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► **To cite this version:**

M. Azaïez, F. Ben Belgacem, J. Casado-Díaz, T. Chacón Rebollo, F. Murat. A New Algorithm of Proper Generalized Decomposition for Parametric Symmetric Elliptic Problems. *SIAM Journal on Mathematical Analysis*, 2018, 50 (5), pp.5426-5445. 10.1137/17M1137164 . hal-01939854

HAL Id: hal-01939854

<https://hal.sorbonne-universite.fr/hal-01939854>

Submitted on 3 Dec 2018

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A new Algorithm of Proper Generalized Decomposition for parametric symmetric elliptic problems

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July 18, 2018

Abstract

We introduce in this paper a new algorithm of Proper Generalized Decomposition for parametric symmetric elliptic partial differential equations. For any given dimension, we prove the existence of an optimal subspace of at most that dimension which realizes the best approximation –in mean parametric norm associated to the elliptic operator– of the error between the exact solution and the Galerkin solution calculated on the subspace. This is analogous to the best approximation property of the Proper Orthogonal Decomposition (POD) subspaces, excepting that in our case the norm is parameter-depending.

We apply a deflation technique to build a series of approximating solutions on finite-dimensional optimal subspaces, directly in the on-line step, and we prove that the partial sums converge to the continuous solution in mean parametric elliptic norm.

We show that the standard PGD for the considered parametric problem is strongly related to the deflation algorithm introduced in this paper. This opens the possibility of computing the PGD expansion by directly solving the optimization problems that yield the optimal sub-spaces.

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1 Introduction

The Karhunen-Loève’s expansion (KLE) is a widely used tool, that provides a reliable procedure for a low dimensional representation of spatiotemporal signals (see [13, 23]). It is referred to as the principal components analysis (PCA) in statistics (see [15, 17, 30]), or called singular value decomposition (SVD) in linear algebra (see [14]). It is named the proper orthogonal decomposition (POD) in mechanical computation, where it is also widely used (see [5]). Its use allows large savings of computational costs, and make affordable the solution of problems that need a large amount of solutions of parameter-depending Partial Differential Equations (see [4, 10, 16, 21, 30, 31, 32, 34]).

However the computation of the POD expansion requires to know the function to be expanded, or at least its values at the nodes of a fine enough net. This makes it rather expensive to solve parametric elliptic Partial Differential Equations (PDEs), as it requires the previous solution of the PDE for a large enough number of values of the parameter (“snapshots”) (see [18]), even if these can be located at optimal positions (see [20]). Galerkin-POD strategies are well suited to solve parabolic problems, where the POD basis is obtained from the previous solution of the underlying elliptic operator (see [19, 26]).

An alternative approach is the Proper Generalized Decomposition that iteratively computes a tensorized representation of the parameterized PDE, that separates the parameter and the independent variables, introduced in [3]. It has been interpreted as a Power type Generalized Spectral Decomposition (see [27, 28]). It has experienced a fast development, being applied to the low-dimensional tensorized solution of many applied problems. The mathematical analysis of the PGD has experienced a relevant development in the last years. The convergence of a version of the PGD for symmetric elliptic PDEs via minimization of the associated energy has been proved in [22]. Also, in [11] the convergence of a recursive approximation of the solution of a linear elliptic PDE is proved, based on the existence of optimal subspaces of rank 1 that minimize the elliptic norm of the current residual.

The present paper is aimed at the direct determination of a variety of reduced dimension for the solution of parameterized symmetric elliptic PDEs. We intend to on-line determine an optimal subspace of given dimension that yields the best approximation in mean (with respect to the parameter) of the error (in the parametric norm associated to the elliptic operator) between the exact solution and the Galerkin solution calculated on the subspace. The optimal POD sub-spaced can no longer be characterized by means of a spectral problem for a compact self-adjoint operator (the standard POD operator) and thus the spectral theory for compact self-adjoint operators does no apply. We build recursive approximations on finite-dimensional optimal subspaces by minimizing the mean parametric error of the current residual, similar to the one introduced in [11], that we prove to be strongly convergent in the “intrinsic” mean parametric elliptic norm. For this reason we call “intrinsic”PGD the method introduced.

In addition, we prove that the method introduced is a genuine extension of both POD and PGD methods, when applied to the solution of parametric elliptic equations. In particular it is strongly related to the PGD method in the sense that the standard formulation of the PGD method actually provides the optimality conditions of the minimization problem satisfied by the optimal 1D sub-spaces. As a consequence of the analysis developed in the paper, the PGD expansion is strongly convergent to the targeted solution in parametric elliptic norm, whenever it is implemented in such a way that all modes are optimal. Furthermore, the characterization of the modes by means of optimization problems opens the door to their computation by using optimization techniques, in addition to the usual Power Iteration algorithm.

The abstract framework considered includes several kind of problems of practical interest,

to which the PGD has been and continues being applied. This is the case of the design analysis in computational mechanics. For instance in the design of energy efficient devices (HVACs) or buildings, it is mandatory to address the heat equation with several structural parameters, for instance the thermal diffusivity or transmittance, and the geometric shape of the device, among others. Also, the optimal design of heterogeneous materials with linear behavior law fits into the framework considered, as the parameters model the structural configuration of the various materials (cf. [29, 33]). Moreover, in practice the structural configuration that optimizes a certain predefined criterion (e.g. construction costs, benefits, etc.) needs to take into account the unavoidable uncertainties in the structural performance. This leads to elliptic problems including modeling of the targeted uncertainty that, when the PDE model is linear, also fits into the abstract framework considered. In addition classical homogenization problems governed by linear symmetric elliptic PDEs formally also fit into this general framework, although the kind of approximation of the solution that is proposed in this work is different than the usual one, that looks for a limit averaged solution. Here we rather approximate the whole family of parameter-depending solutions by a function series.

The method, however, does not apply, for instance, to non-symmetric elliptic forms, neither to non-linear problems.

The present paper focuses on theoretical aspects: We study the existence of the intrinsic POD, and give a convergence result for the deflation algorithm. We keep the quantitative analysis of the convergence as well as numerical investigations for future works.

The paper is structured as follows: In Section 2 we state the general problem of finding optimal subspaces of a given dimension. We prove in Section 3 that there exists a solution for 1D optimal subspaces, characterized as a maximization problem with a non-linear normalization restriction. We extend this existence result in Section 4 to general dimensions. In Section 5 we use the results in Sections 3 and 4 to build a deflation algorithm to approximate the solution of a parametric family of elliptic problems and we show the convergence. Section 6 explains why the method introduced is a genuine extension of both POD and PGD algorithms, and provides a theoretical analysis for the latter. Finally in Section 7 we present the main conclusions of the paper.

2 Statement of the problem

Let H be a separable Hilbert space endowed with the scalar product (\cdot, \cdot) . The related norm is denoted by $\|\cdot\|$. We denote by $B_s(H)$ the space of bilinear, symmetric and continuous forms in H .

Assume given a measure space $(\Gamma, \mathcal{B}, \mu)$, with standard notation, so that μ is σ -finite.

Let $a \in L^\infty(\Gamma, B_s(H); d\mu)$ be such that there exists $\alpha > 0$ satisfying

$$\alpha \|u\|^2 \leq a(u, u; \gamma), \quad \forall u \in H, \quad d\mu\text{-a.e. } \gamma \in \Gamma. \quad (1)$$

For μ -a.e $\gamma \in \Gamma$, the bilinear form $a(\cdot, \cdot; \gamma)$ determines a norm uniformly equivalent to the norm $\|\cdot\|$. Moreover, $\bar{a} \in B_s(L^2(\Gamma, H; d\mu))$ defined by

$$\bar{a}(v, w) = \int_{\Gamma} a(v(\gamma), w(\gamma); \gamma) d\mu(\gamma), \quad \forall v, w \in L^2(\Gamma, H; d\mu) \quad (2)$$

defines an inner product in $L^2(\Gamma, H; d\mu)$ which generates a norm equivalent to the standard one in $L^2(\Gamma, H; d\mu)$.

Let be given a data function $f \in L^2(\Gamma, H'; d\mu)$. We are interested in the variational problem:

$$\text{Find } u(\gamma) \in H \text{ such that } a(u(\gamma), v; \gamma) = \langle f(\gamma), v \rangle, \quad \forall v \in H, \quad d\mu\text{-a.e. } \gamma \in \Gamma, \quad (3)$$

where $\langle \cdot, \cdot \rangle$ denotes the duality pairing between H' and H .

By Riesz representation theorem, problem (3) admits a unique solution for $d\mu$ -a.e. $\gamma \in \Gamma$. On the other hand, we claim that \tilde{u} solution of

$$\tilde{u} \in L^2(\Gamma, H; d\mu), \quad \bar{a}(\tilde{u}, \bar{v}) = \int_{\Gamma} \langle f(\gamma), \bar{v}(\gamma) \rangle d\mu(\gamma), \quad \forall \bar{v} \in L^2(\Gamma, H; d\mu), \quad (4)$$

also satisfies (3): Indeed taking $\bar{v} = v\chi_B$, with $v \in H$ fixed and $B \in \mathcal{B}$ arbitrary, implies that there exists a subset $N_v \in \mathcal{B}$ with $\mu(N_v) = 0$ such that

$$a(\tilde{u}(\gamma), v; \gamma) = \langle f(\gamma), v \rangle, \quad \forall \gamma \in \Gamma \setminus N_v.$$

The separability of H implies that N_v can be chosen independent of v , which proves the claim. By the uniqueness of the solution of (3) this shows that

$$\tilde{u} = u \quad d\mu\text{-a.e. } \gamma \in \Gamma. \quad (5)$$

This proves that u defined by (3) belongs to $L^2(\Gamma, H; d\mu)$ and provides an equivalent definition of u , namely, that u is the solution of (4).

Given a closed subspace Z of H , let us denote by $u_Z(\gamma)$ the solution of the Galerkin approximation of problem (3) on Z , which is defined as

$$u_Z(\gamma) \in Z, \quad a(u_Z(\gamma), z; \gamma) = \langle f(\gamma), z \rangle, \quad \forall z \in Z, \quad d\mu\text{-a.e. } \gamma \in \Gamma, \quad (6)$$

or equivalently as

$$u_Z \in L^2(\Gamma, Z; d\mu), \quad \bar{a}(u_Z, z) = \int_{\Gamma} \langle f(\gamma), z(\gamma) \rangle d\mu(\gamma), \quad \forall z \in L^2(\Gamma, Z; d\mu). \quad (7)$$

For every $k \in \mathbb{N}$, we intend to find the best subspace W of H of dimension smaller than or equal to k that minimizes the mean error (in the norm defined by \bar{a}) between u and u_W . That is, W solves

$$\min_{Z \in \mathbb{G}_{\leq k}} \bar{a}(u - u_Z, u - u_Z), \quad (8)$$

where $\mathbb{G}_{\leq k}$ is the family of subspaces of H of dimension smaller than or equal to k . Note that $\mathbb{G}_{\leq k}$ is a connected component of the Grassmannian variety $\mathbb{G}_{\leq k}$ of H , defined as

$$\mathbb{G}_{\leq k} = \bigcup_{k \geq 0} \mathbb{G}_k,$$

where \mathbb{G}_k is the set formed by all sub-spaces of H of dimension k . The set \mathbb{G}_k is a Hilbert manifold modeled in a particular Hilbert space (see [1, 25]).

Problem (8) will be proved to have a solution in Sections 3 and 4. We will then use this result in Section 5 to approximate the solution u of problem (3) by a deflation algorithm.

Note that when looking at the formulation of the minimization problem (8), it seems that solving it requires the knowledge of the solution u of (3). Such is not the case, since Proposition 2.6 below provides an equivalent formulation of (8) which does not depend on the knowledge of u but only on the data f .

Let us provide some equivalent formulations of problem (8). First we observe that

Proposition 2.1 *For every closed subspace $Z \subset H$, the function u_Z defined by (7) is also the unique solution of*

$$\min_{z \in L^2(\Gamma, Z; d\mu)} \bar{a}(u - z, u - z). \quad (9)$$

Moreover, for $d\mu$ -a.e. $\gamma \in \Gamma$, the vector $u_Z(\gamma)$ is the solution of

$$\min_{z \in Z} a(u(\gamma) - z, u(\gamma) - z; \gamma). \quad (10)$$

Proof: It is a classical property of the Galerkin approximation of the variational formulation of linear elliptic problems that u_Z satisfies (9). Indeed, the symmetry of \bar{a} gives

$$\bar{a}(u - z, u - z) = \bar{a}(u - u_Z, u - u_Z) + 2\bar{a}(u - u_Z, u_Z - z) + \bar{a}(u_Z - z, u_Z - z),$$

for every $z \in L^2(\Gamma, H; d\mu)$, where by (4), (5) and (7) the second term on the right-hand side vanishes, while the third one is nonnegative. This proves (9).

The proof of (10) is the same by taking into account (3) and (6) instead of (4) and (7). ■

As a consequence of Proposition 2.1 and definition (2) of \bar{a} , we have

Corollary 2.2 *A space $W \in \mathbb{G}_{\leq k}$ is a solution of (8) if and only if it is a solution of*

$$\min_{Z \in \mathbb{G}_{\leq k}} \min_{z \in L^2(\Gamma, Z; d\mu)} \bar{a}(u - z, u - z). \quad (11)$$

Moreover

$$\min_{Z \in \mathbb{G}_{\leq k}} \min_{z \in L^2(\Gamma, Z; d\mu)} \bar{a}(u - z, u - z) = \min_{Z \in \mathbb{G}_{\leq k}} \int_{\Gamma} \min_{z \in Z} a(u(\gamma) - z, u(\gamma) - z; \gamma) d\mu(\gamma). \quad (12)$$

Remark 2.3 *Optimization problem (11) is reminiscent of the Kolmogorov k -width related to the best approximation of the manifold $(u(\gamma))_{\gamma \in \Gamma}$ by subspaces in H with dimension k as presented in [24]. In the present minimization problem, we use the norm of $L^2(\Gamma, H; d\mu)$ instead of the norm of $L^\infty(\Gamma, H; d\mu)$ as used there. The minimization problem in [24] can indeed be written as*

$$\min_{Z \in \mathbb{G}_{\leq k}} \operatorname{esssup}_{\gamma \in \Gamma} \min_{z \in Z} a(u(\gamma) - z, u(\gamma) - z; \gamma), \quad (13)$$

if one uses $a(\cdot, \cdot; \gamma)$ as the inner product in H .

The analysis performed in the present paper is strongly based on the Hilbertian framework associated to the minimization in $L^2(\Gamma, H; d\mu)$. To the best of our knowledge few is known about problem (13), in particular there is no proof of existence of solutions. The extension to this problem of the techniques used in the present paper is far from being straightforward, and we intend to discuss this in a future paper. Indeed the $L^\infty(\Gamma, H; d\mu)$ framework is specially interesting whenever uniform error estimates with respect to the parameter are needed. This happens, for instance, when upper bounds for energy consumption (either mechanical, thermal, etc.) should be respected.

For a function $v \in L^2(\Gamma, H; d\mu)$, we denote by $R(v)$ the closure of the vectorial space spanned by $v(\gamma)$ when γ belongs to Γ ; more exactly, taking into account that v is only defined up to sets of zero measure, the correct definition of $R(v)$ is given by

$$R(v) = \bigcap_{\mu(N)=0} \overline{\operatorname{Span}\{v(\gamma) : \gamma \in \Gamma \setminus N\}}. \quad (14)$$

The following result proves that in (14) the intersection can be replaced a single closed spanned space corresponding to a single set $M \in \mathcal{B}$. This proves in particular that it does not reduce to $\{0\}$ if $R(v)$ is not zero $d\mu$ -a.e. $\gamma \in \Gamma$:

Proposition 2.4 *For every $v \in L^2(\Gamma, H; d\mu)$ there exists $M \in \mathcal{B}$, with $\mu(M) = 0$ such that*

$$R(v) = \overline{\operatorname{Span}\{v(\gamma) : \gamma \in \Gamma \setminus M\}}.$$

Proof: For every $N \in \mathcal{B}$, we define P_N as the orthogonal projection of H into

$$R_N := \overline{\operatorname{Span}\{v(\gamma) : \gamma \in \Gamma \setminus N\}}.$$

We also define P as the orthogonal projection of H into $R(v)$.

Let us first prove

$$\forall z \in H, \exists M_z \in \mathcal{B} \text{ with } \mu(M_z) = 0 \text{ such that } Pz = P_{M_z}z. \quad (15)$$

In order to prove this result, we consider $N_n \in \mathcal{B}$, with $\mu(N_n) = 0$, such that

$$\|P_{N_n}z\| \rightarrow \inf_{\mu(N)=0} \|P_Nz\|.$$

Taking $M_z = \cup_n N_n$, we have that $\mu(M_z) = 0$. Moreover, using that $N_n \subset M_z$ implies $R_{M_z} \subset R_{N_n}$, we get

$$\inf_{\mu(N)=0} \|P_Nz\| \leq \|P_{M_z}z\| \leq \|P_{N_n}z\|, \quad \forall n \geq 1.$$

Therefore

$$\|P_{M_z}z\| = \inf_{\mu(N)=0} \|P_Nz\|.$$

Now, we use that for every $N \in \mathcal{B}$ with $M_z \subset N$, $\mu(N) = 0$, we have

$$R_N \subset R_{M_z}, \quad \|P_{M_z}z\| \leq \|P_Nz\|$$

and then

$$P_Nz = P_{M_z}z, \quad \forall N \supset M_z \text{ with } \mu(N) = 0. \quad (16)$$

We take now an arbitrary $N \in \mathcal{B}$ with $\mu(N) = 0$. Using $M_z \subset N \cup M_z$, $\mu(N \cup M_z) = 0$ and (16), we get

$$P_{M_z}z = P_{N \cup M_z}z \in R_{N \cup M_z} \subset R_N, \quad \forall N \in \mathcal{B}, \text{ with } \mu(N) = 0,$$

and so, $P_{M_z}z$ belongs to $R(v)$. On the other hand, observe that $R(v) \subset R_{M_z}$ and the definition of P_{M_z} imply

$$\|z - P_{M_z}z\| \leq \|z - \eta\|, \quad \forall \eta \in R(v)$$

and thus, $P_{M_z}z = Pz$. This proves (15).

Let us now use (15) to prove the statement of Proposition 2.4. We consider an orthonormal basis $\{z_k\}$ of $R(v)^\perp$. By (15), we know that for every $k \geq 1$, there exists $M_{z_k} \in \mathcal{B}$ with $\mu(M_{z_k}) = 0$ such that $P_{M_{z_k}}z_k = 0$. Then, we define

$$M = \bigcup_{k \geq 1} M_{z_k},$$

let us prove that M satisfies the thesis of the Proposition. Clearly $\mu(M) = 0$, moreover, (16) and $M_{z_k} \subset M$ for every $k \geq 1$, imply

$$P_M e_k = 0, \quad \forall k \geq 1.$$

This shows $P_M z = 0$ for every $z \in R(v)^\perp$ and then $R(v)^\perp \subset R_M^\perp$ or equivalently $R_M \subset R(v)$. Since the other contention is immediate, we have then proved $R_M = R(v)$, which finishes the proof. \blacksquare

Taking into account (11), a new formulation of (8) is given by

Proposition 2.5 *If W is a solution of (8), then u_W is a solution of*

$$\min_{\substack{v \in L^2(\Gamma, H; d\mu) \\ \dim R(v) \leq k}} \bar{a}(u - v, u - v). \quad (17)$$

Reciprocally, if \hat{u} is a solution of (17), then $R(\hat{u})$ is a solution of (8) and $\hat{u} = u_{R(\hat{u})}$.

As announced above, the next Proposition provides an equivalent formulation for (8) which does not depend on the knowledge of the solution u of (3), but only on the data f .

Proposition 2.6 *The subspace $W \in \mathbb{G}_{\leq k}$ solves problem (8) if and only if it is a solution of the problem*

$$\max_{Z \in \mathbb{G}_{\leq k}} \int_{\Gamma} \langle f(\gamma), u_Z(\gamma) \rangle d\mu(\gamma), \quad (18)$$

where u_Z is defined by (7).

Proof: As in the proof of the first part of Proposition 2.1, one deduces from (4), (5) and (7) that

$$\bar{a}(u - u_Z, z) = 0, \quad \forall z \in L^2(\Gamma, Z; d\mu).$$

Using the symmetry of \bar{a} , we then have

$$\begin{aligned} \bar{a}(u - u_Z, u - u_Z) &= \bar{a}(u, u) - a(u_Z, u) = \bar{a}(u, u) - \bar{a}(u_Z, u_Z) \\ &= \bar{a}(u, u) - \int_{\Gamma} \langle f(\gamma), u_Z(\gamma) \rangle d\mu(\gamma). \end{aligned}$$

Thus W solves (8) if and only if it solves (18). ■

3 One-dimensional approximations

In Section 4 we shall show the existence of the solution of problem (8) for any arbitrary k . However a particularly interesting case from the point of view of the applications is $k = 1$. We dedicate this section to this special case. Observe that for $Z \in \mathbb{G}_1$, there exists $z \in H \setminus \{0\}$ such that $Z = \text{Span}\{z\}$. The problem to solve can be reformulated as follows.

Lemma 3.1 *Assume $f \not\equiv 0$. Then, the subspace $W \in \mathbb{G}_1$ solves problem (18) if and only if $W = \text{Span}\{w\}$, where w is a solution of*

$$\max_{\substack{z \in H \\ z \neq 0}} \int_{\Gamma} \frac{\langle f(\gamma), z \rangle^2}{a(z, z; \gamma)} d\mu(\gamma). \quad (19)$$

Proof: Let $Z \in \mathbb{G}_1$. Then $Z = \text{Span}\{z\}$, for some $z \in H \setminus \{0\}$, and there exists a function $\varphi : \Gamma \mapsto \mathbb{R}$ such that

$$u_Z(\gamma) = \varphi(\gamma) z, \quad d\mu\text{-a.e. } \gamma \in \Gamma.$$

As $z \neq 0$, then, as $u_Z(\gamma)$ is the solution to the variational equation (6), we derive that

$$\varphi(\gamma) = \frac{\langle f(\gamma), z \rangle}{a(z, z; \gamma)}, \quad d\mu\text{-a.e. } \gamma \in \Gamma.$$

Using this formula we obtain that

$$\int_{\Gamma} \langle f, u_Z(\gamma) \rangle d\gamma = \int_{\Gamma} \frac{\langle f(\gamma), z \rangle^2}{a(z, z; \gamma)} d\mu(\gamma). \quad (20)$$

If the maximum in (18) is obtained by a space of dimension one, then formula (20) proves the desired result.

In contrast, if the maximum in (18) is obtained by the null space, then the maximum in \mathbb{G}_1 is equal to zero. Therefore the right-hand side of (20) is zero for every $z \in H$, which implies that $f = 0$ $d\mu$ -a.e. in Γ , in contradiction with the assumption $f \not\equiv 0$. ■

Remark 3.2 *Since the integrand which appears in (19) is homogenous of degree zero in z , problem (19) is equivalent to*

$$\max_{\substack{z \in H \\ \|z\|=1}} \int_{\Gamma} \frac{\langle f(\gamma), z \rangle^2}{a(z, z; \gamma)} d\mu(\gamma).$$

We now prove the existence of a solution to problem (19).

Theorem 3.3 *Assume $f \not\equiv 0$. Problem (19) admits at least a solution.*

Note that if $f \equiv 0$, then, every vector $w \in H \setminus \{0\}$ is a solution of (19).

Proof: Define

$$M^* := \sup_{\substack{z \in H \\ \|z\|=1}} \int_{\Gamma} \frac{\langle f(\gamma), z \rangle^2}{a(z, z; \gamma)} d\mu(\gamma), \quad (21)$$

and consider a sequence $w_n \subset H$, with $\|w_n\| = 1$ such that

$$\lim_{n \rightarrow \infty} \int_{\Gamma} \frac{\langle f(\gamma), w_n \rangle^2}{a(w_n, w_n; \gamma)} d\mu(\gamma) = M^*. \quad (22)$$

Up to a subsequence, we can assume the existence of $w \in H$, such that w_n converges weakly in H to w . Taking into account that $f(\gamma) \in H'$, $a(\cdot, \cdot, \gamma) \in B_s(H)$ $d\mu$ -a.e. $\gamma \in \Gamma$ and (1) is satisfied, we get

$$\lim_{n \rightarrow \infty} \langle f(\gamma), w_n \rangle = \langle f(\gamma), w \rangle, \quad d\mu\text{-a.e. } \gamma \in \Gamma, \quad (23)$$

$$\liminf_{n \rightarrow \infty} a(w_n, w_n; \gamma) \geq a(w, w; \gamma), \quad d\mu\text{-a.e. } \gamma \in \Gamma. \quad (24)$$

On the other hand, we observe that (1) and $\|w_n\| = 1$ imply

$$|\langle f(\gamma), w_n \rangle| \leq \|f(\gamma)\|_{H'}, \quad \frac{1}{a(w_n, w_n; \gamma)} \leq \frac{1}{\alpha} \quad d\mu\text{-a.e. } \gamma \in \Gamma. \quad (25)$$

If $w = 0$, then (23), (25) and Lebesgue's dominated convergence theorem imply

$$\lim_{n \rightarrow \infty} \int_{\Gamma} \frac{\langle f(\gamma), w_n \rangle^2}{a(w_n, w_n; \gamma)} d\mu(\gamma) = 0,$$

which by (22) is equivalent to $M^* = 0$. Taking into account (1) and the definition (21) of M^* , this is only possible if $f \equiv 0$ is the null function. As we are assuming $f \not\equiv 0$, we conclude that w is different of zero. Then, (25) proves

$$0 \leq \frac{\|f(\gamma)\|_{H'}^2}{\alpha} - \frac{\langle f(\gamma), w_n \rangle^2}{a(w_n, w_n; \gamma)}, \quad d\mu\text{-a.e. } \gamma \in \Gamma,$$

while (23) and (24) prove

$$\liminf_{n \rightarrow \infty} \left(\frac{\|f(\gamma)\|_{H'}^2}{\alpha} - \frac{\langle f(\gamma), w_n \rangle^2}{a(w_n, w_n; \gamma)} \right) \geq \frac{\|f(\gamma)\|_{H'}^2}{\alpha} - \frac{\langle f(\gamma), w \rangle^2}{a(w, w; \gamma)}, \quad d\mu\text{-a.e. } \gamma \in \Gamma. \quad (26)$$

Using (22), Fatou's lemma implies

$$\begin{aligned} \int_{\Gamma} \left(\frac{\|f(\gamma)\|_{H'}^2}{\alpha} - \frac{\langle f(\gamma), w \rangle^2}{a(w, w; \gamma)} \right) d\mu(\gamma) &\leq \liminf_{n \rightarrow \infty} \int_{\Gamma} \left(\frac{\|f(\gamma)\|_{H'}^2}{\alpha} - \frac{\langle f(\gamma), w_n \rangle^2}{a(w_n, w_n; \gamma)} \right) d\mu(\gamma) \\ &= \int_{\Gamma} \frac{\|f(\gamma)\|_{H'}^2}{\alpha} d\mu(\gamma) - M^*, \end{aligned}$$

or equivalently

$$M^* \leq \int_{\Gamma} \frac{\langle f(\gamma), w \rangle^2}{a(w, w; \gamma)} d\mu(\gamma). \quad (27)$$

By definition (21) of M^* , this proves that the above inequality is an equality and that w is a solution of (19). \blacksquare

Remark 3.4 *Actually, in place of (26), one has the stronger result*

$$\liminf_{n \rightarrow \infty} \left(\frac{\|f(\gamma)\|_{H'}^2}{\alpha} - \frac{\langle f(\gamma), w_n \rangle^2}{a(w_n, w_n; \gamma)} \right) = \frac{\|f(\gamma)\|_{H'}^2}{\alpha} - \frac{\langle f(\gamma), w \rangle^2}{\liminf_{n \rightarrow \infty} a(w_n, w_n; \gamma)}, \quad d\mu\text{-a.e. } \gamma \in \Gamma,$$

which by the proof used to prove (27) shows

$$M^* \leq \int_{\Gamma} \frac{\langle f(\gamma), w \rangle^2}{\liminf_{n \rightarrow \infty} a(w_n, w_n; \gamma)} d\mu(\gamma).$$

Combined with

$$M^* = \int_{\Gamma} \frac{\langle f(\gamma), w \rangle^2}{a(w, w; \gamma)} d\mu(\gamma)$$

and (24), this implies

$$a(w, w; \gamma) = \liminf_{n \rightarrow \infty} a(w_n, w_n; \gamma) \quad d\mu\text{-a.e. } \gamma \in \Gamma \quad \text{such that } \langle f(\gamma), w \rangle \neq 0.$$

By (1) and $f \neq 0$, this proves the existence of a subsequence of w_n which converges strongly to w a. e. γ .

Since this proof can be carried out by replacing w_n by any subsequence of w_n , we conclude that the whole sequence w_n (which we extracted just after (22) assuming that it converges weakly to some w) actually converges strongly to w .

The above result may be used to build a computable approximation of a solution of (19). Indeed, for $f \neq 0$, let $\{H_n\}_{n \geq 1}$ be an internal approximation of H , that is a sequence of subspaces of finite dimension of H such that

$$\lim_{n \rightarrow \infty} \inf_{\psi \in H_n} \|z - \psi\| = 0, \quad \forall z \in H.$$

and consider a solution w_n of

$$\max_{\substack{z \in H_n \\ \|z\|=1}} \int_{\Gamma} \frac{\langle f(\gamma), z \rangle^2}{a(z, z; \gamma)} d\mu(\gamma).$$

The existence of such a w_n can be obtained by reasoning as in the proof of Theorem 3.3 or just using Weierstrass theorem because the dimension of H_n is finite.

Taking \tilde{w} a solution of (19) and a sequence $\tilde{w}_n \in H_n$ converging to \tilde{w} in H , we have

$$\begin{aligned} \int_{\Gamma} \frac{\langle f(\gamma), \tilde{w} \rangle^2}{a(\tilde{w}, \tilde{w}; \gamma)} d\mu(\gamma) &= \lim_{n \rightarrow \infty} \int_{\Gamma} \frac{\langle f(\gamma), \tilde{w}_n \rangle^2}{a(\tilde{w}_n, \tilde{w}_n; \gamma)} d\mu(\gamma) \\ &\leq \liminf_{n \rightarrow \infty} \int_{\Gamma} \frac{\langle f(\gamma), w_n \rangle^2}{a(w_n, w_n; \gamma)} d\mu(\gamma) \leq \limsup_{n \rightarrow \infty} \int_{\Gamma} \frac{\langle f(\gamma), w_n \rangle^2}{a(w_n, w_n; \gamma)} d\mu(\gamma) \leq \int_{\Gamma} \frac{\langle f(\gamma), \tilde{w} \rangle^2}{a(\tilde{w}, \tilde{w}; \gamma)} d\mu(\gamma), \end{aligned}$$

and thus

$$\lim_{n \rightarrow \infty} \int_{\Gamma} \frac{\langle f(\gamma), w_n \rangle^2}{a(w_n, w_n; \gamma)} d\mu(\gamma) = \int_{\Gamma} \frac{\langle f(\gamma), \tilde{w} \rangle^2}{a(\tilde{w}, \tilde{w}; \gamma)} d\mu(\gamma) = M^*.$$

This proves that the sequence w_n satisfies (22). Therefore any subsequence of w_n which converges weakly to some w converges strongly to w which is a solution of (19).

4 Higher-dimensional approximations

This section is devoted to the proof of the existence of an optimal subspace which is solution of (8) when $k \geq 1$ is any given number.

Theorem 4.1 *For any given $k \geq 1$, problem (8) admits at least one solution.*

Proof: As in the proof of Theorem 3.3, we use the direct method of the Calculus of Variations. Denoting by m_k

$$m_k = \inf_{Z \in \mathbb{G}_{\leq k}} \bar{a}(u - u_Z, u - u_Z), \quad (28)$$

we consider a sequence of spaces $W_n \in \mathbb{G}_{\leq k}$ such that $w_n := u_{W_n}$ satisfies

$$\lim_{n \rightarrow \infty} \bar{a}(u - w_n, u - w_n) = m_k. \quad (29)$$

Taking into account that by Proposition 2.1

$$Z \subset \tilde{Z} \implies \bar{a}(u - u_{\tilde{Z}}, u - u_{\tilde{Z}}) \leq \bar{a}(u - u_Z, u - u_Z), \quad (30)$$

we can assume that the dimension of W_n is equal to k . Moreover, we observe that (29) implies that w_n is bounded in $L^2(\Gamma, H; d\mu)$.

Let (z_n^1, \dots, z_n^k) be an orthonormal basis of W_n . It holds

$$w_n(\gamma) = \sum_{j=1}^k (w_n(\gamma), z_n^j) z_n^j, \quad d\mu\text{-a.e. } \gamma \in \Gamma. \quad (31)$$

Since the norm of the vectors z_n^j is one, there exists a subsequence of n and k vectors $z^j \in H$ such that

$$z_n^j \rightharpoonup z^j \text{ in } H, \quad \forall j \in \{1, \dots, k\}. \quad (32)$$

Using also

$$|(w_n(\gamma), z_n^j)| \leq \|w_n(\gamma)\|, \quad d\mu\text{-a.e. } \gamma \in \Gamma,$$

we get that (w_n, z_n^j) is bounded in $L^2(\Gamma, H; d\mu)$ for every j and thus, there exists a subsequence of n and k functions $p^j \in L^2(\Gamma; d\mu)$ such that

$$(w_n, z_n^j) \rightharpoonup p^j \text{ in } L^2(\Gamma, H; d\mu), \quad \forall j \in \{1, \dots, k\}. \quad (33)$$

We claim that

$$w_n \rightharpoonup w := \sum_{j=1}^k p^j z^j \text{ in } L^2(\Gamma; d\mu). \quad (34)$$

Indeed, taking into account that w_n is bounded in $L^2(\Gamma, H; d\mu)$ and (31), it is enough to show

$$\lim_{n \rightarrow \infty} \int_{\Gamma} ((w_n, z_n^j) z_n^j, \varphi v) d\mu(\gamma) = \int_{\Gamma} (p^j z^j, \varphi v) d\mu(\gamma), \quad \forall \varphi \in L^2(\Gamma; d\mu), \quad \forall v \in H. \quad (35)$$

This is a simple consequence of

$$\int_{\Gamma} ((w_n, z_n^j) z_n^j, \varphi v) d\mu(\gamma) = (z_n^j, v) \int_{\Gamma} (w_n, z_n^j) \varphi d\mu(\gamma),$$

combined with (32) and (33).

From the continuity and convexity of the quadratic form associated to \bar{a} , as well as from (34) and (29), we have

$$\bar{a}(u - w, u - w) \leq \lim_{n \rightarrow \infty} \bar{a}(u - w_n, u - w_n) = m_k. \quad (36)$$

Using that $W = \text{Span}\{z^1, \dots, z^k\} \in \mathbb{G}_{\leq k}$, and that (see Proposition 2.1)

$$\bar{a}(u - u_W, u - u_W) \leq \bar{a}(u - w, u - w), \quad (37)$$

we conclude that W is a solution of (8). ■

Remark 4.2 From (36), (37), definition (28) of m_k and Proposition 2.1, we have that $w = u_W$ in the proof of Theorem 4.1. Moreover,

$$\bar{a}(u - w, u - w) = m_k = \lim_{n \rightarrow \infty} \bar{a}(u - w_n, u - w_n),$$

which combined with (34) proves that w_n converges strongly to w in $L^2(\Gamma, H; d\mu)$. As in Remark 3.4, this can be used to build a strong approximation of a solution of (8) by using an internal approximation of H .

5 An iterative algorithm by deflation

In the previous section, for any given $k \geq 1$, we have proved the existence of an optimal subspace for problem (8). We use here this fact to build an iterative approximation of the solution of (3) by a deflation approach. We build recursive approximations on finite-dimensional optimal subspaces by minimizing the mean parametric error of the current residual, similar to the one introduced in [11]. Let us denote

$$\Pi_k(v) = \left\{ v_W \mid W \text{ solves } \min_{Z \in \mathbb{G}_{\leq k}} \bar{a}(v - v_Z, v - v_Z), \right\}, \quad \forall v \in L^2(\Gamma, H; d\mu). \quad (38)$$

where v_Z is defined by (7)

The deflation algorithm is as follows

- Initialization:

$$u_0 = 0 \quad (39)$$

- Iteration: Assuming $u_{i-1} \in H$ known for $i = 1, 2, \dots$, set

$$e_{i-1} = u - u_{i-1}, \text{ choose } s_i \in \Pi_k(e_{i-1}), \text{ and define } u_i = u_{i-1} + s_i. \quad (40)$$

Remark 5.1 Note that s_i (and therefore u_i) in general is not defined in a unique way.

Note also that the algorithm (40) does not need the knowledge of the solution u of (4), since $e_{i-1} = u - u_{i-1}$ is directly defined from f and u_{i-1} by

$$\begin{cases} e_{i-1} \in L^2(\Gamma, H; d\mu), \\ \bar{a}(e_{i-1}, v) = \int_{\Gamma} \langle f(\gamma), v(\gamma) \rangle d\mu(\gamma) - \bar{a}(u_{i-1}, v), \quad \forall v \in L^2(\Gamma, H; d\mu). \end{cases} \quad (41)$$

Then Proposition 2.6 applied to the case where f is replaced by the function f_i defined by

$$\int_{\Gamma} \langle f_i(\gamma), v(\gamma) \rangle d\mu(\gamma) = \int_{\Gamma} \langle f(\gamma), v(\gamma) \rangle d\mu(\gamma) - \bar{a}(u_{i-1}, v), \quad \forall v \in L^2(\Gamma, H; d\mu), \quad (42)$$

proves that

$$s_i \in \Pi_k(e_{i-1}) \iff s_i = (e_{i-1})W_i,$$

where W_i is a solution of

$$\max_{Z \in \mathbb{G}_{\leq k}} \left\{ \int_{\Gamma} \langle f(\gamma), (e_{i-1})_Z(\gamma) \rangle d\mu(\gamma) - \bar{a}(u_{i-1}, (e_{i-1})_Z) \right\}, \quad (43)$$

where, in accordance to (7), $(e_{i-1})_Z$ denotes the solution of

$$\begin{cases} (e_{i-1})_Z \in L^2(\Gamma, Z; d\mu), \\ \bar{a}((e_{i-1})_Z, z) = \int_{\Gamma} \langle f(\gamma), z(\gamma) \rangle d\mu(\gamma) - \bar{a}(u_{i-1}, z), \quad \forall z \in L^2(\Gamma, Z; d\mu). \end{cases} \quad (44)$$

This observation allows one to carry out the iterative process without knowing the function u .

Note also that

$$u_i = \sum_{j=1}^i s_j,$$

namely that u_i is the partial sum of the series $\sum_{j \geq 1} s_j$.

Remark 5.2 In this remark we take $k = 1$. Then every space of $\mathbb{G}_{\leq 1}$ is spanned by an element of H , and in particular $W_i = \text{Span}\{w_i\}$ for some $w_i \in H$, then $u_i(\gamma) = \sum_{j=1}^i \Phi_j(\gamma) w_j$, where $\Phi_j(\gamma) \in L^2(\Gamma, d\mu)$ is defined by $s_j = \Phi_j(\gamma) w_j$. Note also that if $w_i = 0$ for some $i \geq 0$, then $f_i = 0$ and thus $u \equiv u_{i-1}$,

The convergence of the algorithm is given by the following theorem. Its proof follows the ideas of [11].

Theorem 5.3 The sequence u_i provided by the least-squares PGD algorithm (39)-(40) strongly converges in $L^2(\Gamma, H; d\mu)$ to the parameterized solution $\gamma \in \Gamma \mapsto u(\gamma) \in H$ of problem (3).

Remark 5.4 In view of the last assertion of Remark 5.1, Theorem 5.3 proves that the series $\sum_{j \geq 1} s_j$ converges in $L^2(\Gamma, H; d\mu)$ to the parametrized solution $\gamma \in \Gamma \mapsto u(\gamma) \in H$ of problem (3).

When $k = 1$, Remark 5.2 implies that the series $\sum_{j \geq 1} \Phi_j(\gamma) w_j$ converges in $L^2(\Gamma, H; d\mu)$ to this parametrized solution.

Proof: By (40) and Proposition 2.5 applied to the case where u is replaced by e_{i-1} , we have that s_i is a solution of

$$\min_{\substack{v \in L^2(\Gamma, H; d\mu) \\ \dim R(v) \leq k}} \bar{a}(e_{i-1} - v, e_{i-1} - v). \quad (45)$$

This proves in particular that s_i is a solution of

$$\min_{\substack{v \in L^2(\Gamma, H; d\mu) \\ R(v) \subset R(s_i)}} \bar{a}(e_{i-1} - v, e_{i-1} - v),$$

and therefore

$$\bar{a}(e_{i-1} - s_i, v) = 0, \quad \forall v \in L^2(\Gamma, H; d\mu) \text{ with } R(v) \subset R(s_i).$$

But (40) implies that

$$e_{i-1} - s_i = e_i, \quad (46)$$

which gives

$$\bar{a}(e_i, v) = 0, \quad \forall v \in L^2(\Gamma, H; d\mu) \text{ with } R(v) \subset R(s_i). \quad (47)$$

Taking $v = s_i$ and using again (46) we get

$$\bar{a}(e_{i-1}, e_{i-1}) = \bar{a}(s_i, s_i) + \bar{a}(e_i, e_i), \quad \forall i \geq 1, \quad (48)$$

and therefore

$$\bar{a}(e_i, e_i) + \sum_{j=1}^i \bar{a}(s_j, s_j) = \bar{a}(e_0, e_0), \quad \forall i \geq 1. \quad (49)$$

Thus, we have

$$e_i \text{ is bounded in } L^2(\Gamma, H; d\mu), \quad (50)$$

$$\sum_{j=1}^{\infty} \bar{a}(s_j, s_j) \leq \bar{a}(e_0, e_0). \quad (51)$$

By (50), there exists a subsequence e_{i_n} of e_i and $e \in L^2(\Gamma, H; d\mu)$, such that

$$e_{i_n} \rightharpoonup e \text{ in } L^2(\Gamma, H; d\mu). \quad (52)$$

On the other hand, since s_{i_n+1} is a solution of (45) with $i-1$ replaced by i_n , we get

$$\begin{aligned} \bar{a}(e_{i_n} - s_{i_n+1}, e_{i_n} - s_{i_n+1}) &\leq \bar{a}(e_{i_n} - v, e_{i_n} - v) = \bar{a}(e_{i_n}, e_{i_n}) - 2\bar{a}(e_{i_n}, v) + \bar{a}(v, v), \\ \forall v \in L^2(\Gamma, H; d\mu), \dim R(v) &\leq k, \end{aligned} \quad (53)$$

and then

$$\bar{a}(e_{i_n} - s_{i_n+1}, e_{i_n} - s_{i_n+1}) - \bar{a}(e_{i_n}, e_{i_n}) \leq -2\bar{a}(e_{i_n}, v) + \bar{a}(v, v), \quad \forall v \in L^2(\Gamma, H; d\mu), \dim R(v) \leq k,$$

or in other terms

$$-2\bar{a}(e_{i_n}, s_{i_n+1}) + \bar{a}(s_{i_n+1}, s_{i_n+1}) \leq -2\bar{a}(e_{i_n}, v) + \bar{a}(v, v), \quad \forall v \in L^2(\Gamma, H; d\mu), \dim R(v) \leq k.$$

Thanks to (50) and (51), the left-hand side tends to zero when n tends to infinity, while in the right-hand side we can pass to the limit by (52). Thus, we have

$$2\bar{a}(e, v) \leq \bar{a}(v, v), \quad \forall v \in L^2(\Gamma, H; d\mu), \dim R(v) \leq k.$$

Replacing in this equality v by tv with $t > 0$, dividing by t , letting t tend to zero and writing the resulting inequality for v and $-v$, we get

$$\bar{a}(e, v) = 0, \quad \forall v \in L^2(\Gamma, H; d\mu), \dim R(v) \leq k.$$

Taking $v = w\varphi$, with $w \in H$, $\varphi \in L^2(\Gamma; d\mu)$, and recalling definition (2) of \bar{a} we deduce

$$\int_{\Gamma} a(e(\gamma), w; \gamma) \varphi(\gamma) d\mu(\gamma) = 0, \quad \forall z \in H, \forall \varphi \in L^2(\Gamma; d\mu),$$

and then for any $w \in H$, there exists a subset $N_w \in \mathcal{B}$ with $\mu(N_w) = 0$ such that

$$a(e(\gamma), w; \gamma) = 0, \quad \forall \gamma \in \Gamma \setminus N_w.$$

The separability of H implies that N_w can be chosen independent of w , and then we have

$$a(e(\gamma), w; \gamma) = 0, \quad \forall w \in H, \text{ } d\mu\text{-a.e. } \gamma \in \Gamma,$$

and therefore

$$e(\gamma) = 0 \quad d\mu\text{-a.e. } \gamma \in \Gamma. \quad (54)$$

This proves that e does not depend on the subsequence in (52) and that

$$e_i \rightharpoonup 0 \text{ in } L^2(\Gamma, H; d\mu). \quad (55)$$

Let us now prove that in (55) the convergence is strong in $L^2(\Gamma, H; d\mu)$. We use that thanks to (46), we have

$$e_i = -\sum_{j=1}^i s_j + e_0, \quad \forall i \geq 1,$$

and so,

$$\bar{a}(e_i, e_i) = - \sum_{j=1}^i \bar{a}(e_i, s_j) + \bar{a}(e_i, e_0), \quad \forall i \geq 1. \quad (56)$$

In order to estimate the right-hand side of the latest equality, we introduce, for $i, j \geq 1$, the function $z_{i,j}$ as the solution of

$$z_{i,j} \in L^2(\Gamma, \mathbb{R}(s_j); d\mu), \quad \bar{a}(z_{i,j}, v) = \bar{a}(e_{i-1}, v), \quad \forall v \in L^2(\Gamma, \mathbb{R}(s_j); d\mu). \quad (57)$$

We have

$$|\bar{a}(e_{i-1}, s_j)| = |\bar{a}(z_{i,j}, s_j)| \leq \bar{a}(z_{i,j}, z_{i,j})^{\frac{1}{2}} \bar{a}(s_j, s_j)^{\frac{1}{2}}. \quad (58)$$

Using (48), (46), the fact that s_i is a solution of (45) and $\dim \mathbb{R}(s_j) \leq k$

$$\bar{a}(e_{i-1}, e_{i-1}) - \bar{a}(s_i, s_i) = \bar{a}(e_{i-1} - s_i, e_{i-1} - s_i) \leq \bar{a}(e_{i-1} - z_{i,j}, e_{i-1} - z_{i,j}).$$

Expanding the right-hand side and using $v = z_{i,j}$ in (57) this gives

$$\bar{a}(z_{i,j}, z_{i,j}) \leq \bar{a}(s_i, s_i),$$

which combined with (58) provides the estimate

$$|\bar{a}(e_{i-1}, s_j)| \leq \bar{a}(s_i, s_i)^{\frac{1}{2}} \bar{a}(s_j, s_j)^{\frac{1}{2}}, \quad \forall i, j \geq 1.$$

Using the latest estimate in (56) and then Cauchy-Schwarz's inequality, we get

$$\left\{ \begin{array}{l} \bar{a}(e_i, e_i) \leq \bar{a}(s_{i+1}, s_{i+1})^{\frac{1}{2}} \sum_{j=1}^i \bar{a}(s_j, s_j)^{\frac{1}{2}} + \bar{a}(e_i, e_0) \\ \leq \bar{a}(s_{i+1}, s_{i+1})^{\frac{1}{2}} i^{\frac{1}{2}} \left(\sum_{j=1}^{\infty} \bar{a}(s_j, s_j) \right)^{\frac{1}{2}} + \bar{a}(e_i, e_0), \quad \forall i \geq 1. \end{array} \right. \quad (59)$$

But the criterion of comparison of two series with nonnegative terms and the facts that (see (51))

$$\sum_{i=1}^{\infty} \frac{1}{i} = \infty, \quad \sum_{i=1}^{\infty} \bar{a}(s_i, s_i) < \infty,$$

prove that

$$\liminf_{i \rightarrow \infty} \bar{a}(s_{i+1}, s_{i+1}) i = \liminf_{i \rightarrow \infty} \frac{\bar{a}(s_{i+1}, s_{i+1})}{\frac{1}{i}} = 0.$$

Since $\bar{a}(e_i, e_i)$ is a decreasing sequence by (48) and since (55) asserts that e_i converges weakly to zero, we can pass to the limit in (59), to deduce

$$\begin{aligned} \lim_{i \rightarrow \infty} \bar{a}(e_i, e_i) &= \liminf_{i \rightarrow \infty} \bar{a}(e_i, e_i) \\ &\leq \liminf_{i \rightarrow \infty} \left(\bar{a}(s_{i+1}, s_{i+1})^{\frac{1}{2}} i^{\frac{1}{2}} \left(\sum_{j=1}^{\infty} \bar{a}(s_j, s_j) \right)^{\frac{1}{2}} + \bar{a}(e_i, e_0) \right) = 0. \end{aligned}$$

This proves that e_i converges strongly to zero in $L^2(\Gamma, H; d\mu)$. Since $e_i = u - u_i$ this finishes the proof of Theorem 5.3. \blacksquare

Remark 5.5 *In many cases the corrections s_i decrease exponentially in the sense that:*

$$\|s_i\| = O(\rho^{-i}) \text{ as } i \rightarrow +\infty, \text{ for some } \rho > 1,$$

where $\|\cdot\|$ denotes the norm in $L^2(\Gamma, H; d\mu)$. This occurs in particular for the standard POD expansion when Γ is an open set of \mathbb{R}^N , μ is the Lebesgue measure and the function $f = f(\gamma)$ is analytic with respect to γ (see [7]). Then $\|s_i\|$ is a good estimator for the error $\|u - u_i\|$.

6 Relationship with POD and PGD methods

The “intrinsic” PGD method developed in the previous sections is a genuine extension of both POD and PGD method.

Indeed, to analyze the connexions with the POD method, let us consider the problem studied in [11], namely

$$(P_k)' \quad \min_{Z \in \mathbb{G}_{\leq k}} \int_{\Gamma} (u(\gamma) - u_Z(\gamma), u(\gamma) - u_Z(\gamma))_H d\mu(\gamma), \quad (60)$$

where $(\cdot, \cdot)_H$ is an inner product on H . In this case a solution of $(P_k)'$ is the space generated by the first k eigenfunctions of the POD operator $\mathcal{P} : H \mapsto H$, which is given by (see below)

$$\mathcal{P}(v) = \int_{\Gamma} (u(\gamma), v)_H u(\gamma) d\mu(\gamma), \quad \forall v \in H.$$

In the present case, due the dependence of a with respect to γ , it does not seem that the problem can be reduced to a spectral problem.

As an example, from now on we fix in this Section

$$k = 1.$$

Then problem (17) can be written as

$$\min_{v \in H, \varphi \in L^2(\Gamma; d\mu)} \int_{\Gamma} a(u(\gamma) - \varphi(\gamma)v, u(\gamma) - \varphi(\gamma)v; \gamma) d\mu(\gamma). \quad (61)$$

Note that problem (61) has at least a solution (see Section 3 above). So, taking the derivative of the functional

$$(v, \varphi) \in H \times L^2(\Gamma; d\mu) \mapsto \int_{\Gamma} a(u(\gamma) - \varphi(\gamma)v, u(\gamma) - \varphi(\gamma)v; \gamma) d\mu(\gamma),$$

we deduce that if $(w, \psi) \in H \times L^2(\Gamma; d\mu)$ is a solution of (61), with $w \neq 0$, then

$$\psi(\gamma) = \frac{a(u(\gamma), w; \gamma)}{a(w, w; \gamma)}, \quad d\mu\text{-a.e. } \gamma \in \Gamma, \quad (62)$$

and w is a solution of the non-linear variational problem

$$\int_{\Gamma} \frac{a(u(\gamma), w; \gamma)}{a(w, w; \gamma)} a(u(\gamma), v; \gamma) d\mu(\gamma) = \int_{\Gamma} \frac{a(u(\gamma), w; \gamma)^2}{a(w, w; \gamma)^2} a(w, v; \gamma) d\mu(\gamma), \quad \forall v \in H. \quad (63)$$

Note that if $w = 0$,

$$\int_{\Gamma} a(u(\gamma) - \varphi(\gamma)v, u(\gamma) - \varphi(\gamma)v; \gamma) d\mu(\gamma) \geq \int_{\Gamma} a(u(\gamma), u(\gamma); \gamma) d\mu(\gamma), \quad \forall v \in H, \forall \varphi \in L^2(\Gamma, d\mu).$$

This implies that $u = 0$ and therefore $f = 0$.

If a does not depend on γ , statement (63) can be written as

$$a \left(\int_{\Gamma} a(u(\gamma), w) u(\gamma) d\mu(\gamma), v \right) = a \left(\frac{\int_{\Gamma} a(u(\gamma), w)^2 d\mu(\gamma)}{a(w, w)} w, v \right), \quad \forall v \in H,$$

which implies that

$$\int_{\Gamma} a(u(\gamma), w) u(\gamma) d\mu(\gamma) = \frac{\int_{\Gamma} a(u(\gamma), w)^2 d\mu(\gamma)}{a(w, w)} w,$$

which proves that w is an eigenvector of the operator

$$v \in H \mapsto \mathcal{P}(v) = \int_{\Gamma} a(u(\gamma), v) u(\gamma) d\mu(\gamma)$$

for the eigenvalue

$$\frac{\int_{\Gamma} a(u(\gamma), w)^2 d\mu(\gamma)}{a(w, w)}.$$

In contrast, when a depends on γ it does not seem that problem (63) corresponds to an eigenvalue problem.

To analyze the relationship with the PGD method, let us remember that this method approximates the solution u of problem (8) by a series similar to that provided by the deflation algorithm introduced in Section 5, namely

$$u(\gamma) = \sum_{i \geq 1} \tilde{\Phi}_i(\gamma) \tilde{w}_i,$$

where the pair $(\tilde{\Phi}_i, \tilde{w}_i) \in L^2(\Gamma, d\mu) \times H$ is recursively obtained as a solution of the non-linear coupled problems

$$\begin{cases} \int_{\Gamma} a(\tilde{\Phi}_i(\gamma) \tilde{w}_i, \tilde{\Phi}_i(\gamma) v; \gamma) d\mu(\gamma) = \int_{\Gamma} \langle \tilde{f}_i(\gamma), \tilde{\Phi}_i(\gamma) v \rangle d\mu(\gamma), \quad \forall v \in H, \\ \int_{\Gamma} a(\tilde{\Phi}_i(\gamma) \tilde{w}_i, \tilde{\Phi}^*(\gamma) \tilde{w}_i; \gamma) d\mu(\gamma) = \int_{\Gamma} \langle \tilde{f}_i(\gamma), \tilde{\Phi}^*(\gamma) \tilde{w}_i \rangle d\mu(\gamma), \quad \forall \tilde{\Phi}^* \in L^2(\Gamma, d\mu), \end{cases} \quad (64)$$

where $\tilde{f}_1 = f$, and \tilde{f}_i is defined by

$$\int_{\Gamma} \langle \tilde{f}_i(\gamma), v(\gamma) \rangle d\mu(\gamma) = \int_{\Gamma} \langle f(\gamma), v(\gamma) \rangle d\mu(\gamma) - \bar{a}(\tilde{u}_{i-1}, v), \quad \forall v \in L^2(\Gamma, H; d\mu), \quad (65)$$

with

$$\tilde{u}_{i-1}(\gamma) = \sum_{j=1}^{i-1} \tilde{\Phi}_j(\gamma) \tilde{w}_j, \quad \text{for } i \geq 2. \quad (66)$$

If problem (64) admits a solution such that $\tilde{w}_i \neq 0$, then the second equation in (64) is equivalent to,

$$a(\tilde{\Phi}_i(\gamma) \tilde{w}_i, \tilde{w}_i; \gamma) = \langle \tilde{f}_i(\gamma), \tilde{w}_i \rangle d\mu - \text{a. e. } \gamma \in \Gamma,$$

which in turn is equivalent to

$$\tilde{\Phi}_i(\gamma) = \frac{\langle \tilde{f}_i(\gamma), \tilde{w}_i \rangle}{a(\tilde{w}_i, \tilde{w}_i; \gamma)} d\mu - \text{a. e. } \gamma \in \Gamma. \quad (67)$$

Then the first equation in (64), is equivalent to the non-linear variational problem

$$\tilde{w}_i \in H, \quad \int_{\Gamma} \frac{\langle \tilde{f}_i(\gamma), \tilde{w}_i \rangle}{a(\tilde{w}_i, \tilde{w}_i; \gamma)} \langle \tilde{f}_i(\gamma), v \rangle d\mu(\gamma) = \int_{\Gamma} \frac{\langle \tilde{f}_i(\gamma), \tilde{w}_i \rangle^2}{a(\tilde{w}_i, \tilde{w}_i; \gamma)^2} a(\tilde{w}_i, v; \gamma) d\mu(\gamma), \quad \forall v \in H. \quad (68)$$

Note that this problem is just problem (63) with w replaced by \tilde{w}_i and f replaced by \tilde{f}_i .

Conversely, if problem (68) admits a solution, then the pair $(\tilde{w}_i, \tilde{\Phi}_i)$, with Φ defined by (67), is a solution on the PGD problem (64).

Consequently the sequence (Φ_i, w_i) provided by the deflation algorithm (39)-(40) is also a solution of the PGD algorithm (64)-(65)-(66), with $\tilde{f}_i = f_i$ for all $i \geq 1$. Thus, if the PGD algorithm is computed in such a way that at each step $\tilde{\Phi}_i \tilde{w}_i = \Phi_i w_i (= s_i)$, the analysis developed in Section 5 proves that the sequence \tilde{u}_i converges in $L^2(\Gamma, H; d\mu)$ to the parametric solution $u(\gamma)$ of problem (3).

However there is the possibility that problem (64) admits several solutions and that some of these do not provide a solution of the optimization problem (45). Then the convergence properties studied in Section 5 may be lost. It is then convenient to solve the PGD problem (64) ensuring that the solution does provide an optimal sub-space.

The previous analysis presents some differences with preceding works on the analysis of convergence of PGD methods applied to the solution of PDEs and optimization problems. Let us describe some of them. In [2] the authors prove the convergence of the PGD for finite dimensional linear systems $A\mathbf{x} = \mathbf{b}$ where $A \in \mathbb{R}^{N \times N}$ is an invertible high dimensional matrix, i.e. $N = N_1 N_2 \cdots N_n$. The solution is searched as a series of rank-one summands, belonging to $\mathbb{R}^N = \mathbb{R}^{N_1} \otimes_a \mathbb{R}^{N_2} \otimes_a \cdots \otimes_a \mathbb{R}^{N_n}$ (where \otimes_a denotes the algebraic tensor product). Also, in [8] the authors prove the convergence of the PGD algorithm applied to the Laplace problem in a tensor product domain,

$$-\Delta u = f \text{ in } \Omega_x \times \Omega_y, \quad u|_{\partial\Omega_x \times \Omega_y} = 0,$$

where $\Omega_x \subset \mathbb{R}$ and $\Omega_y \subset \mathbb{R}$ are two bounded domains. They solve the problem on the tensor space $H_0^1(\Omega_x) \otimes_a H_0^1(\Omega_y)$ which is dense in $H_0^1(\Omega_x \times \Omega_y)$ for the norm of $H_0^1(\Omega_x \times \Omega_y)$. The work [9] proves the convergence of the PGD for the optimization problem: Find $\mathbf{u} \in L^2(\Omega, H^1(I))$ such that $\mathbf{u} \in \arg \min_{\mathbf{v} \in L^2(\Omega, H^1(I))} \mathcal{E}(\mathbf{v})$, where \mathcal{E} is a strongly convex functional, with Lipschitz gradient on bounded sets. This method can be used for high-dimensional nonlinear convex problems. Further, in [12], the authors prove the convergence of a PGD-like algorithm, where the set of rank-one tensors in a tensor space is substituted by a closed cone Σ , to solve the variational problem: Find $\mathbf{u} \in X$ such that $\mathbf{u} \in \arg \min_{\mathbf{v} \in X} \mathcal{E}(\mathbf{v})$, where $\mathcal{E} : X \rightarrow \mathbb{R}$ is a convex functional defined over a reflexive Banach space X . Moreover, in [11] the authors prove the convergence of the PGD for elliptic PDEs in the form $A\mathbf{u} = \mathbf{f}$ where \mathbf{u} and \mathbf{f} belong to a Hilbert tensor space $H = \overline{H_1 \otimes_a H_2 \otimes_a \cdots \otimes_a H_n}^{||| \cdot |||}$. Here the norm $||| \cdot |||^2 = \langle \cdot, \cdot \rangle$ is given by $\langle \cdot, \cdot \rangle = \langle \cdot, \cdot \rangle_1 \langle \cdot, \cdot \rangle_2 \cdots \langle \cdot, \cdot \rangle_n$. This is a generalization of Eckart and Young theorem.

The results reported in the present paper are a generalization of this last work [11] when the operator A depends on a parameter.

7 Conclusion

In this paper we have introduced an iterative deflation algorithm to solve parametric symmetric elliptic equations. It is a Proper Generalized Decomposition algorithm as it builds a tensorized representation of the parameterized solutions, by means of optimal subspaces that minimize the residual in mean quadratic norm. It is intrinsic in the sense that in each deflation step the residual is minimized in the ‘‘natural’’ parametric norm generated by the parametric elliptic operator. It is conceptually close to the Proper Orthogonal Decomposition with the difference that in the POD the residual is minimized with respect to a fixed mean quadratic norm. Due to this difference, spectral theory cannot be applied.

We have proved the existence of the optimal subspaces of dimension less than or equal to a fixed number, as required in each iteration of the deflation algorithm, with a specific analysis for the one-dimensional case. Also, we have proved the strong convergence in the parametric elliptic norm of the deflation algorithm for quite general parametric elliptic operators.

We have further proved that the method introduced is a genuine extension of both POD and PGD methods, and that in particular it provides a theoretical analysis of the PGD method, when this method is applied in such a way that it provides the optimal sub-spaces : The PGD expansion is strongly convergent to the targeted solution in parametric elliptic norm.

We will next focus our research on the analysis of convergence rates of the intrinsic PGD expansion that we introduced. We will analyze whether the standard PGD provides the optimal sub-spaces, and compare the convergence rates with those of the POD expansion, to determine whether the use of optimal modes provides improved convergence rates. We will also work on the use of optimization techniques as an alternative way to compute the optimal modes, rather than the Power Iteration method that is common in PGD computations.

All the results obtained in the present paper refer to *a* symmetric. In a future work we will consider the non-symmetric case.

Acknowledgements

The work of Mejdí Azaiez and Tomás Chacón has been partially supported by the Spanish Government - Feder EU grant MTM2015-64577-C2-1-R.

The work of Juan Casado-Díaz and François Murat has been partially supported by the Spanish Government - Feder EU grant MTM2014-53309-P.

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