times\mathcal{P}_2(d\xi_2)\times\cdots\times\mathcal{P}_d(d\xi_d)$ owing to the assumption of mutual independence. In the present setting, it is further assumed that the random parameters are exponentially integrable, that is there exists $\beta > 0$ such that:

$$\mathbb{E}\{\mathrm{e}^{\beta\|\boldsymbol{\xi}\|}\} = \int_{\mathbb{R}^d} \mathrm{e}^{\beta\|\boldsymbol{\xi}\|} \mathcal{P}_{\boldsymbol{\Xi}}(d\boldsymbol{\xi}) < +\infty\,, \tag{3}$$

where $\|\boldsymbol{\xi}\| = (\sum_{n=1}^d \xi_n^2)^{\frac{1}{2}}$ is the usual Euclidean norm in $\mathbb{R}^d$, and $\mathbb{E}\{\cdot\}$ is mathematical expectation. Together with mutual independence, it ensures that each random variable ξ_n possesses finite moments of all orders, that is $\mathbb{E}\{|\xi_n|^k\} = \int_{\mathbb{R}} |\xi|^k \mathcal{P}_n(d\xi) < +\infty$ for all $k \in \mathbb{N}$. This uniquely defines a sequence of univariate orthonormal polynomials $\{\psi_j^{(n)}\}_{j\in\mathbb{N}}$ associated with the probability measure $\mathcal{P}_n$ for all $1 \le n \le d$, and a sequence of multivariate orthonormal polynomials $\{\psi_{\mathbf{j}}\}_{\mathbf{j}\in\mathbb{N}^d}$ associated with the probability measure $\mathcal{P}_{\boldsymbol{\Xi}}$ given by:

$$\psi_{\mathbf{j}}(\boldsymbol{\xi}) = \prod_{n=1}^{d} \psi_{j_n}^{(n)}(\xi_n)\,, \quad \mathbf{j} = (j_1, j_2, \ldots, j_d) \in \mathbb{N}^d\,, \tag{4}$$

such that $\{\psi_{\mathbf{j}}(\boldsymbol{\xi})\}_{\mathbf{j}\in\mathbb{N}^d}$ constitutes an orthonormal sequence of random variables in the space $L^2(\Omega,\sigma(\boldsymbol{\xi}),\mathcal{P})$ of second-order random variables defined on the probability space endowed with the σ-algebra $\sigma(\boldsymbol{\xi})$ generated by the random parameters $\boldsymbol{\xi}$; see [9, Theorem 3.6]. Alternatively, the polynomial set $\{\psi_{\mathbf{j}}\}_{\mathbf{j}\in\mathbb{N}^d}$ constitutes an orthonormal basis of the functional space $L^2(\mathbb{R}^d,\sigma_B(\mathbb{R}^d),\mathcal{P}_{\boldsymbol{\Xi}}(d\boldsymbol{\xi}))$ of square-integrable functions with respect to $\mathcal{P}_{\boldsymbol{\Xi}}$, where $\sigma_B(\mathbb{R}^d)$ is the Borel σ-algebra on $\mathbb{R}^d$.

Consequently, any random variable u in $L^2(\Omega,\sigma(\boldsymbol{\xi}),\mathcal{P})$ can be expanded in a series of multivariate orthonormal polynomials in the random parameters $\boldsymbol{\xi}$ as:

$$u=\sum_{\mathbf{j}\in\mathbb{N}^d} u_{\mathbf{j}}\psi_{\mathbf{j}}(\boldsymbol{\xi})\,,\quad u_{\mathbf{j}}=\mathbb{E}\{u\psi_{\mathbf{j}}(\boldsymbol{\xi})\}=\int_{\mathbb{R}^d} u\psi_{\mathbf{j}}(\boldsymbol{\xi})\mathcal{P}_{\boldsymbol{\Xi}}(d\boldsymbol{\xi})\,. \tag{5}$$

This is the so-called generalized polynomial chaos expansion. Likewise, the random field $\mathbf{x}\mapsto u(\mathbf{x};\boldsymbol{\xi})$ satisfying (1) has finite energy from physical considerations, so it belongs to $L^2(\mathbb{R}^d,\sigma_B(\mathbb{R}^d),\mathcal{P}_{\boldsymbol{\Xi}}(d\boldsymbol{\xi}))$ and can be expanded as:

$$u(\mathbf{x};\boldsymbol{\xi})=\sum_{\mathbf{j}\in\mathbb{N}^d} u_{\mathbf{j}}(\mathbf{x})\psi_{\mathbf{j}}(\boldsymbol{\xi})\,,\quad u_{\mathbf{j}}(\mathbf{x})=\mathbb{E}\{u(\mathbf{x};\boldsymbol{\xi})\psi_{\mathbf{j}}(\boldsymbol{\xi})\}=\int_{\mathbb{R}^d} u(\mathbf{x};\boldsymbol{\xi})\psi_{\mathbf{j}}(\boldsymbol{\xi})\mathcal{P}_{\boldsymbol{\Xi}}(d\boldsymbol{\xi})\,. \tag{6}$$

In practical numerical applications the foregoing expansions are truncated up to a total order p such that $|\mathbf{j}|=j_1+j_2+\cdots+j_d\le p$. Denoting by $\mathbb{P}^p[\cdot]$ the orthogonal projection onto the space of d-variate polynomials of total degree p in $\xi_1,\xi_2,\ldots,\xi_d$, say V_d^p, we seek for an approximate solution $\mathbb{P}^p[u]$ of (1) in V_d^p as:

$$u(\mathbf{x};\boldsymbol{\xi})\simeq\mathbb{P}^p[u](\mathbf{x};\boldsymbol{\xi})=\sum_{|\mathbf{j}|\le p} u_{\mathbf{j}}(\mathbf{x})\psi_{\mathbf{j}}(\boldsymbol{\xi})=\sum_{j=0}^{P-1} u_j(\mathbf{x})\psi_j(\boldsymbol{\xi})\,,\quad P=\binom{p+d}{d}, \tag{7}$$

by reordering the P multi-indices $\mathbf{j}$ such that $|\mathbf{j}|\le p$. From [9, Theorem 2.2], the sequence $\mathbb{P}^p[u]$ converges to u in the mean-square sense in $L^2(\Omega,\sigma(\boldsymbol{\xi}),\mathcal{P})$ as $p\to+\infty$ provided that the condition (3) is fulfilled.

Now the deterministic functional coefficients $\mathbf{x}\mapsto u_j(\mathbf{x})$ in the truncated series remain unknown since the random field u is unknown. Collocational or weighted versions of (1) together with the above approximation are considered in order to determine them.

§3. Construction of the polynomial chaos expansion

The different methods considered for computing the polynomial expansion coefficients are quoted as intrusive or non intrusive in the mechanical engineering literature. The stochastic Galerkin method is intrusive in that it may require significant alterations of the existing deterministic codes utilized for solving numerically the boundary value problem (1). Generally it also yields coupled equations for the expansion coefficients of its solution. Hence new codes need be developed to handle the larger and coupled systems of equations arising from the Galerkin formulation. The stochastic collocation and regression methods are non intrusive in that they require only repetitive executions of the existing deterministic codes for carefully selected parameter sets. They are the preferred methodologies in CFD, for their applicability is not affected by the complexity and high nonlinearity of the existing flow solvers.

3.1. Stochastic Galerkin method

Similarly to the weak formulation of deterministic problems, on can form the weak form of (1) and seek an approximate solution $u^p \in V_d^p$ such that:

$$\begin{aligned} &\mathbb{E}\{\mathcal{L}(\mathbf{x},\boldsymbol{\xi};u^p)v(\boldsymbol{\xi})\} = 0 \quad \forall v(\boldsymbol{\xi}) \in V_d^p\,, \mathbf{x} \in \mathcal{D}\,, \\ &\mathbb{E}\{\mathcal{B}(\mathbf{x},\boldsymbol{\xi};u^p)v(\boldsymbol{\xi})\} = 0 \quad \forall v(\boldsymbol{\xi}) \in V_d^p\,, \mathbf{x} \in \partial\mathcal{D}\,. \end{aligned} \tag{8}$$

The resulting system becomes a deterministic one in the physical domain $\mathcal{D}$ for the functional coefficients $u_j(\mathbf{x})$, and may be solved by standard discretization techniques *e.g.* finite elements, finite volumes, finite differences, boundary elements, *etc.*; see [13] and references therein for an extensive presentation of this method.

3.2. Stochastic collocation method

Alternatively, one may seek an approximate solution formed by interpolation between solutions of (1) for Q particular choices of the random parameters $\boldsymbol{\xi}$, namely the sampling set $\{\boldsymbol{\xi}^l\}_{1\le l\le Q}$ of so-called nodes, such that:

$$\begin{aligned} &\mathcal{L}(\mathbf{x},\boldsymbol{\xi}^l;u(\mathbf{x};\boldsymbol{\xi}^l)) = 0 \quad \forall l = 1,2,\ldots,Q\,, \mathbf{x} \in \mathcal{D}\,, \\ &\mathcal{B}(\mathbf{x},\boldsymbol{\xi}^l;u(\mathbf{x};\boldsymbol{\xi}^l)) = 0 \quad \forall l = 1,2,\ldots,Q\,, \mathbf{x} \in \partial\mathcal{D}\,. \end{aligned} \tag{9}$$

Then the approximate solution $\mathbb{I}^Q[u]$ to (1) reads as the Lagrange interpolation [14, 23]:

$$u(\mathbf{x};\boldsymbol{\xi}) \simeq \mathbb{I}^Q[u](\mathbf{x};\boldsymbol{\xi}) = \sum_{l=1}^{Q} u(\mathbf{x};\boldsymbol{\xi}^l) L_l(\boldsymbol{\xi})\,, \tag{10}$$

where $\{L_l\}_{1\le l\le Q}$ is the set of d-variate Lagrange polynomials based on the nodes $\{\boldsymbol{\xi}^l\}_{1\le l\le Q}$ chosen so that uniqueness of the interpolation is ensured.

3.2.1. Link with polynomial chaos

Choosing the nodes within a quadrature rule $\boldsymbol{\Theta}(d,Q) = \{\boldsymbol{\xi}^l, w^l\}_{1\le l\le Q}$ tailored such that $\sum_{l=1}^{Q} w^l f(\boldsymbol{\xi}^l)$ is a good approximation of the d-dimensional integral $\int_{\mathbb{R}^d} f(\boldsymbol{\xi})\mathcal{P}_{\boldsymbol{\Xi}}(d\boldsymbol{\xi}) = \mathbb{E}\{f(\boldsymbol{\xi})\}$ for sufficiently smooth functions f, the collocation approach may be considered to compute an approximate solution $\mathbb{P}_Q^p[u]$ defined by:

$$\begin{aligned} \mathbb{P}_Q^p[u](\mathbf{x};\boldsymbol{\xi}) &= \sum_{j=0}^{P-1}\left(\sum_{l=1}^{Q} w^l u(\mathbf{x};\boldsymbol{\xi}^l)\psi_j(\boldsymbol{\xi}^l)\right)\psi_j(\boldsymbol{\xi}) = \sum_{l=1}^{Q} u(\mathbf{x};\boldsymbol{\xi}^l)\left(w^l\sum_{j=0}^{P}\psi_j(\boldsymbol{\xi}^l)\psi_j(\boldsymbol{\xi})\right) \\ &= \sum_{l=1}^{Q} u(\mathbf{x};\boldsymbol{\xi}^l)\tilde{L}_l(\boldsymbol{\xi}) \end{aligned} \tag{11}$$

in view of (7); that is, the quadrature set $\boldsymbol{\Theta}(d,Q)$ is used to evaluate the coefficients $u_j(\mathbf{x})$ in (7). Provided that the quadrature rule $\boldsymbol{\Theta}(d,Q)$ integrates exactly all d-variate polynomials of total order $2p$ and $L_l \in V_d^p$, one has $\tilde{L}_l \equiv L_l$ owing to the orthonormalization of the polynomials $\{\psi_j\}_{0\le j\le P-1}$ which are such that $\mathbb{E}\{\psi_j(\boldsymbol{\xi})\psi_k(\boldsymbol{\xi})\} = \delta_{jk}$, the Kronecker symbol.

3.2.2. Choices of nodal set

The key issue of stochastic collocation is the selection of appropriate sampling sets. A straightforward choice is quadrature nodes and weights as in (11). Multi-dimensional quadrature sets $\boldsymbol{\Theta}(d,Q)=\{\boldsymbol{\xi}^l,w^l\}_{1\leq l\leq Q}$, where $\boldsymbol{\xi}^l$ is the l-th node in $\Gamma=\prod_{n=1}^d\Gamma_n$ and w^l is the corresponding weight, may be constructed from one-dimensional (univariate) quadrature sets by full tensorization or sparse tensorization, following Smolyak's algorithm [18].

Univariate Gauss quadratures $\Theta(1,q_1)$ based on q_1 integration points are tailored to integrate a smooth function $\xi\mapsto f(\xi)$ on $\Gamma_1\equiv[a,b]$ by:

$$\int_{\Gamma_1}f(\xi)W_\Xi(\xi)d\xi\simeq\sum_{l=1}^{q_1-r}w^l f(\xi^l)+\sum_{m=1}^{r}w^{q_1-r+m}f(\xi^{q_1-r+m})\,, \tag{12}$$

such that this rule turns to be exact for univariate polynomials up to the order $2q_1-1-r$. Here r is the number of fixed nodes of the rule, typically the bounds a,b. Depending on the choice of r, different terminologies are used:

- $r=0$ is the classical Gauss rule;
- $r=1$ is the Gauss-Radau rule, choosing $\xi^{q_1}=a$ or $\xi^{q_1}=b$ for instance;
- $r=2$ is the Gauss-Lobatto (GL) rule, choosing $\xi^{q_1-1}=a$ and $\xi^{q_1}=b$ for instance.

Multivariate quadratures may subsequently be obtained by full or sparse tensorization of these one-dimensional rules. Firstly, a fully tensorized grid is obtained by the product rule:

$$\boldsymbol{\Theta}(d,Q)=\bigotimes_{n=1}^{d}\Theta(1,q_n)\,, \tag{13}$$

which contains $Q=\prod_{n=1}^d q_n$ grid points in Γ. Secondly, a sparse quadrature rule can be derived thank to the Smolyak algorithm [18]. The so-called k-th level, d-dimensional Smolyak sparse grid $\widehat{\boldsymbol{\Theta}}(d,k)$ is obtained by the following linear combination of product formulas:

$$\widehat{\boldsymbol{\Theta}}(d,k)=\bigcup_{k+1\leq q_1+\cdots+q_d\leq k+d}\Theta(1,q_1)\otimes\cdots\otimes\Theta(1,q_d)\,. \tag{14}$$

Clearly, the above sparse grid is a subset of the full tensor product grids. It typically contains $Q\sim(2d)^k/k!$ nodes in Γ whenever $d\gg1$ and k is fixed. By a direct extension of the arguments divised in [15], it can be shown that provided the univariate quadrature rules $\Theta(1,q)$ are exact for all univariate polynomials of order up to $2q-1$ (Gauss rules) or $2q-3$ (GL rules), the foregoing rule is exact for all d-variate polynomials of at least total order up to $2k-1$ or $2k-3$, respectively. In [17] it has been observed that sparse quadratures outperform tensorized quadratures with non-nested underlying one-dimensional rules whenever $d\geq4$, though. If $\Theta(1,q_i)$ is now Clenshaw-Curtis univariate quadrature of i-th level for $i>1$, such that:

$$\xi^l=-\cos\frac{(l-1)\pi}{q_i-1}\,,\quad 1\leq l\leq q_i=2^{i-1}+1\,,$$

then $\Theta(1,q_i)\subset\Theta(1,q_{i+1})$, that is the univariate Clenshaw-Curtis rules $\Theta(1,q_i)$ are nested. Consequently the multivariate rules are nested as well, $\widehat{\boldsymbol{\Theta}}(d,k)\subset\widehat{\boldsymbol{\Theta}}(d,k+1)$. The total number of nodes is significantly reduced compared to non nested rules. Nested Clenshaw-Curtis rules are however exact for all multivariate polynomials of at least total order k [1].

3.3. Regression methods

In regression approaches, the P expansion coefficients in (7) are determined on the basis of a set of observations $\{u(\cdot;\boldsymbol{\xi}^l\}_{1\leq l\leq Q}$, obtained by computations or measurements, of the random variable or field u for some particular choices of the random parameters $\boldsymbol{\xi}$, again the sampling set $\{\boldsymbol{\xi}^l\}_{1\leq l\leq Q}$. They consist in solving a weighted least-squares minimization problem:

$$\mathbf{U} \simeq \mathbf{U}^\star = \arg\min_{\mathbf{V}\in\mathbb{R}^P} \frac{1}{2}\,(\mathbf{y}-\boldsymbol{\Phi}\mathbf{V})^\mathsf{T}\,\mathbf{W}\,(\mathbf{y}-\boldsymbol{\Phi}\mathbf{V})\;, \tag{15}$$

where $\mathbf{y} = (u(\cdot;\boldsymbol{\xi}^1), u(\cdot;\boldsymbol{\xi}^2), \ldots, u(\cdot;\boldsymbol{\xi}^Q))^\mathsf{T}$ is the vector of observations, $[\boldsymbol{\Phi}]_{lj} = \psi_j(\boldsymbol{\xi}^l)$ is the so-called $Q\times P$ measurement matrix, $\mathbf{W}$ is a $Q\times Q$ weighting matrix, and $\mathbf{U} = (u_0, u_1, \ldots, u_{P-1})^\mathsf{T}$ is the sought vector of coefficients. This is the approach retained in *e.g.* [2], for which numerous methods are available to solve this optimization problem whenever $Q \geq P$. Alternatively, one may consider the situation whereby $Q < P$ and more particularly $Q \ll P$, that is, underdetermined systems. This can be achieved thanks to some recent results pertaining to the resolution of under-sampled linear systems promoting sparsity of the sought solution, known as compressed sensing or compressive sampling [4, 8]. A review of the application of this approach to generalized polynomial chaos expansions is proposed in [11]; see also [12, 17] for applications in aerodynamics and aeroelasticity. The compressed sensing approach consists in reformulating the least-squares minimization problem (15) as a convex minimization problem with some sparsity constraint, namely:

$$\mathbf{U} \simeq \mathbf{U}^\star = \arg\min_{\mathbf{V}\in\mathbb{R}^P} \{\|\mathbf{V}\|_1\;;\; \|\mathbf{y}-\boldsymbol{\Phi}\mathbf{V}\|_2 \leq \varepsilon\}\;, \tag{16}$$

for some tolerance $0 \leq \varepsilon \ll 1$ on the polynomial chaos truncation (7). Here the ℓ_m-norm is $\|\mathbf{a}\|_m = (\sum_{j=0}^{P-1} \left|a_j\right|^m)^{\frac{1}{m}}$ for $m > 0$, and $\|\mathbf{a}\|_0 = \#\{j;\, a_j \neq 0\}$ otherwise. Sparsity means that only a small fraction of the sought coefficients $\mathbf{U}$ are non negligible. The latter problem is known as basis pursuit denoising [6]. It is uniquely solvable thanks to some *ad hoc* mixing properties of the measurement matrix $\boldsymbol{\Phi}$.

One of them is the restricted isometry property (RIP) or uniform uncertainty principle. For each integer $S \in \mathbb{N}^*$, the isometry constant δ_S of $\boldsymbol{\Phi}$ is defined as the smallest number such that:

$$(1-\delta_S)\,\|\mathbf{U}_S\|_2^2 \leq \|\boldsymbol{\Phi}\mathbf{U}_S\|_2^2 \leq (1+\delta_S)\,\|\mathbf{U}_S\|_2^2$$

for all S-sparse vectors $\mathbf{U}_S \in \{\mathbf{V}\in\mathbb{R}^P;\; \|\mathbf{V}\|_0 \leq S\}$. Then $\boldsymbol{\Phi}$ is said to satisfy the RIP of order S if, say, δ_S is not too close to 1. This property amounts to saying that all S-column submatrices of $\boldsymbol{\Phi}$ are numerically well-conditioned, or S (or less) columns selected arbitrarily in $\boldsymbol{\Phi}$ are nearly orthogonal. Consequently, they form a near isometry so that $\boldsymbol{\Phi}$ approximately preserves the Euclidean norm of S-sparse vectors. The following theorem by Candès *et al.* [4, 5] then states that (16) can be solved efficiently:

Theorem 1. *Assume $\delta_{2S} < \sqrt{2}-1$. Then the solution $\mathbf{U}^\star$ to (16) satisfies:*

$$\left\|\mathbf{U}^\star - \mathbf{U}\right\|_2 \leq C_0\,\frac{\|\mathbf{U}_S - \mathbf{U}\|_1}{\sqrt{S}} + C_1\varepsilon$$

for some $C_0, C_1 > 0$ depending only on δ_{2S}. Here $\mathbf{U}_S$ is $\mathbf{U}$ with all but the S largest entries set to zero.

This result calls for several comments. First, the coefficients $\mathbf{U}$ are actually nearly sparse, rather than strictly sparse, in the sense that only a small fraction of them contribute significantly to the output statistics while the others are not strictly null. Opportunely, the foregoing theorem deals with all signals and not only the S-sparse ones. In addition, it also allows noiseless recovery if $\varepsilon = 0$. Second, it is deterministic and does not involve any probability for a successful recovery. Lastly, the ℓ_1-minimization strategy is non adapted because it identifies the sparsity pattern, that is the order (location) of the negligible coefficients in the polynomial chaos basis, and the leading coefficients at the same time. The algorithm can therefore efficiently capture the relevant information of a sparse vector without trying to comprehend that vector [5]. This is clearly a much desirable feature for practical industrial applications. Additionally, the RIP prompts the use of unstructured observation sets $\{\boldsymbol{\xi}^l\}_{1\leq l\leq Q}$, typically selected randomly, for an efficient recovery by basis pursuit. Structured sets may also be considered, though, as proposed in [21].

3.4. Application to uncertainty quantification

Once the polynomial expansion (7) has been derived, the first moments and/or cumulants of the random field u can be computed with this expansion. Owing to the orthonormality of the polynomials, the mean and variance for example are:

$$\mu(\mathbf{x}) = \mathbb{E}\{u(\mathbf{x};\boldsymbol{\xi})\} = u_0(\mathbf{x})\,, \quad \sigma^2(\mathbf{x}) = \mathbb{E}\{(u(\mathbf{x};\boldsymbol{\xi}) - \mu(\mathbf{x}))^2\} = \sum_{j=1}^{P-1} u_j^2(\mathbf{x})\,.$$

Sensitivity indices may be computed alike [19]. They quantify the fraction of variance of the solution u which can be related to the variation of each random parameter. Denoting by $\mathcal{J}_n$ the set of indices corresponding to the polynomials depending only on the n-th variable parameter ξ_n, the main-effect Sobol' indices are given by:

$$\mathcal{S}_n(\mathbf{x}) = \frac{\operatorname{Var}\mathbb{E}\{u(\mathbf{x};\boldsymbol{\xi})|\xi_n\}}{\operatorname{Var}u(\mathbf{x};\boldsymbol{\xi})} = \frac{1}{\sigma^2(\mathbf{x})}\sum_{j\in\mathcal{J}_n} u_j^2(\mathbf{x})\,. \tag{17}$$

More generally, if $\mathcal{J}_{n_1 n_2 \ldots n_s}$ is the set of indices corresponding to the polynomials depending only on the parameters $\xi_{n_1}, \xi_{n_2}, \ldots \xi_{n_s}$, the s-fold joint sensitivity indices are:

$$\mathcal{S}_{n_1 n_2 \ldots n_s}(\mathbf{x}) = \frac{\operatorname{Var}\mathbb{E}\{u(\mathbf{x};\boldsymbol{\xi})|\xi_{n_1}, \xi_{n_2}, \ldots \xi_{n_s}\}}{\operatorname{Var}u(\mathbf{x};\boldsymbol{\xi})} = \frac{1}{\sigma^2(\mathbf{x})}\sum_{j\in\mathcal{J}_{n_1 n_2 \ldots n_s}} u_j^2(\mathbf{x})\,.$$

§4. Discussion

Because of the high complexity of fluid flow solvers, non intrusive uncertainty quantification techniques have been primarily developed in aerodynamic and aeroelastic simulations. They are used to compute the sensitivities of output quantities of interest that are required to evaluate the objective function of an optimization process, for example. Polynomial surrogate models have commonly been considered in this respect. In most applications the polynomial expansion coefficients are evaluated by Gauss quadratures (see section 3.2.2). However

this approach becomes computationally very demanding for parametric spaces of high dimensions, even if sparse rules are utilized: this is the so-called curse of dimensionality. Observing that the output quantities of interest of complex systems depend only weekly on the multiple cross-interactions between the variable inputs, one may argue that only low-order polynomials significantly contribute to their surrogates. This feature favors reconstruction techniques benefiting from such a sparse structure, as compressed sensing (see section 3.3). It should be noted that the "sparsity-of-effects" principle invoked here has already been outlined in [16]. It may be established rigorously for parameterized, possibly non linear elliptic-parabolic equations in the framework analyzed in [7]. The results obtained with aerodynamic and aeroelastic simulations involving complex fluid flows solved by Reynolds-averaged Navier-Stokes equations (RANS) with turbulence transport closure models corroborate to a large extend this expected trend. Such examples are described in [17] for the case of a two-dimensional rigid profile with random Mach number, angle-of-attack, and thickness-to-chord ratio; and in [12] for the case of a three-dimensional flexible wing-fuselage configuration with random Mach number, lift force, and wing structural stiffness. Efficient non-adapted polynomial reconstructions with sampling sets orders of magnitude smaller than the ones required by the usual techniques are achieved. The (global) quantities of interest considered in these applications are typically the drag force and pitching moment of the profiles, which integrate the (local) pressure fields along them.

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