Abstract

The Proper Generalized Decomposition or, in short, PGD is a technique that reduces calculation and storage cost drastically and presents some similarities with the Proper Orthogonal Decomposition, in short POD. It was initially introduced for the analyze and reduction of statistical and experimental data, the a posteriori decomposition techniques, also known as Karhunen-Loeve Expansion, Singular Value decomposition or Principal Component Analysis, are now used in the context of model reduction. Its are also related with the so-called n-best term approximation problem. In this paper we study and analyze the different mathematical and computational problems appearing in the optimization procedures related with the Proper Generalized Decomposition and its relative n-best term approximation problem.

Keywords: Proper Generalized Decomposition, Tensor Product Hilbert Space, Best Approximation.

1 Introduction

The main goal of this paper is to use of a separated representation of the solution of a class of elliptic problems, which allows to define a tensor product approximation basis as well as to decouple the numerical integration of a high dimensional model in each dimension. The milestone of this methodology is the use of shape functions given by a tensorial based construction. This fact has advantages as the manipulation of only one dimensional polynomials and its derivatives, that provides a better computational performance and simplified implementation and use one-dimensional integration rules. Moreover, it makes possible the solution of models defined in spaces of more than hundred dimensions in some specific applications. This problem is closely related with the decomposition of a tensor as a sum of rank-one tensors, that it can be considered as a higher order extension of the matrix Singular Value Decomposition.

It is well-known, from the Lax-Milgram Lemma, that if V is a Hilbert space, $\mathcal{A}(\cdot,\cdot)$ is a bounded, $V-$elliptic bilinear form on V, and $\ell \in V'$. Then there is a unique solution of the problem

$$\text{Find } u \in V \text{ such that } \mathcal{A}(u,v) = \ell(v) \text{ for all } v \in V. \tag{1}$$

A generalized paradigm is that if $V = V_1 \otimes \ldots \otimes V_d$ then the intensive use of tensor techniques can help to the computer scientist to ”avoid the curse of dimensionality”.

The Proper Generalized Decomposition (PGD) method has been recently proposed [1, 17, 21] for the a priori construction of separated representations of an element u in a tensor product space $V = V_1 \otimes \ldots \otimes V_d$, which is the solution of a problem of type (1) with a symmetric bilinear form. A rank-n approximated separated representation u_n of u is defined by

$$u_n = \sum_{i=1}^{n} v_i^1 \otimes \ldots \otimes v_i^d \tag{2}$$

The concept of separated representation was introduced by Beylkin and Mohlenkamp in [4] and it is related with the problem of constructing the approximate solutions of some classes of problems in high-dimensional spaces by means a separable function. In particular, for a given map

$$u : [0,1]^d \subset \mathbb{R}^d \longrightarrow \mathbb{R},$$

we say that it has a *separable representation* if

$$u(x_1,\ldots,x_d) = \sum_{j=1}^{\infty} u_1^{(j)}(x_1)\cdots u_d^{(j)}(x_d) \tag{3}$$

Now, consider a mesh of $[0,1]$ in the x_k-variable given by N_k-mesh points, $1 \leq k \leq d$, then we can write a discrete version of (3) by

$$u(x_{i_1},\ldots,x_{i_d}) = \sum_{j=1}^{\infty} u_1^{(j)}(x_{i_1})\cdots u_d^{(j)}(x_{i_d}), \tag{4}$$

where $1 \leq i_k \leq N_k$ for $1 \leq k \leq d$. Observe that for each $1 \leq k \leq d$, if $\mathbf{x}_k^j \in \mathbb{R}^{N_k}$ denotes the vector with components $u_k^{(j)}(x_{i_k})$ for $1 \leq i_k \leq N_k$, then (4) it is equivalent to

$$\mathbf{u} = \sum_{j=1}^{\infty} \mathbf{x}_1^j \otimes \cdots \otimes \mathbf{x}_d^j. \tag{5}$$

We point out that (5) is an useful expression to implemented numerical algorithms using the MATLAB and OCTAVE function `kron`.

This paper is organized as follows. In the next section we introduce the tensor product Hilbert spaces. In Section we give the definition of progressive representation in tensor product Hilbert spaces and introduce the existence theorem for the progressive separated representation in Tensor Product Hilbert Spaces using a class of energy functionals. Next, in 4 we propose two algorithms in order to construct the PGD approach for general elliptic problems. Finally, in Section 5 some numerical examples are given.

2 Tensor product sums on tensor product Hilbert spaces

Let $V = \bigotimes_{i=1}^{d} V_i$ be a tensor product Hilbert space where V_i, for $i = 1, 2, \dots, d$, are separable Hilbert spaces. We denote by $(\cdot, \cdot)$ and $\|\cdot\|$ a general inner product on V and its associated norm. We introduce norms $\|\cdot\|_i$ and associated inner products $(\cdot,\cdot)_i$ on V_i, for $i = 1, 2, \dots, d$. These norms and inner products define a particular norm on V, denoted $\|\cdot\|_V$, defined by

$$\| \otimes_{i=1}^{d} v_i \|_V = \prod_{i=1}^{d} \|v_i\|_i,$$

for all $(v_1, v_2, \dots, v_d) \in \mathbf{V}$, where $\mathbf{V}$ is the product space $V_1 \times \cdots \times V_d$. The associated inner product $(\cdot,\cdot)_V$ is defined by

$$\left(\otimes_{i=1}^{d} u_i, \otimes_{i=1}^{d} v_i \right)_V = \prod_{i=1}^{d} (u_i, v_i)_i,$$

Recall that V, endowed with inner product $(\cdot,\cdot)_V$, is in fact constructed by taking the completion under this inner product.

Now, we introduce the set of V of vectors that can be written as a sum of tensor rank 1 elements. For each $n \in \mathbb{N}$, we define the set of rank-n tensors

$$\mathcal{S}_n = \{u \in V : \text{rank}_{\otimes} u \leq n\},$$

introduced in [11] in the following way. Given $u \in V$ we say that $u \in \mathcal{S}_1$ if $u = u_1 \otimes u_2 \otimes \cdots \otimes u_d$, where $u_i \in V_i$, for $i = 1, \dots, d$. For $n \geq 2$ we define inductively $\mathcal{S}_n = \mathcal{S}_{n-1} + \mathcal{S}_1$, that is,

$$\mathcal{S}_n = \left\{ u \in V : u = \sum_{i=1}^{k} u^{(i)},\, u^{(i)} \in \mathcal{S}_1 \text{ for } 1 \leq i \leq k \leq n \right\}.$$

Note that $\mathcal{S}_n \subset \mathcal{S}_{n+1}$ for all $n \geq 1$. We will say for $u \in V$ that $\text{rank}_{\otimes} u = n$ if and only if $u \in \mathcal{S}_n \setminus \mathcal{S}_{n-1}$.

We first consider the following important property of the set $\mathcal{S}_1$ and inner product $\|\cdot\|_V$.

Lemma 1 *$\mathcal{S}_1$ is weakly closed in $(V, \|\cdot\|_V)$.*

Since equivalent norms induce the same weak topology on V, we have the following corollary.

Corollary 2 *If the norm $\|\cdot\|$ on V is equivalent to the norm $\|\cdot\|_V$, then $\mathcal{S}_1$ is weakly closed in $(V, \|\cdot\|)$.*

Corollary 3 *If the V_i are finite-dimensional vectors spaces, then $\mathcal{S}_1$ is weakly closed in $(V, \|\cdot\|)$ whatever the norm $\|\cdot\|$.*

3 An existence theorem for the progressive separated representation in Tensor Product Hilbert Spaces using a class of energy functionals

Now we want to construct a class of energy functional on $\mathcal{S}_1$, with respect to a given inner product $(\cdot,\cdot)$ on V, with associated norm $\|\cdot\|$. The results of this section are due to Falcó and Nouy [10]. We make the following assumption on the inner product.

Assumption 4 *We consider that the inner product $(\cdot,\cdot)$, with associated norm $\|\cdot\|$, is such that $\mathcal{S}_1$ is weakly closed in $(V, \|\cdot\|)$.*

Let us recall that by Corollary 2, the particular norm $\|\cdot\|_V$ verifies Assumption 4. Now, we introduce for the norm $\|\cdot\|$ and for each $r \in V$ the functional $\mathcal{E}_r : V \longrightarrow \mathbb{R}$ by

$$\mathcal{E}_r(v) = \frac{1}{2}\|v\|^2 - (r, v) = \frac{1}{2}\|r - v\|^2 - \frac{1}{2}\|r\|^2.$$

The following result gives the main properties of the energy functional $\mathcal{E}_r$.

Theorem 5 *For each $r \in V$ there exists $v^* \in \mathcal{S}_1$ such that*

$$\mathcal{E}_z(v^*) = \min_{v \in \mathcal{S}_1} \mathcal{E}_z(v). \tag{6}$$

Moreover,

$$\mathcal{E}_z(v^*) = -\frac{1}{2}\|v^*\|^2, \tag{7}$$

$$\|z - v^*\|^2 = \|z\|^2 - \|v^*\|^2, \tag{8}$$

and

$$(r - v^*, v^*) = 0. \tag{9}$$

Definition 6 (Progressive separated representation of $u \in V$) *For a given $z \in V$, take $z_0 = 0$ and for $n \geq 1$, proceed as follows:*

$$\begin{aligned} r_n &= z - z_{n-1} && (10) \\ z_n &= z_{n-1} + v_n, \text{ where } v_n \in \operatorname{argmin}_{v \in \mathcal{S}_1} \mathcal{E}_{r_n}(v). && (11) \end{aligned}$$

z_n is called an optimal rank-n progressive separated representation of z with respect to the norm $\| \cdot \|$.

We introduce the following definition of the *progressive rank*. Note that in general, the progressive rank of an element $z \in V$ is different from the optimal rank $\operatorname{rank}_{\otimes}(z)$.

Definition 7 (Progressive rank) *We define the progressive rank of an element $u \in V$, denoted by $\operatorname{rank}_{\sigma}(z)$, as follows:*

$$\operatorname{rank}_{\sigma}(z) = \min\{n : z_n = 0\} \tag{12}$$

where z_n is the progressive separated representation of z, defined in definition 6, where by convention $\min(\emptyset) = \infty$.

Theorem 8 (Existence of the Progressive Separate Representation) *For $z \in V$, the sequence $\{z_n = \sum_{i=1}^{n} v_i\}_{n \geqslant 0}$ defined in definition 6 verifies:*

$$z = \lim_{n \to \infty} z_n = z_{\operatorname{rank}_{\sigma}(z)} = \sum_{i=1}^{\operatorname{rank}_{\sigma}(z)} v_i.$$

Moreover, for each $0 \leq n \leq \operatorname{rank}_{\sigma}(z) - 1$ it follows

$$\|z - z_n\|^2 = \|z\|^2 - \sum_{i=1}^{n} \|v_i\|^2 = \sum_{i=n+1}^{\operatorname{rank}_{\sigma}(z)} \|v_i\|^2 \tag{13}$$

and

$$\frac{\|r_n\|}{\|z\|} = \prod_{j=1}^{n-1} \sin \theta_i, \tag{14}$$

where θ_i is the angle between r_i and v_i, that is,

$$\theta_i = \arccos \frac{(r_i, v_i)}{\|r_i\| \|v_i\|}.$$

4 A variational formulation of the Proper Generalized Decomposition

4.1 Formulation of the problem

We consider the following variational problem, defined on the a tensor product Hilbert space $(V, \|\cdot\|_V)$:

$$u \in V, \quad \mathcal{A}(u,v) = \ell(v) \quad \forall v \in V \tag{15}$$

where $\mathcal{A}(\cdot,\cdot) : V \times V \longrightarrow \mathbb{R}$ is a continuous, $V-$elliptic bilinear form, *i.e.* such that for all $u, v \in V$,

$$|\mathcal{A}(u,v)| \leq M\|u\|_V\|v\|_V, \tag{16}$$

$$\mathcal{A}(v,v) \geq \alpha\|v\|_V^2 \tag{17}$$

for constants $M > 0$ and $\alpha > 0$.

Now, we introduce the operator $A : V \longrightarrow V$ associated with $\mathcal{A}$, and defined by

$$\mathcal{A}(u,v) = (Au, v)_V \tag{18}$$

for all $u, v \in V$. We also introduce the element $l \in V$ associated with L and defined by

$$\ell(v) = (l, v)_V \tag{19}$$

for all $v \in V$.. The existence of A and l is ensured by the Riesz representation theorem. Problem (15) can be rewritten in an operator form:

$$Au = l \tag{20}$$

4.2 The Proper Generalized Decomposition a continuous, $V-$elliptic bilinear symmetric form

Assume that for all $u, v \in V$,

$$\mathcal{A}(u,v) = \mathcal{A}(v,u). \tag{21}$$

From the assumptions on the bilinear form $\mathcal{A}(\cdot,\cdot)$, we know that A is bounded, self-adjoint, and positive definite. As usual, we will denote by $(\cdot,\cdot)_A$ the inner product induced by the operator A, where for all $u, v \in V$

$$(u,v)_A = (Au,v)_V = (u, Av)_V,$$

We denote by $\|u\|_A = (u,u)_A^{1/2}$ the associated norm. Note that if $A = I$ the identity operator, then $\|\cdot\|_A = \|\cdot\|_V$.

From properties of operator A, the norm $\|\cdot\|_A$ is equivalent to $\|\cdot\|_V$. Therefore, by Corollary 2, the set $\mathcal{S}_1$ is weakly closed in $(V, \|\cdot\|_A)$ and then, $\|\cdot\|_A$ verifies assumption 4. Then we consider in this case for each $r \in V$ the map

$$\mathcal{E}_{A^{-1}r}(v) = \frac{1}{2}\|v\|_A - (A^{-1}r, v)_A = \frac{1}{2}\|v\|_A - (r, v)_V.$$

Definition 9 (PGD for self-adjoint operators) *Let $z_0 = 0$ and for $n \geq 1$,*

$$\begin{aligned} r_n &= l - Az_{n-1} && (22)\\ z_n &= z_{n-1} + v_n, \text{ where } v_n \in \operatorname{argmin}_{v \in \mathcal{S}_1} \mathcal{E}_{A^{-1}r_n}(v). && (23) \end{aligned}$$

From Theorem 8 we obtain that

$$\lim_{n\to\infty} \|A^{-1}r_n\|_A = 0,$$

that is $\lim_{n\to\infty} z_n = A^{-1}l$ in the $\|\cdot\|_A$-norm. Since $\|\cdot\|_A$ is equivalent to $\|\cdot\|_V$, then the sequence $\{z_n\}_{n\geq 0}$ also converges to $A^{-1}l$ in the $\|\cdot\|_V$-norm. Observe, that the convergence rate given in (14) is $\|\cdot\|_A$-norm dependent, more precisely,

$$\frac{\|A^{-1}r_n\|_A}{\|A^{-1}l\|_A} = \prod_{j=1}^{n-1} \sin\theta_i,$$

where

$$\theta_i = \arccos \frac{(A^{-1}r_i, z_i)_A}{\|A^{-1}r_i\|_A \|z_i\|_A}.$$

A natural question arises in this context: How we compute a minimum of $\mathcal{E}_{A^{-1}r}$ over $\mathcal{S}_1$ for a given $r \in V$? Note that if

$$v = \bigotimes_{i=1}^{d} v_i \in \operatorname{argmin}_{z \in \mathcal{S}_1} \mathcal{E}_{A^{-1}r}(z)$$

then

$$\frac{d}{dt}\mathcal{E}_{A^{-1}r}\left(\bigotimes_{i=1}^{d}(v_i + tw_i)\right)\Bigg|_{t=0} = 0 \qquad (24)$$

holds for all $(w_1, \ldots, w_d) \in V_1 \times \cdots \times V_d$. Equation (24) is equivalent to show that the following Euler-Lagrange Equation:

$$\sum_{i=1}^{d}\left(r - A\left(\bigotimes_{i=1}^{d} v_i\right), v_1 \otimes \cdots \otimes v_{i-1} \otimes w_i \otimes v_{i+1} \otimes \cdots \otimes v_i\right)_V = 0 \qquad (25)$$

holds for all $(w_1, \ldots, w_d) \in V_1 \times \cdots \times V_d$.

4.2.1 A special case

Now, assume that $A = \sum_{k=1}^{n_A} \bigotimes_{i=1}^{d} A_i^k$ and $r = \sum_{k=1}^{n_r} \otimes_{i=1}^{d} r_i^k$ are given also in rank-one form. Then the Euler-Lagrange equation appears as

$$\sum_{i=1}^{d} \left(\sum_{k=1}^{n_r} \prod_{j=1, j\neq i}^{d} (r_j^k, v_j)_j r_i^k - \sum_{s=1}^{n_A} \prod_{j=1, j\neq i}^{d} (A_j^s v_j, v_j)_j A_i^s v_i, w_i \right)_i = 0 \tag{26}$$

for all $(w_1, \ldots, w_d) \in V_1 \times \cdots \times V_d$. Then

$$\left(\sum_{k=1}^{n_r} \prod_{j=1, j\neq i}^{d} (r_j^k, v_j)_j r_i^k - \sum_{s=1}^{n_A} \prod_{j=1, j\neq i}^{d} (A_j^s v_j, v_j)_j A_i^s v_i, w_i \right)_i = 0 \tag{27}$$

for $1 \leq i \leq d$ and for all $(w_1, \ldots, w_d) \in V_1 \times \cdots \times V_d$. Now, consider an n-dimensional subspace $\mathrm{span}\,\{w_i^1, \ldots, w_i^n\}$ of V_i, for each $1 \leq i \leq d$, and define the vector $\mathbf{v}_i \in \mathbb{R}^n$ by means

$$(\mathbf{v}_i)_\alpha = v_i^\alpha \text{ where } v_i = \sum_{\alpha=1}^{n} v_i^\alpha w_i^\alpha.$$

On the other hand introduce the symmetric matrices $\mathbb{A}_j^s \in \mathbb{R}^{n\times n}$ and the vectors $\mathbf{r}_j^k \in \mathbb{R}^n$ by

$$(\mathbb{A}_j^s)_{\alpha,\beta} = (A_j^s w_j^\beta, w_j^\alpha)_j \text{ and } (\mathbf{r}_j^k)_\alpha = (r_j^k, w_j^\alpha)_j.$$

Note that we can write

$$(\mathbf{r}_1^k \otimes \cdots \otimes \mathbf{r}_d^k)_{\alpha_1,\ldots,\alpha_d} = \prod_{j=1}^{d} (r_j^k, w_j^{\alpha_j})_j = \left(\otimes_{j=1}^d r_j^k, \otimes_{j=1}^d w_j^{\alpha_i} \right)_V,$$

for $1 \leq k \leq n_r$.

Under the above notation the PGD run as follows. Start with $\mathbf{u} = \mathbf{0} \in \mathbb{R}^{n^d}$ and $r_j^k = l_j^k$, here we assume that $l = \sum_{k=1}^{n_l} \otimes_{i=1}^{d} l_i^k$, thus $n_r = n_l$. Then we compute $\{\mathbf{v}_1, \ldots, \mathbf{v}_d\} \subset \mathbb{R}^n$ as follows. Note, that (27) can be written as

$$\sum_{k=1}^{n_r} \prod_{j=1, j\neq i}^{d} \langle \mathbf{r}_j^k, \mathbf{v}_j \rangle_2 \, \mathbf{r}_i^k - \sum_{s=1}^{n_A} \prod_{j=1, j\neq i}^{d} \langle \mathbf{v}_j, \mathbb{A}_j^s \mathbf{v}_j \rangle_2 \, \mathbb{A}_i^s \mathbf{v}_i = \mathbf{0} \tag{28}$$

for $1 \leq i \leq d$, here $\langle \cdot, \cdot \rangle_2$ denotes the usual inner product in $\mathbb{R}^2$. The strategy to solve the above non-linear system can be seen in Algorithm **??**.

From Algorithm **??** we can update the solution $\mathbf{u} = \mathbf{u} + \mathbf{v}_1 \otimes \cdots \otimes \mathbf{v}_d$ and the residual by consider $n_r = n_r + n_A$ and

$$\mathbf{r}_j^{n_r+k} = \mathbb{A}_j^k \mathbf{v}_j \text{ for } 1 \leq k \leq n_A \text{ and } 1 \leq j \leq d.$$

We remark that under this notation we have

$$\begin{aligned}(\mathbb{A}_1^k\mathbf{v}_1 \otimes \cdots \otimes \mathbb{A}_d^k\mathbf{v}_d)_{\alpha_1,\ldots,\alpha_d} &= \prod_{j=1}^d (\mathbb{A}_j^k\mathbf{v}_j)_{\alpha_j} \\ &= \prod_{j=1}^d \left(A_j^k v_j, w_j^{\alpha_j}\right)_j \\ &= \left(\otimes_{j=1}^d A_j^k v_j, \otimes_{j=1}^d w_j^{\alpha_j}\right)_V\end{aligned}$$

for $1 \leq k \leq n_A$. In consequence at step $N \geq 1$ the residual can be written as

$$\mathbf{r}_N = \sum_{k=1}^{n_r} \otimes_{j=1}^d \mathbf{r}_j^k \in \mathbb{R}^{n^d},$$

where $n_r = n_r + N n_A$. The proposal algorithm is given in Algorithm 1.

4.3 The Proper Generalized Decomposition a continuous, $V-$elliptic bilinear form

We consider for each $r \in V$ the map

$$\begin{aligned}\mathcal{E}_r(Av) &= (\mathcal{E}_r \circ A)(v) \\ &= \frac{1}{2}\|Av\|_V - (r, Av)_V \\ &= \frac{1}{2}\|v\|_{A^*A} - (A^*r, v)_V \\ &= \frac{1}{2}\|v\|_{A^*A} - ((A^*A)^{-1}A^*r, v)_{A^*A}.\end{aligned}$$

Thus since A^*A is a self-adjoint operator, then the norm $\|\cdot\|_{A^*A}$ is equivalent to the $\|\cdot\|_V$-norm and in consequence $\mathcal{S}_1$ is also weakly closed in the $\|\cdot\|_{A^*A}$-norm. Moreover, $(\mathcal{E}_r \circ A)$ in the $\|\cdot\|_V$-norm is equal to $\mathcal{E}_{(A^*A)^{-1}A^*r}(v)$ in the $\|\cdot\|_{A^*A}$-norm.

Definition 10 (PGD for non self-adjoint operators) *Let* $z_0 = 0$ *and for* $n \geq 1$,

$$r_n = b - Az_{n-1} \tag{29}$$

$$z_n = z_{n-1} + v_n, \text{ where } v_n \in \arg\min_{v \in \mathcal{S}_1} \mathcal{E}_{r_n}(Av). \tag{30}$$

From Theorem 8 we obtain

$$\lim_{n\to\infty} \|(A^*A)^{-1}A^*r_n\|_{A^*A} = \lim_{n\to\infty} \|A(A^*A)^{-1}A^*r_n\|_V = \lim_{n\to\infty} \|r_n\|_V = 0.$$

Thus, in this case the sequence $\{z_n\}_{n\geq 0}$ also converges to the solution $A^{-1}l$ in the $\|\cdot\|_V$-norm. Here the convergence rate (14) is given by the expression:

$$\frac{\|(A^*A)^{-1}A^*r_n\|_{A^*A}}{\|(A^*A)^{-1}A^*b\|_{A^*A}} = \frac{\|r_n\|_V}{\|b\|_V} = \prod_{j=1}^{n-1} \sin\theta_i, ,$$

where

$$\theta_i = \arccos \frac{((A^*A)^{-1}A^*r_i, v_i)_{A^*A}}{\|(A^*A)^{-1}A^*r_i\|_{A^*A}\|v_i\|_{A^*A}} = \arccos \frac{(r_i, Av_i)_V}{\|r_i\|_V\|Av_i\|_V}$$

In order to solve the associated minimization problem for a given $r \in V$, we have that if

$$\bigotimes_{i=1}^{d} v_i \in \operatorname{argmin}_{z\in\mathcal{S}_1}\mathcal{E}_r(Az)$$

then the following Euler-Lagrange equation

$$\sum_{i=1}^{d}\left(A^*r - A^*A\left(\bigotimes_{i=1}^{d} v_i\right), v_1\otimes\cdots\otimes v_{i-1}\otimes w_i\otimes v_{i+1}\otimes\cdots\otimes v_i\right)_V = 0,$$

or equivalently

$$\sum_{i=1}^{d}\left(r - A\left(\bigotimes_{i=1}^{d} v_i\right), A(v_1\otimes\cdots\otimes v_{i-1}\otimes w_i\otimes v_{i+1}\otimes\cdots\otimes v_i)\right)_V = 0 \quad (31)$$

holds for all $(w_1,\ldots,w_d) \in V_1\times\cdots\times V_d$.

4.3.1 A special case

Now, assume that $A = \sum_{k=1}^{n_A}\bigotimes_{i=1}^{d} A_i^k$ and $r = \sum_{k=1}^{n_r}\otimes_{i=1}^{d} r_i^k$ are given also in rank-one form. Then the Euler-Lagrange equation appears as

$$\sum_{i=1}^{d}\sum_{s=1}^{n_A}\left(\sum_{k=1}^{n_r}\prod_{j=1,j\neq i}^{d}(r_j^k, A_j^s v_j)_j r_i^k - \sum_{t=1}^{n_A}\prod_{j=1,j\neq i}^{d}(A_j^t v_j, A_j^s v_j)_j A_i^t v_i, A_i^s w_i\right)_i = 0 \quad (32)$$

for all $(w_1,\ldots,w_d) \in V_1\times\cdots\times V_d$. Then

$$\sum_{s=1}^{n_A}\left(\sum_{k=1}^{n_r}\prod_{j=1,j\neq i}^{d}(r_j^k, A_j^s v_j)_j r_i^k - \sum_{t=1}^{n_A}\prod_{j=1,j\neq i}^{d}(A_j^t v_j, A_j^s v_j)_j A_i^t v_i, A_i^s w_i\right)_i = 0 \quad (33)$$

for $1 \leq i \leq d$ and for all $(w_1,\ldots,w_d) \in V_1\times\cdots\times V_d$. In a similar way as in the symmetric case, let be consider an n-dimensional subspace $\operatorname{span}\{w_i^1,\ldots,w_i^n\}$ of V_i, for each $1 \leq i \leq d$, and in this case we define the vector $\mathbf{v}_i \in \mathbb{R}^n$ as follows:

$$(\mathbf{v}_i)_\alpha = v_i^\alpha \text{ where } v_i = \sum_{\alpha=1}^{n} v_i^\alpha w_i^\alpha.$$

In this case, the symmetric matrix $\mathbb{A}_j^{k,i} \in \mathbb{R}^{n\times n}$ and the vector $\mathbf{r}_j^{k.i} \in \mathbb{R}^n$ are

$$(\mathbb{A}_j^{k,i})_{\alpha,\beta} = (A_j^k w_j^\beta, A_j^i w_j^\alpha)_j \text{ and } (\mathbf{r}_j^{k,i})_\alpha = (r_j^k, A_j^i w_j^\alpha)_j.$$

Now, (33) with this notation can be written as follows

$$\sum_{s=1}^{n_A}\sum_{k=1}^{n_r}\prod_{j=1,j\neq i}^{d}\langle \mathbf{r}_j^{k,s}, \mathbf{v}_j\rangle_2\, \mathbf{r}_i^{k,s} - \sum_{t=1}^{n_A}\prod_{j=1,j\neq i}^{d}\langle \mathbf{v}_j, \mathbb{A}_j^{t,s}\mathbf{v}_j\rangle_2\, \mathbb{A}_i^{t,s}\mathbf{v}_i = \mathbf{0} \tag{34}$$

for $1 \leq i \leq d$. The proposal algorithm is given in Algorithm 2.

5 A case study: The first passage time and the Poisson equation in $(0,1)^d$

Our first case to study is based on the well-known FeynmanKac representation of the solution to the Dirichlet problem for Poissons equation. Recall that the Dirichlet problem for Poissons equation is

$$\begin{cases} -\Delta u = f \text{ in } \Omega \subset \mathbb{R}^d \\ u|_{\partial\Omega} = 0. \end{cases} \tag{35}$$

where $f = f(x_1, x_2, \ldots, x_d)$ is a given function and $\Delta = \sum_{i=1}^d \frac{\partial^2}{\partial x_i^2}$ is the Laplace operator. The solution of this problem at $\mathbf{x}_0 \in \mathbb{R}^d$, given in the form of the path-integral with respect to standard d-dimensional Brownian motion $\mathbf{W}_t$ is as follows

$$u(\mathbf{x}_0) = \mathbb{E}\left[\int_0^{\tau_{\partial\Omega}} 2f(\mathbf{W}_t)dt\right] \tag{36}$$

Here

$$\tau_{\partial\Omega} = \inf\{t : \mathbf{W}_t \in \partial\Omega\}$$

is the first-passage time and $\mathbf{W}_{\tau_{\partial\Omega}}$ is the first-passage location on the boundary, $\partial\Omega$. We assume that $\mathbb{E}[\tau_{\partial\Omega}] < \infty$ for all $\mathbf{x}_0 \in \Omega$ and f and u are continuous and bounded in Ω, and that the boundary, $\partial\Omega$, is sufficiently smooth so as to ensure the existence of a unique solution, $u(\mathbf{x})$, that has bounded and continuous first- and second-order partial derivatives in any interior subdomain

Example 11 *Firstly, we consider the following problem in 3D: Solve for*

$$(x_1, x_2, x_3) \in \Omega = (0,1)^3 :$$

$$-\Delta u = (2\pi)^2 \cdot 3 \cdot \sin(2\pi x_1 - \pi)\sin(2\pi x_2 - \pi)\sin(2\pi x_3 - \pi), \tag{37}$$

$$u|_{\partial\Omega} = 0, \tag{38}$$

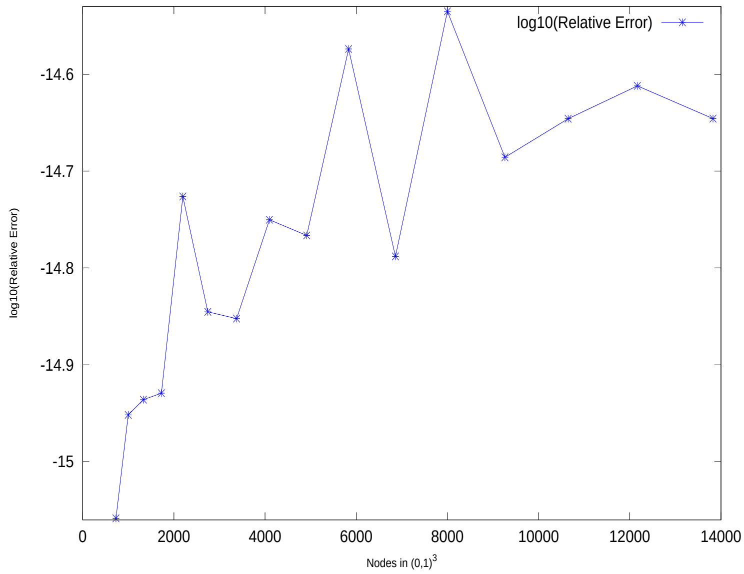

Figure 1: The relative error $\|\mathbf{u}_1 - A^{-1}\mathbf{f}\|_2 / \|A^{-1}\mathbf{f}\|_2$ in logarithmic scale.

which has as closed form solution

$$u(x_1, x_2, x_3) = \sin(2\pi x_1 - \pi)\sin(2\pi x_2 - \pi)\sin(2\pi x_3 - \pi).$$

We used the separable representation Algorithm 1) with parameter values `iter_max` $= 5$, `rank_max` $= 1000$ *and* $\varepsilon = 0.001$. *The algorithm give us an approximated solution* $\mathbf{u}_1 \in \mathcal{S}_1$. *In Figure 1 we represent the relative error of the solution computed using the separable representation algorithm, using logarithmic scale, as a function of the number of nodes used in the discretization of the Poisson equation. All the computations were performed using the GNU software* OCTAVE *in a AMD 64 Athlon K8 with 2Gib of RAM.*

In Figure 2 we represent the CPU time, in logarithmic scale, used in solving the standard FEM linear system against the separable representation algorithm. In both cases all the linear systems involved were solved using the standard linear system solver (A\b) of OCTAVE.

Example 12 *Finally we are addressing some highly multidimensional models. To this end we solve numerically (35) for* $(x_1, \ldots, x_d) \in \Omega = (0, \pi)^d$ *where*

$$f = \sum_{k=1}^{d} -(1+k)\sin^{(-1+k)}(x_k)\left(-k\cos^2(x_k) + \sin^2(x_k)\right) \prod_{k'=1, k' \neq k}^{d} \sin^{(1+k')}(x_{k'}),$$

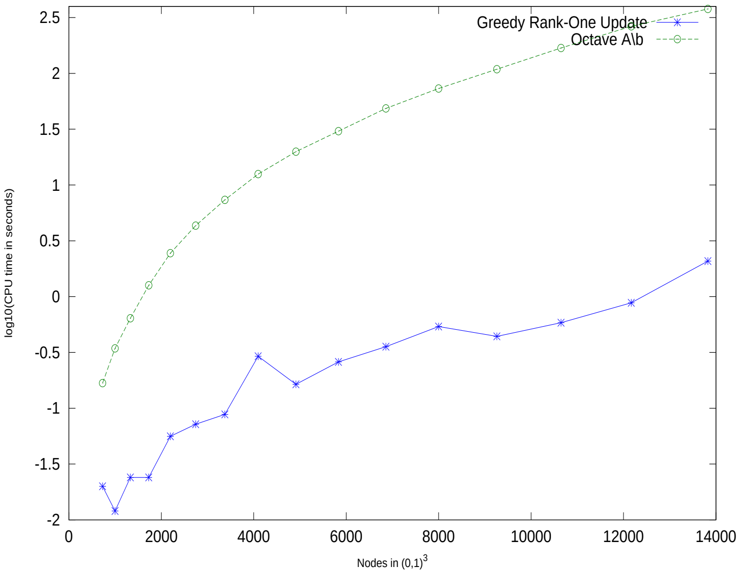

Figure 2: The CPU time, in seconds, used in solving the linear system as a function of the number of nodes employed in the discretization of the Poisson Equation.

which has as closed form solution

$$u(x_1, \ldots, x_d) = \prod_{k=1}^{d} \sin^{(k+1)}(x_k).$$

Here we consider the true solution $\mathbf{u}$ *given by* $\mathcal{U}_{i_1,\ldots,i_d} = u(\widehat{x}_{i_1+1}, \ldots, \widehat{x}_{i_d+1})$. *For* $d = 10$ *we use the parameter values* `iter_max` $= 2$, `rank_max` $= 10$ *and* $\varepsilon = 0.001$. *In a similar way as above the algorithm give us an approximated solution* $\widehat{\mathbf{u}} \in \mathcal{S}_1$. *In Figure 3 we represent the absolute error* $\|\widehat{\mathbf{u}} - \mathbf{u}\|_2$ *as a function of* $h = \pi/N$ *for* $N = 5, 10, 20, \ldots, 160$ *in* $\log_{10}$*-scale. By using similar parameters values the problem has been solved for* $d = 100$ *in about 20 minutes.*

References

[1] A. Ammar, B. Mokdad, F. Chinesta, and R. Keunings. A new family of solvers for some classes of multidimensional partial differential equations encountered in kinetic theory modelling of complex fluids. *Journal of Non-Newtonian Fluid Mechanics*, 139(3):153–176, 2006.

[2] A. Ammar, B. Mokdad, F. Chinesta, and R. Keunings. A new family of solvers for some classes of multidimensional partial differential equations encountered in kinetic theory modelling of complex fluids part II: Transient simulation using

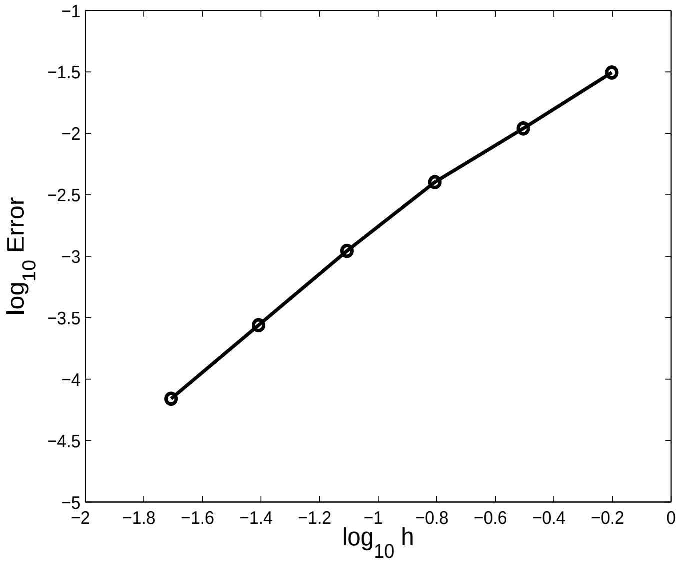

Figure 3: The absolute error $\|\widehat{\mathbf{u}} - \mathbf{u}\|_2$ as a function of $h = \pi/N$ for $N = 5, 10, 20, \ldots, 160$ in $\log_{10}$-scale.

space-time separated representations. *Journal of Non-Newtonian Fluid Mechanics*, 144(2–3):98–121, 2007.

[3] A. Ammar, F. Chinesta, and A. Falcó. On the convergence of a Greedy Rank-One Update Algorithm for a class of Linear Systems. *Archives of Computational Methods in Engineering*, In press.

[4] G. Beylkin and M. J. Mohlenkamp. Algorithms for Numerical Analysis in High Dimensions. *SIAM J. Sci. Comput.* Vol 26, No. 6 (2005). pp. 2133–2159.

[5] J. Chen and Y. Saad. On The Tensor Svd And The Optimal Low Rank Orthogonal Approximation Of Tensors. *Siam Journal On Matrix Analysis And Applications*, 30(4):1709–1734, 2008.

[6] F. Chinesta, A. Ammar and E. Cueto. Recent advances in the use of the proper generalized decomposition for solving multidimensional models. *Archives of Computational Methods in Engineering*, In press.

[7] R. F. Curtain and A. J. Prichard *Functional Analysis in Modern Applied Mathematics*. Academic Press, 1977.

[8] L. De Lathauwer, B. De Moor, and J. Vandewalle. A multilinear singular value decomposition. *SIAM J. Matrix Anal. Appl.*, 21(4):1253–1278, 2000.

[9] L De Lathauwer, B De Moor, and J Vandewalle. On the best rank-1 and rank-(R1,R2,...,R-N) approximation of higher-order tensors. *Siam Journal On Matrix Analysis And Applications*, 21(4):1324–1342, 2000.

[10] A. Falcó and A. Nouy. A Proper Generalized Decomposition for the solution of elliptic problems in abstract form by using a functional Eckart-Young approach. *Submmited*, 2010.

[11] V. de Silva and L.-H. Lim. Tensor rank and ill-posedness of the best low-rank approximation problem. *SIAM Journal of Matrix Analysis & Appl.*, 30(3):1084–1127, 2008.

[12] A. Doostan and G. Iaccarino. A least-squares approximation of partial differential equations with high-dimensional random inputs. *Journal of Computational Physics*, 228(12):4332–4345, 2009.

[13] D. Dureisseix, P. Ladevèze, and B. A. Schrefler. A computational strategy for multiphysics problems — application to poroelasticity. *International Journal for Numerical Methods in Engineering*, 56(10):1489–1510, 2003.

[14] Carl Eckart and Gale Young. The Approximation Of One Matrix By Another Of Lower Rank. *Psychometrika*, 1(3):211–218, 1936.

[15] T.G. Kolda. Orthogonal tensor decompositions. *SIAM J. Matrix Analysis & Applications*, 23(1):243–255, 2001.

[16] TG Kolda. A counterexample to the possibility of an extension of the Eckart-Young low-rank approximation theorem for the orthogonal rank tensor decomposition. *Siam Journal On Matrix Analysis And Applications*, 24(3):762–767, 2003.

[17] P. Ladevèze. *Nonlinear Computational Structural Mechanics - New Approaches and Non-Incremental Methods of Calculation*. Springer Verlag, 1999.

[18] P. Ladevèze and A. Nouy. On a multiscale computational strategy with time and space homogenization for structural mechanics. *Computer Methods in Applied Mechanics and Engineering*, 192:3061–3087, 2003.

[19] P. Ladevèze, J.C. Passieux, and D. Néron. The LATIN multiscale computational method and the Proper Generalized Decomposition. *Computer Methods in Applied Mechanics and Engineering*, In press.

[20] C. Le Bris, T. Lelievre, and Y. Maday. Results and questions on a nonlinear approximation approach for solving high-dimensional partial differential equations. *Constructive Approximation*, 30(3):621-651, 2009.

[21] A. Nouy. A generalized spectral decomposition technique to solve a class of linear stochastic partial differential equations. *Computer Methods in Applied Mechanics and Engineering*, 196(45-48):4521–4537, 2007.

[22] A. Nouy. Generalized spectral decomposition method for solving stochastic finite element equations: invariant subspace problem and dedicated algorithms. *Computer Methods in Applied Mechanics and Engineering*, 197:4718–4736, 2008.

[23] A. Nouy. Recent developments in spectral stochastic methods for the numerical solution of stochastic partial differential equations. *Archives of Computational Methods in Engineering*, 16(3):251–285, 2009.

[24] A. Nouy. Proper generalized decompositions and separated representations for the numerical solution of high dimensional stochastic problems. *Archives of Computational Methods in Engineering*, In press.

[25] A. Nouy. A priori model reduction through Proper Generalized Decomposition for solving time-dependent partial differential equations. *Computer Methods in Applied Mechanics and Engineering*, In press.

[26] A. Nouy and P. Ladevèze. Multiscale computational strategy with time and space homogenization: a radial-type approximation technique for solving micro problems. *International Journal for Multiscale Computational Engineering*, 170(2):557–574, 2004.

[27] A. Nouy and O.P. Le Maître. Generalized spectral decomposition method for stochastic non linear problems. *Journal of Computational Physics*, 228(1):202–235, 2009.

Algorithm 1 PGD symmetric case

1: **procedure** PGDSYM($\sum_{k=1}^{n_l} \otimes_{j=1}^{d} l_j^k, \sum_{k=1}^{n_A} \bigotimes_{j=1}^{d} A_j^k, \varepsilon, \texttt{tol}, \texttt{rank\_max}$)

2: $\quad (\mathbb{A}_j^s)_{\alpha,\beta} = (A_j^s w_j^\beta, w_j^\alpha)_j$ for $1 \leq j \leq d$ and $1 \leq s \leq n_A$.

3: $\quad (\mathbf{r}_j^k)_\alpha = (l_j^k, w_j^\alpha)_j$ for $1 \leq j \leq d$ and $1 \leq k \leq n_l$.

4: $\quad \mathbf{u} = \mathbf{0}$

5: $\quad$ **for** $i = 0, 1, 2, \dots,$ $\texttt{rank\_max}$ **do**

6: $\quad\quad$ Initialize $\mathbf{v}_i^0 \in \mathbb{R}^n$ for $i = 1, 2 \dots, d$. ▷ We solve $\min_{v \in \mathcal{S}_1} \mathcal{E}_{A^{-1} r_n}(v)$ by a fixed point strategy

7: $\quad\quad$ $\texttt{distance} \leftarrow 1.$

8: $\quad\quad$ **while** $\texttt{distance} \geq \varepsilon$ **do**

9: $\quad\quad\quad$ **for** $k = 1, 2, \dots, d$ **do**

10: $\quad\quad\quad\quad \mathbf{v}_k^1 \leftarrow \mathbf{v}_k^0$

11: $\quad\quad\quad\quad \mathbf{v}_k^0 \leftarrow \left[\sum_{s=1}^{n_A} \prod_{j=1, j\neq k}^{d} \langle \mathbf{v}_j, \mathbb{A}_j^s \mathbf{v}_j \rangle_2 \, \mathbb{A}_k^s \right]^{-1} \sum_{c=1}^{n_l} \prod_{j=1, j\neq k}^{d} \langle \mathbf{r}_j^c, \mathbf{v}_j \rangle_2 \, \mathbf{r}_k^c$

12: $\quad\quad\quad$ **end for**

13: $\quad\quad\quad$ $\texttt{distance} \leftarrow \max_{1 \leq i \leq d} \|\mathbf{v}_i^0 - \mathbf{v}_i^1\|_2$

14: $\quad\quad$ **end while**

15: $\quad\quad \mathbf{u} \leftarrow \mathbf{u} + \mathbf{v}_1^0 \otimes \cdots \otimes \mathbf{v}_d^0$

16: $\quad\quad$ **for** $k = 1, \dots, n_A$ **do** ▷ We update the residual

17: $\quad\quad\quad \mathbf{r}_j^{n_l+k} = -\mathbb{A}_j^k \mathbf{v}_j^0$ for $1 \leq j \leq d$.

18: $\quad\quad$ **end for**

19: $\quad\quad n_l \leftarrow n_l + n_A.$ ▷ Here we update the residual tensor rank

20: $\quad\quad$ $\texttt{residual(i)} = \sum_{k=1}^{n_l} \prod_{j=1}^{d} \|\mathbf{r}_j^k\|_2$

21: $\quad\quad$ **if** $\texttt{residual(i)} < \varepsilon$ or $|\texttt{residual(i)} - \texttt{residual(i)}| < \texttt{tol}$ **then goto** 13

22: $\quad\quad$ **end if**

23: $\quad$ **end for**

24: $\quad$ **return** $\mathbf{u}$ and $\texttt{residual(rank\_max)}$

25: $\quad$ **break**

26: $\quad$ **return** $\mathbf{u}$ and $\texttt{residual(i)}$

27: **end procedure**

Algorithm 2 PGD non-symmetric case

procedure PGD($\sum_{k=1}^{n_l} \otimes_{j=1}^{d} l_j^k, \sum_{k=1}^{n_A} \bigotimes_{j=1}^{d} A_j^k, \varepsilon, \texttt{tol}, \texttt{rank\_max}$)

    $(\mathbb{A}_j^{k,i})_{\alpha,\beta} = (A_j^k w_j^\beta, A_j^i w_j^\alpha)_j$ for $1 \leq j \leq d$ and $1 \leq k, i \leq n_A$.

    $(\mathbf{r}_j^{k,i})_\alpha = (l_j^k, A_j^i w_j^\alpha)_j$ for $1 \leq j \leq d$, $1 \leq k \leq n_l$ and $1 \leq i \leq n_A$.

    $\mathbf{u} = \mathbf{0}$

    for $i = 0, 1, 2, \ldots, \texttt{rank\_max}$ **do**

        Initialize $\mathbf{v}_i^0 \in \mathbb{R}^n$ for $i = 1, 2 \ldots, d$. ▷ We solve $\min_{v \in \mathcal{S}_1} \mathcal{E}_{A^{-1} r_n}(v)$ by a fixed point strategy

        $\texttt{distance} \leftarrow 1.$

        while $\texttt{distance} \geq \varepsilon$ **do**

            for $k = 1, 2, \ldots, d$ **do**

                $\mathbf{v}_k^1 \leftarrow \mathbf{v}_k^0$

$$\mathbf{v}_k^0 \leftarrow \left[\sum_{s=1}^{n_A} \sum_{t=1}^{n_A} \prod_{j=1, j \neq k}^{d} \langle \mathbf{v}_j, \mathbb{A}_j^{t,s} \mathbf{v}_j \rangle_2 \, \mathbb{A}_k^{t,s} \right]^{-1} \sum_{s=1}^{n_A} \sum_{c=1}^{n_r} \prod_{j=1, j \neq k}^{d} \langle \mathbf{r}_j^{c,s}, \mathbf{v}_j \rangle_2 \, \mathbf{r}_k^{c,s}$$

            end for

            $\texttt{distance} \leftarrow \max_{1 \leq i \leq d} \|\mathbf{v}_i^0 - \mathbf{v}_i^1\|_2$

        end while

        $\mathbf{u} \leftarrow \mathbf{u} + \mathbf{v}_1^0 \otimes \cdots \otimes \mathbf{v}_d^0$

        for $k = 1, \ldots, n_A$ **do** ▷ We update the residual

            $\mathbf{r}_j^{n_l+k,s} = -\mathbb{A}_j^{k,s} \mathbf{v}_j^0$ for $1 \leq j \leq d$ and $1 \leq s \leq n_A$.

        end for

        $n_l \leftarrow n_l + n_A$. ▷ Here we update the residual tensor rank

        $\texttt{residual(i)} == \sum_{k=1}^{n_l} \prod_{j=1}^{d} \|\mathbf{r}_j^k\|_2$

        if $\texttt{residual(i)} < \varepsilon$ or $|\texttt{residual(i)} - \texttt{residual(i)}| < \texttt{tol}$ **then goto** 13

        end if

    end for

    return $\mathbf{u}$ and $\texttt{residual(rank\_max)}$

    break

    return $\mathbf{u}$ and $\texttt{residual(i)}$

end procedure