Compressive sensing adaptation for polynomial chaos expansions

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Abstract

Basis adaptation in Homogeneous Chaos spaces rely on a suitable rotation of the underlying Gaussian germ. Several rotations have been proposed in the literature resulting in adaptations with different convergence properties. In this paper we present a new adaptation mechanism that builds on compressive sensing algorithms, resulting in a reduced polynomial chaos approximation with optimal sparsity. The developed adaptation algorithm consists of a two-step optimization procedure that computes the optimal coefficients and the input projection matrix of a low dimensional chaos expansion with respect to an optimally rotated basis. We demonstrate the attractive features of our algorithm through several numerical examples including the application on Large-Eddy Simulation (LES) calculations of turbulent combustion in a HIFiRE scramjet engine.

Keywords: Polynomial Chaos, basis adaptation, compressive sensing, $\ell_1$-minimization, dimensionality reduction, uncertainty propagation

1. Introduction

While the use of computer codes to represent complex physical phenomena has always been an integral part of uncertainty quantification (UQ), efforts toward adopting more realistic models often face computational challenges that must be overcome before meaningful quantitative analysis becomes possible. The need for a statistical exploration of the solution space is arguably the most pressing of these challenges, requiring repetitive simulation of the numerical code. The associated computational burden quickly becomes prohibitive, especially in the context of complex physical systems where each of these simulations is, by itself, already testing the limits of computational resources. In many important instances, the map from input random parameters to output quantities is highly nonlinear, limiting the value of standard statistical sampling techniques. In such cases, $L_2$-based formalisms, such as polynomial chaos (PC) expansions have shown promise\textsuperscript{[24, 35, 45, 37]}, though, by explicitly tracking each input stochastic parameter, they are subject to the curse of dimensionality\textsuperscript{[4]}. The latter is manifested by a factorial growth of the number of parameters and therefore result in an overwhelming increase of the numerical simulations required to systematically explore the parameter space. Significant efforts have been expanded recently to leverage the mathematical structure provided by an $L_2$ resolution to alleviate that computational burden with rigorous and tractable error control\textsuperscript{[12, 52]}. While no single approach works universally, successful model reduction strategies have addressed these challenges with either the construction of a model surrogate that replaces
the expensive initial model \cite{24, 44}, or the representation of the model output as a mapping from a reduced input space \cite{16, 31, 12, 52, 11, 53}.

In this paper, we concentrate our efforts on approximating nonlinear response surfaces by polynomial chaos expansions that consist of linear series of terms that are orthogonal with respect to the probability measure of input variables. The foundation of these representations was pioneered in the context of stochastic finite elements \cite{20, 21, 22, 23, 24, 25, 57}, and the Hilbertian structure of the underlying $L_2$ space permitted the development of non-intrusive approaches for estimating the expansion coefficients \cite{35, 3, 36}. More recently, basis enrichment \cite{25}, least-squares \cite{5, 11, 12, 43} and $\ell_1$-minimization methods \cite{7, 15, 18, 43} were suggested as enhancements or alternatives to the spectral perspective. Further, recent advances of $\ell_1$-minimization have demonstrated additional sparsity enhancement by adaptively selecting the basis terms \cite{47, 32}.

A recently introduced dimension reduction technique consists of a basis adaptation procedure \cite{52} which constructs polynomial chaos expansions for specific quantities of interest (QoIs) using only a small number of Gaussian variables that are linear combinations of the original basis. These combinations are specifically adapted to the QoI in question and are obtained through a learning process which involves exploring the solution space through a limited number of samples. Standard basis adaptation procedures involve choosing these linear combinations through a rotation matrix computed according to particular sparse grid rules, following a low-dimensional quadrature rule for evaluating the adapted expansion for the QoI. While basis adaptation was shown to be effective for reduced representation of random fields \cite{54} and design optimization under uncertainty \cite{50}, the overall computational cost (while linear in the dimension) can be further reduced.

The main contribution of the paper is a novel algorithm that efficiently and simultaneously computes the basis rotation as well as the corresponding chaos coefficients using a fixed number of model evaluations independent of the choice of reduced dimensionality, and as a result departing from the restrictive traditional pseudo-spectral approaches. This is achieved by incorporating an $\ell_1$-minimization procedure on Hermite Chaos expansions with respect to variables that are assumed to be orthogonal projections of the original input variables through a projection map that is computed jointly with the $\ell_1$-minimization. As was emphasized in the original basis adaptation method \cite{52}, our approach applies specifically to the Hermite Chaos with Gaussian input variables, as the distribution of the projected variables would otherwise be arbitrary, resulting in non optimal polynomial representation, due to the loss of the orthogonality property. A recent attempt to adapt the basis of non-Hermite Chaos \cite{57}, has been restricted to projections on 1-dimensional bases, as those can be easily mapped to uniformly distributed inputs and the Legendre Chaos can then be employed. This however required an a priori indication that such a 1-dimensional adaptation exists, which was validated using a gradient-based criterion to compute the rotation, that again relies on pseudo-spectral approaches and we therefore restrain from such exploitations here. The advantages of our algorithm are highlighted on an example of extreme scale computation for a realistic engineering application, involving large-eddy simulations (LES) of supersonic turbulent reactive flows inside a scramjet engine combustor, where the input space is high dimensional and a very limited number of these expensive simulations is available.

Few previous works for achieving dimensionality reduction within the context of PC or generic polynomial surrogates are known to the authors. Namely, a similar heuristic algorithm has been proposed in the past \cite{63}, where the combination of an $\ell_1$-minimization approach for computing the chaos coefficients together with the active subspace method for estimating a rotation matrix, has resulted in improved sparsity in the PC expansion. Furthermore, an approach for generic polynomial ridge functions was proposed in \cite{28} where both the coefficients and the projection matrix are estimated using least squares minimization. First, for the coefficients, their well-known least squares solution that involves a Moore-Penrose pseudoinverse of the measurement matrix, was substituted in the objective function. The implicit dependence of the pseudoinverse on the projection matrix results in replacing the two step procedure by a single optimization problem that is referred to as variable projection approach. Our work, as is explained below, offers a new alternative that retains the benefits of a sparse solution ensured by the use of $\ell_1$-minimization as in the first reference, while the least squares solution for the rotation matrix allows for a data-driven adaptation as in the second approach.

This paper is structured as follows. Section 2.1 describes the use of PC expansion as a response surface, specifically the Hermite (Homogeneous) Chaos for both standard Gaussian variables and rotated Gaussian
variables produced from the basis adaptation procedure. Section 2.2 provides the main ingredients of compressive sensing, which are combined with basis adaptation to estimate the new expansion coefficients. The overall method is then demonstrated on a series of numerical examples in Section 3, including a 12-dimensional ridge function, a 20-dimensional Burgers’ equation, and an 11-dimensional scramjet combustor application. The paper then ends with conclusions in Section 4.

2. Methodology

2.1. Polynomial Chaos Expansion

2.1.1. Homogeneous Chaos

Throughout this paper, let us assume the quantity $u := u(\xi)$, that can be written as a function of uncorrelated Gaussian variables $\xi = (\xi_1, \ldots, \xi_d)$, is a square integrable function, that is $u \in L^2(\Omega, F, P)$, where $F := F(\mathcal{G})$ is the $\sigma$-algebra generated from the Gaussian Hilbert space $\mathcal{G} = \operatorname{span}\{\xi_i\}_{i=1}^d$. It is known [59, 6, 24] that $u$ admits a series expansion of the form

$$u(\xi) = \sum_{\alpha \in J_d} c_\alpha \psi_\alpha(\xi),$$

where $\alpha = (\alpha_1, \ldots, \alpha_d) \in J_d := \mathbb{N}^d \cup \{0\}$ are finite-dimensional multiindices with norm $|\alpha| = \alpha_1 + \cdots + \alpha_d$, and the basis functions $\psi_\alpha$ are defined as the tensor product

$$\psi_\alpha(\xi) = \prod_{i=1}^d \psi_{\alpha_i}(\xi_i)$$

with

$$\psi_n(\xi) = \frac{h_n(\xi)}{\sqrt{n!}}$$

and $h_n$ is the standard 1-dimensional Hermite polynomials of order $n$ which is orthogonal with respect to the Gaussian measure with density $p(\xi) = (2\pi)^{-1/2} \exp(-\xi^2/2)$ and has norm $\|h_n\| = 1$, $n \in \mathbb{N}$. The Hilbert structure of $L^2(\Omega, F, P)$ is characterized by the inner product defined as

$$\langle \psi_\alpha(\xi), \psi_\beta(\xi) \rangle := \mathbb{E}\{\psi_\alpha \psi_\beta\} = \int_{\mathbb{R}^d} \psi_\alpha(\xi) \psi_\beta(\xi) p(\xi) d\xi$$

where $p(\xi) = \prod_{i=1}^d p(\xi_i)$, $\|\psi_\alpha\| = (\mathbb{E}\{\psi_\alpha^2\})^{1/2}$, thus the orthogonality condition is given by

$$\langle \psi_\alpha(\xi), \psi_\beta(\xi) \rangle = \|\psi_\alpha\|^2 \delta_{\alpha, \beta},$$

where $\delta_{\alpha, \beta}$ is the Dirac delta function taking the value of 1 if $\alpha = \beta$ and 0 otherwise. Eq. (3) suggests that $\|\psi_\alpha\| = 1$, and so the polynomials are normalized. We refer to Eq. (2) as the polynomial chaos expansion of $u$.

In practice, we work with truncated versions of (3). For $Q \in \mathbb{N}$, $J_d^Q := \{\alpha \in J_d : |\alpha| \leq Q\}$, we assume that $u$ can be accurately approximated by

$$u(\xi) \approx \sum_{\alpha \in J_d^Q} c_\alpha \psi_\alpha(\xi).$$

This truncated expansion of order $Q$ consists of

$$N_Q = \binom{d + Q}{Q} = \frac{(d + Q)!}{d!Q!}$$

basis terms whose coefficients $\{c_\alpha\}_{\alpha \in J_d^Q}$ need to be computed.
2.1.2. Adaptation on the Gaussian basis

From the above, it is clear that all \( u \) that are \( \mathcal{F} \)-measurable can be expressed as a function of any basis of \( \mathcal{G} \). This encompasses any set of uncorrelated standard normal random variables that spans \( \mathcal{G} \), since the latter generates identical Chaos spaces of higher order. Assume \( A : \mathbb{R}^d \to \mathbb{R}^d \) is a unitary matrix (\( AA^T = I \)) that serves as a linear operator from \( \mathbb{R}^d \) to itself, and taking \( \xi \) to be an \textit{initially} chosen basis, then

\[
\eta = A\xi
\]

defines a new set of independent standard normal random variables that spans \( \mathcal{G} \), and therefore generating the same \( \sigma \)-algebra \( \mathcal{F}(\mathcal{G}) \). As a result, any \( u \in L^2(\Omega, \mathcal{F}, P) \) can also be expanded as

\[
u := u(\eta) = \sum_{\beta \in \mathcal{J}_Q^d} \tilde{c}_\beta \psi_\beta(\eta) = \sum_{\beta \in \mathcal{J}_Q^d} \tilde{c}_\beta \psi_\beta(A\xi) = \sum_{\gamma \in \mathcal{J}_Q^{d_0}} \tilde{c}_\gamma \psi_\gamma(W\xi),
\]

where from the almost sure equality \( u(\xi) \overset{a.s.}{=} u(\eta) \) we have that

\[
c_\alpha = \sum_{\beta \in \mathcal{J}_Q^d} \tilde{c}_\beta (\psi_\beta(A\xi), \psi_\alpha(\xi)).
\]

Of high interest is the \( A \) that leads to an expansion of \( u(\eta) \) (for a given fixed order \( Q \)) that depends primarily only on a small number of components. In other words, we would like to construct \( \tilde{\eta} = (\eta_1, \ldots, \eta_{d_0})^T \) with \( d_0 \ll d \) such that

\[
u(\xi) \approx u(\tilde{\eta}) = u(W\xi) = \sum_{\gamma \in \mathcal{J}_Q^{d_0}} \tilde{c}_\gamma \psi_\gamma(W\xi),
\]

where the coefficients of the terms \( \psi_\gamma(\eta) \) for \( \gamma \in \mathcal{J}_Q^d \setminus \mathcal{J}_Q^{d_0} \) are assumed to take small values and therefore can be neglected. Here, \( W \) is the matrix from decomposing the isometry

\[
A = \begin{bmatrix} W \\ V \end{bmatrix}
\]

where \( W^T \in M_{d_0}^n \), \( V^T \in M_{d-d_0}^n \) with \( M_m^n \) being the set of \( n \times m \) matrices with orthogonal columns

\[
M_m^n = \{ U \in \mathbb{R}^{n \times m} : U^T U = I_m \},
\]

and is also known as the Stiefel manifold [58].

Several criteria for choosing the isometry \( A \) have been proposed in [52], but relying on knowing either the QoI cumulative distribution function or its low (e.g., first or second) order PC coefficients in a \( \xi \)-expansion. Both approaches require prior computations to construct \( A \), which do not provide information on the reduced dimensionality \( d_0 \), and can be computationally inefficient as they are mainly associated with non-intrusive pseudo-spectral methods. Our goal is to develop a novel way of simultaneously computing optimal projection matrices and estimating the resulting expansion coefficients, with the flexibility of utilizing non-structured samples instead of quadrature nodes.

2.2. Compressive Sensing

2.2.1. \( \ell_1 \)-minimization for polynomial regression

To estimate the chaos coefficients \( c = \{ c \}_{c \in \mathcal{J}_Q^d} \), we employ compressive sensing (CS) techniques [7, 15] that seek sparse PC representations. CS is particularly advantageous for scenarios where \( c \) is indeed sparse, \( \xi \) is high-dimensional, and a very limited number of model evaluations are available. These methods make use of the fact that a PC expansion is linear with respect to its coefficients:

\[
u \approx \Psi c,
\]
where \( \mathbf{u} = (\hat{u}^{(1)}, \ldots, \hat{u}^{(N)})^T \) is the vector of output data, \( \{\xi^{(i)}\}_{i=1}^N \) is the set of input points corresponding to the data outputs, and \( \Psi \) is the measurement matrix with entries \((\Psi)_{ij} = \psi_j(\xi^{(i)}), \ i = 1, \ldots, N, \ j \in \mathcal{I}_k\). We also denote the full dataset with \( \mathcal{D} = \{\{\xi^{(i)}\}_{i=1}^N, \{\hat{u}^{(i)}\}_{i=1}^N\} \), that is the set of all available data points. In practice, as we will see next, the training data, that is the data points used to infer any parameters of interest, will be either \( \mathcal{D} \) or a subset of it. The influence of the coefficients is typically observed to quickly decay with higher order polynomials, an effect that makes the \( \ell_1 \)-minimization a suitable method when one is interested in obtaining a sparse solution.

We focus on the following form of \( \ell_1 \)-minimization:

\[
P_{1,\epsilon} := \left\{ \arg \min_{\mathbf{c}} \|\mathbf{c}\|_1 \quad s.t. \quad \|\mathbf{u} - \Psi \mathbf{c}\|_2 \leq \epsilon \right\}.
\]

The \( P_{1,\epsilon} \) problem is known as the Basis Pursuit Denoising problem. When \( \epsilon = 0 \) is chosen to enforce an exact fit on the data, it is known as Basis Pursuit problem. Equivalence with the Least Absolute Shrinkage Operator (LASSO) \([51]\) problem can also be shown under proper choices of the regularization and tolerance parameters \([16]\).

2.2.2. Cross validation for choosing \( \epsilon \)

In order to obtain a solution for the \( P_{1,\epsilon} \) problem that is useful for subsequent predictions, one needs to choose \( \epsilon > 0 \) properly to avoid overfitting or underfitting the data. Small values of \( \epsilon \) might result in overfitting the training data without necessarily providing accurate predictions on points outside the training set. Large values of \( \epsilon \) on the other hand will penalize heavily on the sparsity of the solution without taking into account the observations. We use cross-validation to find a suitable choice of \( \epsilon \). We divide the \( N \) observations into two sets consisting of \( N_t \) and \( N_v \) samples \((N = N_t + N_v)\) that will serve as the training and validation data respectively and we denote with \( \Psi_t \) and \( \Psi_v \), the corresponding measurement matrices. We solve \( P_{1,\epsilon} \) using only the \( N_t \) training data points and for a discrete set of values \( \epsilon_{tr} \) to obtain \( \mathbf{c}_{tr} \). For each solution we compute the validation error \( \epsilon_v = \|\mathbf{u}_v - \Psi_v \mathbf{c}_{tr}\|_2 \) and choose \( \epsilon_{tr} \) such that \( \epsilon_v \) is minimized. The procedure is summarized in Algorithm 1. Alternative cross validation procedures can be preferable when large datasets are considered. These particularly involve partitioning the data into \( K \) sets (folds), each consisting of \( n_k = N/K \) points and repeat the above procedure \( K \) times, where each time one fold serves as the validation set while the remaining points are the training set (leave-\( n_k \)-out cross validation) \([32, 30]\). Such procedures, however, are beyond our scope.

**Algorithm 1:** Cross validation algorithm for estimation of \( \epsilon_v \)

Arbitrarily choose \( N_t \) out of \( N \) data points in \( \mathcal{D} \), denote it with \( \mathcal{D}_{tr} \) and set \( \mathcal{D}_v = \mathcal{D} \setminus \mathcal{D}_{tr} \). Choose a span of \( J \) values \( \{\epsilon_{tr}\}_j, \ j = 1, \ldots, J \)

for \( j = 1 \) to \( J \) do

\[ \mathbf{c}_{tr} \leftarrow \text{Solution of } P_{1,\epsilon_{tr}} \text{ using data } \mathcal{D}_{tr} \]

\[ \epsilon_{tr} = \|\mathbf{u}_{tr} - \Psi_{tr} \mathbf{c}_{tr}\|_2. \]

end

Return \( \epsilon = \sqrt{\frac{N}{N_t}} \epsilon^* \) where \( \epsilon^* = \min_j \epsilon_{tr} \).

In the above algorithm note that the \( \sqrt{\frac{N}{N_t}} \) scaling is motivated by the fact that the validation error on the validation samples becomes large as the values of \( \epsilon_{tr} \) increase, while it is smaller than the error \( \|\mathbf{u} - \Psi \mathbf{c}_{tr}\|_2 \) when using the full set \( \mathcal{D} \) \([12]\).

2.2.3. \( \ell_1 \)-minimization using adapted PCE

Assuming now that the observed model output admits a representation of the form \([12]\), one might be interested in finding the best projection matrix \( \mathbf{W} \) such that the observed data can be explained as emerging
from a $d_0$-dimensional PC expansion over polynomials of $\tilde{\eta}$, for a given $d_0 \ll d$. The linear model in this case is written as
\[ u \approx \Psi \mathbf{c}. \] (17)

Here $u$ and $c$ are as in [16] while the measurement matrix has entries $(\Psi_{ij})_{ij} = \psi_j(\tilde{\eta}^{(i)})$, where $\tilde{\eta}^{(i)} = W \xi^{(i)}$, $i = 1, \ldots, N$, $j \in J_{d_0}$. The $\ell_1$-minimization problem can be restated as
\[ \mathcal{P}_{1,\epsilon}^W := \left\{ \arg \min_c \|c\|_1 \text{ s.t. } \|u - \Psi \mathbf{c}\|_2 \leq \epsilon \right\} \] (18)

where with $\mathcal{P}_{1,\epsilon}^W$ we emphasize the dependence of the solution on the projection matrix $W$.

In practice, the projection matrix is not known a priori and needs to be estimated using a criterion that will guarantee some sense of optimality. Provided that all we have available is the data set $D$, a natural choice is to minimize the $\ell_2$ error of the model fit to the data, that is to solve
\[ W^* = \arg\min_{W} ||\Psi \mathbf{c} - u||_2, \] (19)

where $W$ appears only in the measurement matrix $\Psi_W$ and we assume that a candidate for $c$ (e.g., an initial guess) is available. This motivates an iterative procedure, to be described in the next section. To further justify our choice, it can be easily shown that this criterion is equivalent to the maximum likelihood estimate in the Bayesian context [47], see Appendix B for details. We emphasize that the above is a constrained optimization problem since the unknown parameters are required to satisfy the orthonormality conditions; in other words, the solution is restricted within the Stiefel manifold $\mathcal{M}_{d_0}^d$.

2.2.4. Computational algorithm

We have described the $\ell_1$-minimization problem for adapted PC expansions that requires knowledge of $W$, while the estimation of $W$ requires the knowledge of $\mathbf{c}$. In what follows, we propose a two-step optimization scheme that can address the challenge of solving this coupled optimization problem. The algorithm is simply based on the idea that the two optimization problems can be interchangeably solved such that the solution of the one is kept fixed while solving the other, until some convergence criterion is satisfied. Although, at first sight, this two step approach appears to be quite heuristic, it can, in fact, be interpreted as a coordinate descent algorithm that converges to the maximum a posteriori solution corresponding to a Bayesian formalism of the problem, see Appendix B for detailed explanation. The pseudocode for this idea is summarized in Algorithm 2.

Algorithm 2: Compressive sensing with built-in basis adaptation

Require: Observed inputs $\{x^{(i)}\}_{i=1}^N$, observed outputs $\{u^{(i)}\}_{i=1}^N$, choice of $d_0 < d$, initial guess $c^0 \in \mathbb{R}^{(d_0)^2}$, $W^0 \in \mathcal{M}_{d_0}^d$, maximum number of iterations $M_{\text{iter}}$, convergence tolerances $\epsilon_1$ and $\epsilon_2$, fitting error $\epsilon$. Set $i = 1$.

repeat
\begin{align*}
&\text{Compute } \{\eta^{(i)}\}_{i=1}^N \text{ and } \Psi_{W^t-1}, \text{ where } \eta^{(i)} = W^{tt-1} \xi^{(i)}, i = 1, \ldots, N \text{ and } [\Psi_{W^{t-1}}]_{kl} = \psi_l(\eta^{(k)}) \\
&c^{it} \leftarrow \arg\min_c ||c||_1 \text{ subject to } ||u - \Psi W^{t-1} c||_2 < \epsilon \\
&W^{it} \leftarrow \arg\min_W ||u - \Psi W^{it} c||_2 \\
&it \leftarrow it + 1
\end{align*}
until relative change in $||c||_1$ is less than $\epsilon_1$, and change in $F(W)$ is less than $\epsilon_1$ or it = $M_{\text{iter}}$

While the proposed algorithm involves iterating between two tractable subproblems ($\ell_1$ and $\ell_2$-minimizations), it does not address how to choose $d_0$, and the issue of increasing dimensionality of both arguments $c$ and $W$ when one increases $d_0$. More specifically, upon solving (18) for a small value $d_0$, one may decide that the resulting PC expansion is not accurate enough, and therefore, the need to increase $d_0$ and repeat the procedure. The number of expansion coefficients increases factorially with $d_0$ while the number of entries
in $W$ increases geometrically, and the combined effect can result in an expensive-to-solve problem as we move to larger $d_0$ values. In practice, the growth mainly affects the constrained optimization problem with respect to $W$, and the convergence to a global minimum can become slow.

Another drawback of the proposed procedure is the possibility to be stuck in a local minimum. This is mainly due to the fact that the objective function to be optimized with respect to $W$ is generally non-convex. In addition, it can be observed that for a given $d_0$, the optimal solution provides a PC expansion with respect to a germ $\eta$ that can itself be rotated along the $d_0$-dimensional space, resulting in an infinite number of possible expansions that are almost surely equal and with the same $\ell_2$ value, while the $\ell_1$ norms of the chaos coefficients are not necessarily equal. This property is further explained in Appendix C. As a result, the algorithm might not converge to the global maximum likelihood value when minimizing with respect to $W$.

In order to reduce the number of parameters in our optimization problem, and thus improve its efficiency, we also propose a second algorithm that computes the rows of $W$ by successively solving the optimization problem with respect to each row at a time while fixing the entries of the rows that have already been estimated; the pseudocode is presented in Algorithm 3. This algorithm replaces the problem of minimizing the $\ell_2$ error with respect to $d_0 \times d$ parameters with that of solving $d_0$ minimization problems with $d$ parameters each time (note that the increase of the number of chaos coefficients at each problem does not add up significant computational complexity). While this new variant mitigates the computational burden at each iteration, the challenge of local minima remains. To further assist convergence to the global minimum, we repeat the procedure multiple times from different initial conditions and select the solution corresponding to the lowest minimum. At small values of $d'$, it is possible that the linear system is overdetermined and ordinary least squares (OLS) can be employed instead of $P_{1,\epsilon}$. One can therefore replace the corresponding step with an OLS solution until the problem becomes underdetermined as $d'$ is increased. Both approaches are expected to perform similarly as the $P_{1,\epsilon}$ solution tends toward the OLS solution for large values of $N$.

**Algorithm 3:** Successive row estimation of the projection matrix

Require : Observed inputs $\{\xi^{(i)}\}_{i=1}^N$, observed outputs $\{u^{(i)}\}_{i=1}^N$, choice of $1 < d_0 < d$, initial guess $c^0 \in \mathbb{R}^{[d_0]}$, $w^0 \in M_1^d$, maximum number of iterations $M_{\text{iter}}$, convergence tolerances $\epsilon_{\ell_1}$ and $\epsilon_{\ell_2}$, fitting error $\epsilon$.

Initialize: Set $d' = 1$ and use Algorithm 2 to solve (18) and obtain $W^* \in M_1^d$ and $c^* \in \mathbb{R}^{[d_0]}$.

for $d' = 2$ to $d_0$ do
  - Set $W^d = W^*$.
  - Generate random initial guess $c^0 \in \mathbb{R}^{[d_0]}$, $w^0 \in M_1^d$ such that $W^{d'} \cdot w^{0T} = 0 \in \mathbb{R}^{d'-1}$ and set $W^0 = [W^{dT} \cdot w^{0T}]^T$.
  - Employ Algorithm 2 to obtain new $W^* \in M_1^d$ and $c^* \in \mathbb{R}^{d'}$ while the first $d' - 1$ rows of $W^*$ are kept fixed (and equal to $W^d$).
end

In all numerical examples presented in this paper, we perform the $\ell_1$-minimization problem by employing the Douglas-Rachford algorithm [19] [10], that is a splitting technique of finding a zero of the sum of two maximally monotone operators. For the optimization with respect to the projection matrix subject to orthogonality constraints, we make use of the Sequential Quadratic Programming (SQP) algorithm [38], Ch. 18) that solves a sequence of subproblems that optimize a quadratic model of the objective function. SQP requires knowledge of the gradients of the objective function which are derived in Appendix A. Another alternative for optimization problems with orthogonal constraints would be to follow a Crank-Nicolson-like update scheme [53]. However, our implementations primarily focus on Algorithm 3 which involves optimization with respect to one matrix row at a time, and we do not pursue extensive exploration of more sophisticated optimization algorithms at this time.
3. Examples

A set of numerical examples are presented below to demonstrate the performance of our methodology. The algorithm is validated in Sec. 3.1 on a synthetic example where the exact adaptation and solutions are known. In Sec. 3.2 the technique is applied on a high-dimensional benchmark UQ problem: the stochastic Burgers’ equation with a 20-dimensional random forcing term. We compare two cases where the first has a relatively benign random forcing with decaying amplitudes, and the other has non-decaying amplitudes to further challenge our algorithm. We end this section with a realistic engineering application involving LES of turbulent reactive flows in a scramjet engine combustor (Sec. 3.3), where engine performance QoIs are functions of 11 uncertain input parameters, and a full-dimensional chaos expansion would be infeasible due to the computational requirements of the simulations.

3.1. Ridge function with known adaptation

We consider the function \( u : \mathbb{R}^d \rightarrow \mathbb{R} \) that is given by

\[
   u(\xi) = \sum_{i=1}^{d} \xi_i + 0.25 \left( \sum_{i=1}^{d} \xi_i \right)^2 + 0.025 \left( \sum_{i=1}^{d} \xi_i \right)^3
\]

which is a PC expansion due to its polynomial form, and the coefficients can easily be identified. Since \( \sum_{i=1}^{d} \xi_i \) is a zero-mean Gaussian with variance equal to \( d \), the above expression can be rewritten as a function of the transformed standard Gaussian variable

\[
   \eta_1 = d^{-1/2} \sum_{i=1}^{d} \xi_i,
\]

resulting in

\[
   u(\eta_1) = d^{1/2} \eta_1 + 0.25d\eta_1^2 + 0.025d^{3/2}\eta_1^3
\]

\[
   = c_0 + c_1\psi_1(\eta_1) + c_2\psi_2(\eta_1) + c_3\psi_3(\eta_1),
\]

where

\[
   c = \begin{pmatrix}
   c_0 \\
   c_1 \\
   c_2 \\
   c_3 \\
   \end{pmatrix} = \begin{pmatrix}
   0.25 \\
   d^{1/2} + 0.075d^{3/2} \\
   0.25d^{1/2} \\
   0.025d^{3/2} \\
   \sqrt{d} \\
   \sqrt{3}d^{1/2} \\
   \end{pmatrix}
\]

We set \( d = 12 \), therefore \( |J_{12}^{1/2}| = 455 \) and we construct synthetic data that consists of \( N = 180 \) Monte Carlo samples \( (N/|J_{12}^{1/2}| \approx 0.4) \). We execute Algorithm 3 and obtain the solutions for 1d, 2d, and 3d expansions. Fig. 1 shows all three density functions (left) and isometry values for the 1d and 2d cases (right). It is clear that the densities coincide since \( u(\xi) \) can be written as a univariate function. The first row of the isometry is indeed as in (21) while the values of the second row are in fact insignificant since the series coefficients that correspond to \( \eta_2 \) (and cross terms) are zero. Fig. 2 shows the plot of \( u \) as a function of \( \eta_1 \) (left) and as a bivariate function of \( (\eta_1, \eta_2) \) (right). Since the coefficients corresponding to \( \eta_2 \) are zero, the function exhibits no variation along \( \eta_2 \). Fig. 3 shows the bivariate (2d) expansions obtained after performing 10 independent runs of Algorithm 2 and a comparison of one run from each algorithm. Interestingly we observe that at each run, Algorithm 2 converges to an arbitrary rotation and the corresponding coefficients result in an expansion \( u(\eta_1', \eta_2') \) that itself is a rotation of \( u(\eta_1, \eta_2) \) obtained by Algorithm 3. That is due to the fact that the observations incorporated in the \( \ell_2 \) error term are each time mapped to different rotated inputs. Thus both algorithms capture the same PC expansion but Alg. 2 fails to detect a dominant direction.
3.2. Stochastic Burgers’ equation

Let us consider the following initial boundary value problem (IBVP):

\[
\begin{align*}
\frac{\partial v}{\partial t} + v \frac{\partial v}{\partial x} &= \nu \frac{\partial^2 v}{\partial x^2} + \sigma \sum_{l=1}^{M} \xi_l \phi_l(x,t), \quad x \in [0, 2\pi], \quad t \in [0, 1] \\
v(x,0) &= 1 + \sin(2x) \\
v(0,t) &= v(2\pi,t) = 1 + \sin(\pi t)
\end{align*}
\]

where \( \xi_l, l = 1, \ldots, M \) are i.i.d. standard normal random variables. For the random forcing term we consider two cases: (i) \( \phi_l(x,t) = \cos(2lx) \cos(2l\pi t)/\sqrt{l} \) where the strength of the random Gaussians decays as a function of \( l \) and (ii) \( \psi_l(x,t) = \cos(2lx) \cos(2l\pi t)/M \) where all terms contribute equally although their coefficients maintain varying (increasing) frequencies. For our numerical implementations below we discretize \([0, 2\pi] \times [0, 1]\) into a rectangular 500 \times 500 grid and solve the IBVP using an implicit Newton’s method. The scalar QoI which we seek to expand in a PC series with respect to \( \xi = (\xi_1, \ldots, \xi_M) \) is the spatial average of the solution to the IBVP at \( t = 1 \),

\[
u(\xi) := \frac{1}{2\pi} \int_0^{2\pi} v(x,1; \xi)dx.
\]
For both cases we take $M = 20$ with $\nu = 1/2$ and $\sigma = 2$. For case (i) we set the order of the approximating expansion expansion to be $Q = 6$ and we generate 1000 Monte Carlo samples as our synthetic data while for (ii) we reduce the order to $Q = 3$ and the number of samples is set to 700.

Fig. 4 shows the plots of the estimated 1d and 2d expansions obtained from Algorithm 3 for the two cases. For case (i), the expansions provide a good fit to the data. This can be partially explained by the fact that $Q$ is higher but most importantly because the decay in the random forcing proportional to $1/\sqrt{l}$ quickly makes $\xi$'s insignificant, and the QoI depends on only a few inputs, thus making it easy to identify a rotation in a low dimensional space. On the contrary, in case (ii) clearly both expansions provide a quite poor fit on the data and the need to increase $d_0$ is apparent. A comparison of the coefficients of the 1d and 2d expansions for (i) indicates that the polynomial terms that depend on $\eta_1$ are dominant compared to those that depend on $\eta_2$. In addition, a look at the entries of the first row of the projection matrix for the two cases confirms our assumption above regarding the increasing significance of the $\xi$'s as we move from case (i) to case (ii). In the first, only two entries have significant amplitudes, while in the second, the values exhibit fluctuations that result in $\eta_1$ being strongly dependent on all $\xi$'s. Fig. 5 shows the density functions of the PC expansions obtained for the two cases. For (i) we compare the PC expansions of dimension up to 2 as we find no reason to pursue estimation of higher dimensional expansions. For (ii) we display the densities for expansions of dimensionality up to 10 where it is observed that no convergence is yet achieved. For comparison, we also display the empirical densities (histograms) of the QoI based on 5000 samples that are drawn by directly solving eq. (24). The coefficients of all successive PC expansions are pairwise compared in Fig. 6. We observe that by using the computed rotation found for $d' - 1$, each successive run of the algorithm for $d' - 1$ augmented with the additional nonzero coefficients corresponding to $\eta_0$ plus cross terms. Overall, the method performs effectively in both cases. However, only in the first case we manage to obtain a reduced PC expansion that can be used as an approximation of our QoI. This is due to the different effect on the random forcing on the QoI and independent of our algorithm. Nevertheless, for the second and more challenging case we still manage to draw our conclusions at a fixed computation cost, that of performing 700 runs of the PDE solver, in constrast to using quadrature methods which would require far more model evaluations. For instance, using a level 1 quadrature rule to compute first order coefficients as in [52], and then using a level 3 (to account for $Q = 3$ in this case) quadrature rule on the reduced basis from $d_0 = 1$ up to 10, would require a total of 8501 evaluations!

3.3. Turbulent reactive flows in a scramjet engine combustor

UQ for supersonic reactive flows using large eddy simulations (LES) has only recently become feasible owing to both algorithmic advances and increasing computational power and resources. This development
Figure 4: Top: Plot of the QoI as a function of its 1d input for case (i) (left) and case (ii) (right). Middle: Plot of the QoI as a function of its 2d input for case (i) (left) and case (ii) (right). Bottom: Coefficients of 1d and 2d expansions for case (i) (left) and comparison of the first row of $W$ for the two cases (right).
Figure 5: Density functions of the PC expansions for $d_0 = 1, 2$ in case (i) (left) and for $d_0 = 1, \ldots, 10$ in case (ii) (right). To allow comparison with the true pdf of each QoI, we also display the histograms that correspond to an empirical distribution and are based on 5000 MC samples drawn by solving eq. (24) directly.

Figure 6: Case (ii): Plot of chaos coefficients for expansions with consecutive increase in dimensionality, from 1d-2d (top left) to 9d-10d (bottom right). To improve visibility along the y-axis, the zeroth order coefficient is ignored in the comparison of 6d-7d and higher orders.
has allowed researchers to explore beyond the commonly used Reynolds-averaged Navier-Stokes (RANS) model \[64\]. Even with the use of RANS, hybrid RANS/LES, or Detached Eddy simulations (DES) \[48\], construction of accurate response surfaces for QoIs faces insurmountable challenges due to the large number of simulations required to explore the often high-dimensional space of uncertain model parameters. Indeed, systematic UQ studies for supersonic combusting ramjet (scramjet) engines is currently rare, with a few exceptions \[60, 12\]. Only very recently, CS methods were used for constructing PC surrogates for scramjet computations \[30\] and global sensitivity analysis studies were presented \[29\].

3.3.1. The model

We concentrate on a scramjet configuration studied under the HIFiRE (Hypersonic International Flight Research and Experimentation) program \[13, 14\], where the flight test payload (Figure 7) involves a cavity-based hydrocarbon-fueled dual-mode scramjet. A ground test rig, designated the HIFiRE Direct Connect Rig (HDCR) (Figure 7), was developed to duplicate the isolator/combustor layout of the flight test hardware \[27, 49\]. Mirroring the HDCR setup, we aim to simulate and assess flow characteristics inside the isolator/combustor portion of the scramjet.

We simulate reactive flow through the HDCR. The rig consists of a constant-area isolator (planar duct) attached to a combustion chamber. It includes four primary injectors that are mounted upstream of flame stabilization cavities on both the top and bottom walls. Four secondary injectors along both walls are positioned downstream of the cavities. The primary fuel injectors are located at \(x = 244\) mm from the inlet and aligned at \(15^\circ\) from the wall, while the secondary injectors are at \(x = 419\) mm and aligned at \(90^\circ\) from the wall. All injectors have a diameter of \(d = 3.175\) mm. Flow travels from left to right in the \(x\)-direction (streamwise), and the geometry is symmetric about the centerline in the \(y\)-direction. Numerical simulations take advantage of this symmetry by considering a domain that covers only the bottom half of this configuration. To further reduce the computational cost, we consider one set of primary/secondary injectors and impose periodic conditions in the \(z\)-direction (spanwise). The overall computational domain is highlighted by the red lines in Figure 8. JP-7 surrogate fuel \[42\] is inserted through these injectors, containing 36% methane and 64% ethylene by volume. A reduced, three-step mechanism is employed to characterize the combustion process, and its kinetic parameters are tuned for the current simulations \[34\].

LES calculations are then performed using the RAPTOR code framework developed by Oefelein \[40, 39\]. The solver has been optimized to meet the strict algorithmic requirements imposed by the LES formalism. The theoretical framework solves the fully coupled conservation equations of mass, momentum, total-energy, and species for a chemically reacting flow. It is designed to handle high Reynolds number, high-pressure, real-gas and/or liquid conditions over a wide Mach operating range. It also accounts for detailed thermodynamics and transport processes at the molecular level. RAPTOR employs non-dissipative, discretely conservative, staggered, finite-volume differencing, which eliminates numerical contamination due to artificial dissipation and produces high quality LES results.

Figure 7: HIFiRE Flight 2 payload (left) \[31\] and HDCR cut view (right) \[27\].
3.3.2. Input parameters and quantities of interest

In our example, we allow a total of 11 input parameters to be variable and uncertain, shown in Table 1 along with the range of admissible values. Their distributions are assumed uniform across the ranges indicated and, for the purpose of constructing a Hermite Chaos expansion, are further mapped to Gaussian variables as explained in the next section. We focus on two QoIs: (1) burned equivalence ratio ($\phi_B$) and (2) stagnation pressure loss ratio ($R_P$). These QoIs reflect the overall scramjet performance, and are based on time-averaged variables. The data utilized in the current analysis are from 2D simulations on the $(x,y)$ plane of the scramjet computational domain (bottom of Fig. 8), using grid resolution where cell size is 1/16 of the injector diameter $d = 3.175$ mm.

- **Burned equivalence ratio** ($\phi_B$) is defined to be equal to $\phi_B \equiv \phi_T \eta_c$, where $\phi_T$ is the total equivalence ratio imposed on the system, and $\eta_c$ is the combustion efficiency based on static enthalpy quantities [49, 26]:

  $$\eta_c = \frac{H(T_{\text{ref}}, Y_e) - H(T_{\text{ref}}, Y_{\text{ref}})}{H(T_{\text{ref}}, Y_{\text{e, ideal}}) - H(T_{\text{ref}}, Y_{\text{ref}})}.$$  

  (26)

  Here $H$ is the total static enthalpy, the “ref” subscript indicates a reference condition derived from the inputs, the “e” subscript is for the exit, and the “ideal” subscript is for the ideal condition where all fuel is burnt to completion. The reference condition corresponds to that of a hypothetical non-reacting mixture of all inlet air and fuel at thermal equilibrium. The numerator, $H(T_{\text{ref}}, Y_e) - H(T_{\text{ref}}, Y_{\text{ref}})$, thus reflects the global heat released during the combustion, while the denominator represents the total heat release available in the fuel-air mixture.

- **Stagnation pressure loss ratio** ($R_P$) is defined as

  $$R_P = 1 - \frac{P_{s,e}}{P_{s,i}},$$  

  (27)

  where $P_{s,e}$ and $P_{s,i}$ are the wall-normal-averaged stagnation pressure quantities at the exit and inlet planes, respectively.
Table 1: Uncertain model parameters. The uncertain distributions are assumed uniform across the ranges shown.

| Notation | Range |
|----------|-------|
| Inlet boundary conditions |       |
| Stagnation pressure | $p_0$ [1.406, 1.554] × 10^9 Pa |
| Stagnation temperature | $T_0$ [1472.5, 1627.5] K |
| Mach number | $M_0$ [2.259, 2.761] |
| Turbulence intensity horizontal component | $I_i$ [0, 0.05] |
| Turbulence length scale | $L_i$ [0.8] × 10^{-3} m |
| Ratio of turbulence intensity vertical to horizontal components | $R_i$ [0.8, 1.2] |
| Fuel inflow boundary conditions |       |
| Turbulence intensity magnitude | $I_f$ [0, 0.05] |
| Turbulence length scale | $L_f$ [0.8] × 10^{-3} m |
| Turbulence model parameters |       |
| Modified Smagorinsky constant | $C_R$ [0.01, 0.06] |
| Turbulent Prandtl number | $Pr_t$ [0.5, 1.7] |
| Turbulent Schmidt number | $Sc_t$ [0.5, 1.7] |

3.3.3. Results

In order to construct Hermite Chaos expansions, we first introduce the normalized physical parameters

$$\theta = (\theta_1, \ldots, \theta_{11}) := \left( \frac{p_0}{p_0}, \frac{T_0}{T_0}, \frac{M_0}{M_0}, \frac{C_R}{C_R}, \frac{Pr_t}{Pr_t}, \frac{Sc_t}{Sc_t}, \frac{L_i}{L_i}, \frac{L_f}{L_f}, \frac{I_i}{I_i}, \frac{I_f}{I_f} \right)$$

where $|\cdot|$ denotes the range of each parameter as that is shown in Table 1 and the bar denotes that the parameters are shifted towards zero (lower bound value is subtracted), hence all parameters are normalized to $\theta_i \in [0, 1]$. Next $\theta$ is mapped to Gaussian random germs $\xi = (\xi_1, \ldots, \xi_{11})$ via the relation $\theta_i = \Phi(\xi_i), i = 1, \ldots, 11$ where $\Phi(\cdot)$ is the standard normal cumulative distribution function.

PC expansions of $u_1 := \phi_B$ and $u_2 := R_p$ of order $Q = 4$ are constructed using Algorithm 5 for $d_0 = 1, 2, 3, 4$ and 5 on a data set consisting of 256 Monte Carlo samples, shown in Fig. 9. For each choice of $d_0$ and for both QoIs, it is observed that the algorithm converges to a solution after only 4-5 interchanges over the $\ell_1$-minimization procedures. In addition, for each $d_0$ the cross validation procedure is repeated independently in order to re-estimate $\epsilon$. As $d_0$ increases, the set of values $\epsilon^*_d$ is upper-bounded by the value chosen at $d_0 - 1$, and so the value for $\epsilon$ decreases. This agrees with intuition which suggests that by increasing the dimensionality of the adapted expansion, we should expect the fit on data to improve.

Fig. 10 shows plots of the resulting 1d and 2d adaptations for the QoIs along with density functions of the 5 PC expansions. This is further supported by the comparison of density functions of the 5 PC expansions, which show almost identical shape for both QoIs. Fig. 11 shows the values of the first two rows of computed projection matrices that define $\eta_1$ and $\eta_2$ from $\xi$, for each of the QoIs. Assuming that a 1d or 2d expansion can be used as a functional representation of each QoI, these values can be used as a measure of sensitivity to each $\xi_i$ as each of the values determines the impact of the corresponding $\xi_i$ on the variance of $\eta_1$ and $\eta_2$. Overall we observe that the first row values weigh the $\xi_i$’s in a similar way for the two QoIs. The values of the second row are slightly different for each case, however several entries maintain an agreement.

We also explore the dependence of the algorithm performance with respect to the number of data samples. Fig. 12 shows the 11 values of the projection vector $w$ for a 1d adaptation when the number of samples varies from 40 to 256 with 10-sample batch being added at a time (and 16 at the final step from 240 to 256). One can observe small fluctuations in the values when the samples vary from 40 to over 100 when they start to converge, which suggests that the isometry could be safely recovered with about 120 samples. Next, all the computed 1d expansions are shown in Fig. 13 along with all 256 data points in order to
assess the quality of the fit. Overall one can conclude that for both QoIs, even the expansions obtained with very few data points provide about the same fit on the data along the whole range of the Gaussian germ $\eta_1$ and they only start diverging from each other around the tails of the distribution that is past the $-2, 2$ values which correspond to areas where $\eta_1$ can be found with probability less than 0.05. At last, plots of the $\ell_2$ errors $\|u - \Psi^{wc^*}\|^2$ versus the dimensionality of the chaos expansion are shown in Fig. 14 for $N = 40, 110, 180$ and 256 verifying our initial intuition that the data fit should be improving as we move towards higher dimensions. Overall our approach has provided a thorough understanding and description of statistics of two complex and highly nonlinear quantities of interest in this computationally expensive study of turbulent combustion in the HiFIRE scramjet engine that would be otherwise infeasible, given this limited number of available model evaluations. Accurate description of the probability distribution of the two QoI’s had been achieved with as low as 120 samples, whereas our 1-dimensional expansions and specifically the their projections indicate that the stagnation temperature and Mach number are the dominant parameters affecting $\phi_B$ and stagnation pressure and turbulence length scale are the two most dominant parameters affecting $R_p$. Moreover, tasks such as computing joint distributions and joint probabilities of the QoI’s can now be performed in an efficient manner due to the availability of their analytical representations with respect to a low dimensional input.

4. Conclusions

We presented a novel method for dimension reduction of polynomial chaos expansions by combining compressive sensing with basis adaptation. Starting with a low dimension, the new algorithm finds an optimal rotated PC expansion by alternating between two subproblems: computing the chaos coefficients via $\ell_1$-minimization, and constructing an orthogonal rotation matrix through $\ell_2$-minimization. The appropriate reduced dimension can then be selected by assessing the convergence of data fit, statistics, and distribution of the quantities of interest being represented.

The main advantage of the new method is its efficiency in estimating chaos expansions on a reduced dimension and with a usually significantly smaller number of samples compared to a full dimensional PC expansion. It also advances the basis adaptation framework by coupling it with compressive sensing algorithms, thus offering flexibility to avoid the computational burden associated with the use of quadrature methods for estimation of their coefficients in pseudo-spectral approaches, particularly in high dimensions.
Figure 10: Top: 1d chaos expansions with rotated inputs evaluated at the input data points. Middle: 2d chaos expansions with rotated inputs evaluated over the $[-4, 4]^2$ domain. The data points in both cases are plotted as functions of the rotated inputs. Bottom: Density functions for up to 5d chaos expansions. Left column results corresponds to $\phi_B$ while right column corresponds to $R_{\bar{B}}$. 
Figure 11: Comparison of the values of the first (left) and second (right) rows of the projection matrix for the two QoIs.

Figure 12: Estimated projection vector values of the 1d expansion versus number of samples used for $\phi_B$ (left) and $R_{\bar{F}}$ (right).

Figure 13: Plots of all the 1d PC expansions of $\phi_B$ (left) and $R_{\bar{F}}$ (right), computed for a number of samples varying from $N = 40$ to $N = 256$. All 256 samples are also shown.
A promising future direction of this research would definitely involve testing its applicability to more computationally expensive or physically complex problems and to even higher dimensions. From a theoretical point of view, our methodology can be shown to be a special case of a Bayesian Compressive Sensing approach in the spirit of the work of Sargsyan [47] and our solution is the \textit{maximum a posteriori} (MAP) estimate, corresponding to a Laplace and Uniform (on the Stiefel manifold) priors on the coefficients and the projection matrix respectively and a Gaussian Likelihood function. More general prior and likelihood function choices could lead to a more thorough understanding of the behavior of the MAP solution and the computational challenges of the algorithm. Furthermore, techniques for sampling from distributions defined on Stiefel manifolds as in [9] would enable estimation of posterior distributions of projection matrices and would be another step towards the ultimate goal that is the fully Bayesian solution of the problem. Recent progress on this direction has shown that an approach for sampling from the marginal posteriors of the coefficients and the rotation matrix, using a combination of variational inference and hamiltonian Monte Carlo on the Stiefel manifold, can result in an efficient way of exploring the joint posterior [55], though more generic approaches are yet to be developed.

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Appendix A. Gradient of the $\ell_2$ error

Here we seek to derive the gradient of the $\ell_2$ error function

$$ J(W) = ||u - \Psi_W c||^2 = (u - \Psi_W c)^T (u - \Psi_W c) $$

with respect to the entries of $W$. For arbitrary $\theta := (W)_{ij}$ we get

$$ \frac{\partial J(W)}{\partial \theta} = -2u^T \frac{\partial \Psi_W}{\partial \theta} c + c^T \left( \Psi_W^T \frac{\partial \Psi_W}{\partial \theta} + \frac{\partial \Psi_W}{\partial \theta} \right) c. $$

19
where \( \partial_{\theta} \Psi \) is the matrix with entries \( \frac{\partial(\Psi \omega)}{\partial \theta} = \partial_{\theta}(\Psi \xi^{(k)}) \). For each multi-index \( \beta \) and for \( \epsilon_i \) being the multi-index with value 1 as its \( i \)-th entry and zero elsewhere, we have

\[
\frac{\partial \psi_{\beta}(\Psi \xi)}{\partial \theta} = \sum_{r=1}^{d_n} \frac{\partial \psi_{\beta}}{\partial \eta_r} \frac{\partial \eta_r}{\partial \theta} = \frac{\partial \psi_{\beta}}{\partial \eta_r} \frac{\partial \eta_r}{\partial \theta} = \sqrt{\beta} \psi_{\beta-\epsilon_i}(\eta) \xi_j
\]

(3.3)

where the last equality makes use of the fact that \( \psi^{(r)}(\eta) = \sqrt{r} \psi_{n-1}(\eta) \) and that gives

\[
\frac{\partial}{\partial \eta_i} \psi_{\beta}(\eta) = \psi^{(r)}(\eta_i) \prod_{j=1, j \neq i}^{N} \psi_{\beta_j}(\eta_j) = \sqrt{\beta} \psi_{\beta-\epsilon_i}(\eta).
\]

A.4

Appendix B. Bayesian problem formulation and maximum a posteriori solutions

In order to clarify the motivation for our proposed methodology that was used to estimate the coefficients \( c \) and the projection matrix \( W \), we reformulate the problem in a Bayesian setting. As our starting point, we treat both \( c \) and \( W \) as random quantities that are assigned prior distributions, say \( p(c, W) = p(c)p(W) \), where clearly the factorization implies independence between \( c \) and \( W \). The prior can then be updated to a posterior distribution conditioned on available data \( D \) given by

\[
p(c, W|D) \propto \mathcal{L}(D|c, W)p(c)p(W),
\]

(3.1)

where the data is defined as \( D = \{(\xi^{(i)})_{i=1}^{N}, \{\hat{u}^{(i)}\}_{i=1}^{N}\} \), that is the set of available model input/output pairs. The likelihood considered here is Gaussian

\[
\mathcal{L}(D|c, W) = (2\pi\sigma^2)^{-N/2} \exp \left\{-\frac{1}{2\sigma^2}||u - \Psi wc||^2_2\right\},
\]

(3.2)

where \( u = (\hat{u}^{(1)}, \ldots, \hat{u}^{(N)})^T \) is the vector of output data, \( \{\xi^{(i)}\}_{i=1}^{N} \) is the set of input points corresponding to the data outputs, and \( \Psi \) is the measurement matrix with entries \( (\Psi W)_{ij} = \psi_{j}(W \xi^{(i)}) \), \( i = 1, \ldots, N \), \( j \in J^\beta \).

For the coefficients we assume a Laplace prior that has been commonly used as a sparsity-inducing prior and is given as

\[
p(c) = (\tau/2)^{|J^\beta|+1} \exp \left\{-\tau \sum_{i=0}^{|J^\beta|} |c_i| \right\},
\]

(3.3)

while for \( W \), provided that naturally one has no prior information regarding the optimal projection, we choose a uniform prior. Taking into account the pairwise orthogonality constraints among the rows of \( W \), the probability measure is defined on the Stiefel manifold \( \mathcal{M}^d_{d_n} \) and its constant density is

\[
p(W) = \frac{\Gamma_{d_n}(d/2)}{2^{d_n}d_n!d/2},
\]

(3.4)

where \( \Gamma_{d_n}(\cdot) \) is the \( d_n \)-ivariate Gamma function. Combining the above priors and the likelihood together, one can easily see that the maximum a posteriori (MAP) estimate satisfies

\[
c^*, W^* = \arg\max_{c, W} \{-\mathcal{F}(c, W)\} = \arg\min_{c, W} \{\mathcal{F}(c, W)\}
\]

(3.5)

where

\[
\mathcal{F}(c, W) \propto -\log \mathcal{L}(D|c, W) + \tau ||c||_1 = \frac{1}{2\sigma^2}||u - \Psi wc||^2_2 + \tau ||c||_1,
\]

(3.6)

Note that for the case where standard PC expansions are used and no projection matrix is involved, optimization of the objective function \( \mathcal{F} \) above, with respect to \( c \) only, reduces to the classical compressive
Algorithm 4: Coordinate descent for minimization of (B.6)

Choose \( c_0, W_0 \), tolerance tol, set \( n = 0 \)
while Change in \( F \) is less than tol do
  \( c_{n+1} \leftarrow \arg \min_c \{ F(c_n, W_n) \} \)
  \( W_{n+1} \leftarrow \arg \min_W \{ F(c_{n+1}, W_n) \} \)
  \( n \leftarrow n + 1 \)
end
Return \( c^*, W^* := c_n, W_n \).

sensing problem or its Bayesian counterpart. In the general case however, one way of making the optimization problem tractable, is to employ a coordinate descent algorithm that breaks the problem into two easier subproblems that are solved within a loop as described in Algorithm 4.

As mentioned above, even when \( W \) is present in \( \Psi_W \), minimization of \( F(c, W) \) with respect to \( c \) only, is the lagrangian version of the LASSO problem, or equivalently, the \( \ell_1 \)-minimization problem. On the other hand, the \( F(c, W) \) is minimized with respect to \( W \), the regularization term \( \tau ||c||_1 \) can be ignored and the problem reduces to minimizing the misfit term \( ||u - \Psi_W c||_2^2 \) or equivalently, the negative log-likelihood. In other words, Algorithm 4 becomes Algorithm 2 and that justifies the heuristic two-step optimization problem in our methodology.

Appendix C. On the equivalence of solutions of the \( \ell_2 \) error

Here we explain in some more detail the connection between Algorithms 2 and 3. Assume that \( c^* \) and \( W^* \) are the outcome of Alg. 2. For the corresponding expansion
\[
    u(\eta) = \sum_{\alpha} c_{x_\alpha} \psi_{\alpha}(\eta),
\]
with \( \eta = W^* \xi \), let \( B \) be any \( d_0 \times d_0 \) isometry matrix and set \( \zeta = B\eta \). The expansion can be rewritten as
\[
    u(\eta) \xrightarrow{\text{a.s.}} \tilde{u}(\zeta) = \sum_{\beta} \tilde{c}_{\beta} \psi_{\beta}(\zeta).
\]
Denoting with \( \tilde{c} \) the vector of new coefficients and with \( \Psi_{BW^*} \) the new measurement matrix and using the almost sure equality of the two expansions we get that
\[
    \min_{W^*} ||u - \Psi_{W^*} c||_2 = ||u - \Psi_{W^*} c^*||_2 = ||u - \Psi_{BW^*} \tilde{c}||_2
\]
that is \( BW^* \) provides the same fit on the data. Intuitively, Alg. 2 can attain a particular minimum for many different rotation matrices, depending each time on the starting values of \( W \) which in general are chosen randomly. Equality of the corresponding coefficients of course is not guaranteed. Each set of coefficients attains a minimum \( \ell_1 \) norm only for the corresponding \( \Psi_W \).

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