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ON THE MATCHING OF EIGENSOLUTIONS TO PARAMETRIC PARTIAL DIFFERENTIAL EQUATIONS

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Abstract. In this paper a novel numerical approximation of parametric eigenvalue problems is presented. We motivate our study with the analysis of a POD reduced order model for a simple one dimensional example. In particular, we introduce a new algorithm capable to track the matching of eigenvalues when the parameters vary.

1 INTRODUCTION

The study of parametric eigenvalue problems arising from partial differential equations with multidimensional (possibly stochastic) parameter space, is still the object of very limited research. Starting from the pioneer work presented in [2] it is apparent that the analysis of parametric eigenvalue problems cannot be simply considered as a generalization of the theory developed for parametric/stochastic *source* partial differential equations [6, 9, 7, 5, 8, 18, 3]. Indeed, parametric eigenvalue problems lack a fundamental regularity condition needed for the analysis of parametric source problems; this is the consequence of possible eigenvalue crossings occurring when the parameters vary. When a crossing occurs, clearly the eigenvalues involved in the crossing are not smooth functions of the parameters and the corresponding eigenspaces are

not even continuous if the eigenvalues are sorted by their magnitude. The question addressed in this paper concerns the matching of the eigenvalues across their intersections so that a new sorting of the eigenmodes can be introduced that restores the smoothness of eigenvalues and eigenspaces with respect to the parameters.

A reduced basis approximation of an isolated eigenmode has been presented and analyzed in [15], while in [16] the reduced basis model approach is applied to the simultaneous approximation of multiple eigenvalues. The latter reference can be considered as the state of the art in reduced order modeling for eigenvalue problems.

A reduced order model for the approximation of eigenvalue problems was considered in [4] and an algorithm for tracking the matching of the eigenvalues is under development [1]. The latter takes inspiration from reduced order model techniques for the parametric-in-frequency Helmholtz equation [14, 11, 12, 10, 13, 17].

The aim of this paper is twofold. On one side, we provide the reader with a convincing example of the necessity of tracking the matching of the eigenvalues for different parameters values. Indeed, the lack of prior knowledge of the behavior of the eigenvalues, in terms of dependence on the parameters and of their possible crossings, may lead to unexpected results. On the other side, we introduce a greedy algorithm that can be used to successfully match the eigenmodes and we describe some of its properties.

In Section 2 we describe our abstract problem. In Section 3 we present a one dimensional example from which it is clear how crucial is to detect the crossings of eigenvalues, and finally in Section 4 we introduce our matching algorithm.

2 PROBLEM SETTING

Let $(H, (\bullet,\bullet)_H)$ and $(V, (\bullet,\bullet)_V)$ be Hilbert spaces such that $V \subset H \simeq H' \subset V'$ gives a standard Hilbert triplet and V is compact subset of H. Moreover, let $\mathcal{M} \subset \mathbb{R}^P$ be a P-dimensional parametric domain, with $P \geq 1$, and $a, b\colon V \times V \times \mathcal{M} \to \mathbb{R}$ two parameter-dependent bilinear forms such that, for all $\mu \in \mathcal{M}$, $a(\bullet,\bullet;\mu)$ is symmetric and coercive, namely, there exist a positive constant α such that

$$\begin{aligned} &a(v,v;\mu) \geq \alpha \|v\|_V^2 \qquad \forall\, v \in V \\ &a(w,v;\mu) = a(v,w;\mu) \quad \forall\, w, v \in V \end{aligned} \tag{1}$$

and $b(\bullet,\bullet;\mu)$ is equivalent to the scalar product of H, namely, there exist positive constants c_b, C_b such that

$$c_b(w,v)_H \leq b(w,v) \leq C_b(w,v)_H \quad \forall\, w, v \in V. \tag{2}$$

Given a window of values $[\lambda_{min}, \lambda_{max}] \subset \mathbb{R}_+$ we are interested in the following parametric eigenvalue model problem: for each $\mu \in \mathcal{M}$, find eigenvalues $\lambda(\mu) \in [\lambda_{min}, \lambda_{max}]$ and non-vanishing eigenfunctions $u(\mu) \in V$ such that, for all $v \in V$ it holds

$$a(u(\mu), v; \mu) = \lambda(\mu) b(u(\mu), v; \mu). \tag{3}$$

3 A MOTIVATING EXAMPLE

Let $\mathcal{M}$ be the interval $[-0.9, 0.9]$ and consider the following μ-dependent boundary value problem, with $\mu \in \mathcal{M}$:

$$\begin{cases} -\operatorname{div}(A(\mu)\nabla u(\mu)) = \lambda(\mu)u(\mu) & \text{in } \Omega = (0,1)^2 \\ u(\mu) = 0 & \text{on } \partial\Omega \end{cases} \tag{4}$$

where the diffusion $A(\mu) \in \mathbb{R}^{2\times 2}$ is given by the diagonal matrix

$$A(\mu) \coloneqq \begin{pmatrix} 1 & 0 \\ 0 & 1+\mu \end{pmatrix}.$$

The weak formulation of (4) reads: for all $\mu \in \mathcal{M}$, find $(\lambda(\mu), u(\mu)) \in \mathbb{R}_+ \times H^1_0(\Omega)$, with $u(\mu)$ non vanishing, such that, for all $v \in H^1_0(\Omega)$ it holds

$$\int_\Omega (A(\mu)\nabla u(\mu)) \cdot \nabla v \, dx = \lambda(\mu) \int_\Omega u(\mu) v \, dx. \tag{5}$$

Problem (5) is a particular case of the general problem (3) when choosing the spaces $V = H^1_0(\Omega)$, $H = L^2(\Omega)$, (equipped with the natural inner products $(\bullet,\bullet)_{H^1}$ and $(\bullet,\bullet)_{L^2}$) and the bilinear forms

$$\begin{aligned} a(w, v; \mu) &\coloneqq \int_\Omega (A(\mu)\nabla w) \cdot \nabla v \, dx, \\ b(w, v; \mu) &\coloneqq \int_\Omega wv \, dx. \end{aligned} \tag{6}$$

Notice that $a(\bullet,\bullet;\mu)$ is symmetric and coercive, with coercivity constant $\alpha = (1 + C_P^2)^{-1}$, C_P being the Poincaré constant, and $b(\bullet,\bullet;\mu)$ coincides with the L^2-inner product, i.e., the chain of inequalities (2) is a chain of equalities with constants $c_b = C_b = 1$.

The analytical eigensolutions to (4) can be explicitly computed by separation of variables, and they are given by:

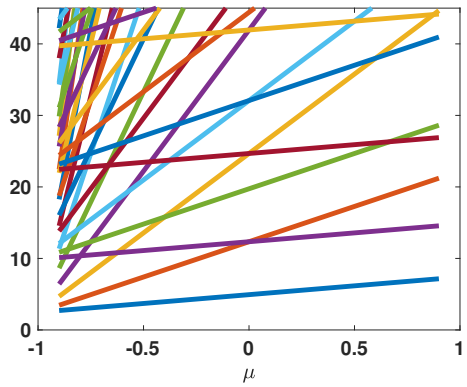
$$\begin{array}{ll} \lambda_{n,m}(\mu) & = \frac{\pi^2}{4}(m^2 + (1+\mu)n^2) \\ u_{n,m} & = \cos\left(\frac{m\pi}{2}x\right)\cos\left(\frac{n\pi}{2}y\right) \end{array} \qquad \forall\, m, n \in \mathbb{N}. \tag{7}$$

In particular, we underline that the eigenfunctions $\{u_{n,m}\}_{n,m\in\mathbb{N}}$ are independent of the parameter $\mu \in \mathcal{M}$, in contrast to the eigenvalues $\{\lambda(\mu)_{n,m}\}_{n,m\in\mathbb{N}}$. This property makes the problem particularly simple and suitable for our preliminary considerations. Figure 1a shows the exact eigenvalues corresponding to the formula in Equation (7), while Figure 1b shows the first six approximating eigenvalues sorted according to their magnitude and denoted $\lambda_{1,h}, \ldots, \lambda_{6,h}$.

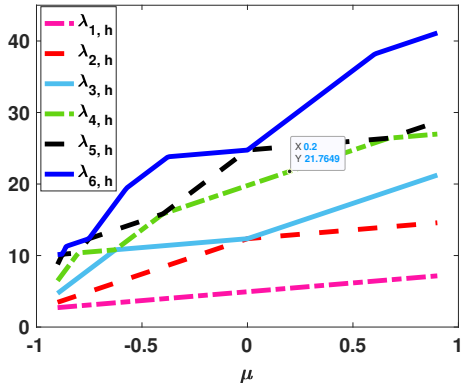
3.1 Reduced basis approximation of the first eigenvalue

We are interested in computing an approximation to the first eigenpair $(\lambda_1(\mu), u_1(\mu))$ as μ varies in the parametric interval $\mathcal{M}$. Consider the uniform decomposition of $\mathcal{M}$

$$\mathcal{M}_T = \{-0.9 + (j-1)\Delta\mu,\, j = 1, \ldots, T\} = \{\mu_j,\, j = 1, \ldots, T\}$$



(a) Exact eigenvalues $\lambda_{n,m}(\mu)$ given by formula (7), for $\mu \in \mathcal{M}$.



(b) First six eigenvalues $\lambda_{1,h}, \ldots, \lambda_{6,h}$ computed by the FEM and sorted according to their magnitutde, for $\mu \in \mathcal{M}$.

with $\Delta\mu = 0.1$ and $T = 19$. On a given regular (fine) mesh of Ω, we compute the eigensolutions $\{(\lambda_{1,h}^{(j)}, u_{1,h}^{(j)}),\ j = 1, \ldots, T\}$ corresponding to $\mathcal{M}_T$ via the piecewise linear finite element method (FEM). We collect the T computed eigenfunctions into the snapshot matrix $S_1 = [u_{1,h}^{(1)} | \cdots | u_{1,h}^{(T)}] \in \mathbb{R}^{N_h \times T}$, where N_h denotes the number of degrees of freedom. By performing the singular value decomposition (SVD), we derive the following representation of the snapshot matrix:

$$S_1 = U \Sigma Z^T,$$

where $U \in \mathbb{R}^{N_h \times N_h}$, $Z \in \mathbb{R}^{T \times T}$ are unitary matrices and $\Sigma \in \mathbb{R}^{N_h \times T}$ is a rectangular diagonal matrix.

Theoretically we expect S to have rank one because the first eigenvalue is well separated by the others and the first eigenspace is independent of μ. Numerically, we observe that the first singular value is well separated by the others even if it is not the only non vanishing one. Indeed, for any fixed (relatively large) tolerance $tol < 1.e-3$, several singular vectors N_{tol} will be considered in the truncated SVD expansion of S_1 (see Figure 2). For $tol > 1.e-1$, only the first singular vector will be considered in the singular value decomposition, namely, $N_{tol} = 1$. The reduced basis proper orthogonal decomposition (RB-POD) approximation to the first eigenpair $(\lambda_1(\mu), u_1(\mu))$ of (5) is obtained by projection onto the one-dimensional space spanned by the first singular eigenvector. Looking at the results summarized in Table 1, we note that the first RB-POD eigenvalue is a good approximation of the first FE eigenvalue $\lambda_1(\mu)$, for $\mu \in \{-0.75, -0.25, 0.25, 0.75\}$. Slightly better approximations are also obtained for $N_{tol} = 2$ (see Table 2).

3.2 Reduced basis approximation of the third eigenvalue

We now follow the same strategy as before, with the aim of approximating the third eigenpair $(\lambda_3(\mu), u_3(\mu))$ of problem (5), for $\mu \in \mathcal{M}$. Denote by S_3 the snapshot matrix $S_3 = [u_{3,h}^{(1)} | \cdots | u_{3,h}^{(T)}] \in \mathbb{R}^{N_h \times T}$ collecting the third eigenfunctions $u_{3,h}^{(j)}$ with $\mu_j \in \mathcal{M}_T$. Theoretically, we expect S_3 to have rank 3, because of two eigenvalue crossings (see Figure 1b). The singular

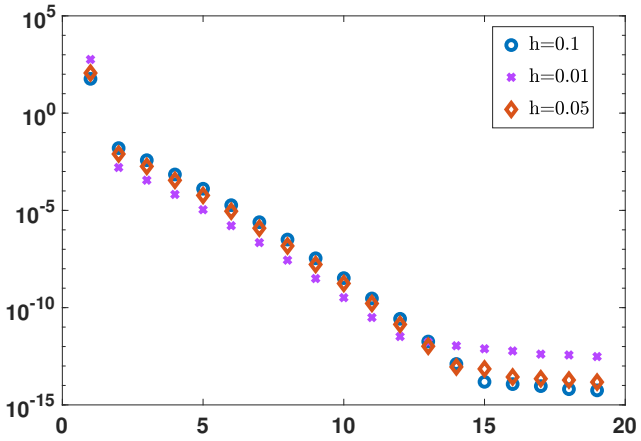


Figure 2: Singular values of the snapshot matrix S_1 for successively refined meshes of Ω with maximum diameter denoted as h.

h	μ	FEM based first eigenvalue	RB-POD based first eigenvalue
0.1	-0.75	3.09172930	3.09178369
	-0.25	4.32853369	4.32853489
	0.25	5.56526834	5.56528610
	0.75	6.80197424	6.80203730
0.05	-0.75	3.08606437	3.08607518
	-0.25	4.32052203	4.32052233
	0.25	5.55496589	5.55496949
	0.75	6.78940395	6.78941665
0.01	-0.75	3.08432204	3.08432252
	-0.25	4.31805168	4.31805169
	0.25	5.55178071	5.55178087
	0.75	6.78550948	6.78551005

Table 1: Comparison between the FE and RB-POD approximation to the first eigenpair $(\lambda_1(\mu), u_1(\mu))$ of problem (5), using a one-dimensional RB space, spanned by the first singular vector of S_1.

h	μ	FEM based first eigenvalue	RB-POD based first eigenvalue
0.1	-0.75	3.09172930	3.09172950
	-0.25	4.32853369	4.32853469
	0.25	5.56526834	5.56526837
	0.75	6.80197424	6.80197627
0.05	-0.75	3.08606437	3.08606442
	-0.25	4.32052203	4.32052230
	0.25	5.55496589	5.55496590
	0.75	6.78940395	6.78940447
0.01	-0.75	3.08432204	3.08432204
	-0.25	4.31805168	4.31805169
	0.25	5.55178071	5.55178071
	0.75	6.78550948	6.78550950

Table 2: Comparison between the FE and RB-POD approximation to the first eigenpair $(\lambda_1(\mu), u_1(\mu))$ of problem (5), using a two-dimensional RB space, spanned by the first two singular vectors of S_1.

values of S_3 are depicted in Figure 3, and the approximation results for $N_{tol} = 3$ are summarized in Table 3. Even though the results might look satisfactory, it is important to observe that the numbers reported in the last column of Table 3 correspond to the second eigenvalue of the 3×3 reduced model.

Actually, in this case we know the exact solution and, after careful inspection, it was possible to realize that the approximation of the solution we are interested in, corresponds to the second eigenvalue of the 3×3 system. This comes from the fact that the three element of the reduced basis correspond to the three eigenvalues associated with the three modes belonging to the third eigenmode. More precisely, looking at Figure 1b, the curve corresponding to $\lambda_{3,h}$, is made of three straight pieces and that's the reason why we are expecting the rank of the snapshot matrix to be equal to three. If we now isolate from the figure of the exact values 1a the three straight lines corresponding to the three selected eigenfunctions, then we see that the curve we are interested in is always the one related to the second eigenfunction out of those three.

We can deduce that, in general, it is essential to know some information about the structure of the exact solution. In particular, a fundamental question that needs to be addressed is how to match computed eigenvalues for different values of the parameter μ.

4 THE MATCHING OF EIGENVALUES

The motivating example of the previous section demonstrates that the reduced order techniques available in the literature are inappropriate for tracking the eigenpair solutions to the parameter-dependent eigenvalue problem (3). This section describes the crucial ingredient of a novel algorithm under development, which is able to overcome this obstacle.

The algorithm performs an a priori matching between two sets of eigensolutions. Given two values of the parameter μ_i, $\mu_k \in \mathcal{M}$, and the corresponding set of eigenpairs

$$\{(\lambda_j(\mu_i), u_j(\mu_i))\}_{j=1}^{m_i} \qquad \{(\lambda_\ell(\mu_k), u_\ell(\mu_k))\}_{\ell=1}^{m_k}$$

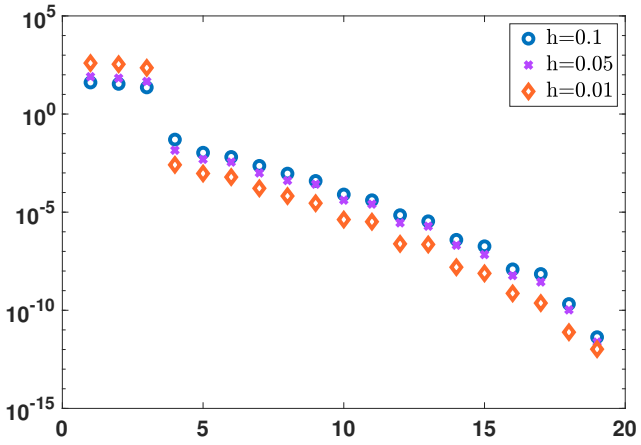


Figure 3: Singular values of the snapshot matrix S_3.

h	μ	FEM based third eigenvalue	RB-POD based third eigenvalue
0.1	-0.75	8.14338931	8.14352843
	-0.25	11.78888922	11.78893305
	0.25	14.89196477	14.89205929
	0.75	19.85303433	19.85335723
0.05	-0.75	8.05008647	8.05010991
	-0.25	11.73700317	11.73701402
	0.25	14.82575077	14.82577826
	0.75	19.76686171	19.76695884
0.01	-0.75	8.02024667	8.02024755
	-0.25	11.72081569	11.72081613
	0.25	14.80523805	14.80523912
	0.75	19.74028492	19.74028861

Table 3: Comparison between the FE and RB-POD approximation to the third eigenpair $(\lambda_3(\mu), u_3(\mu))$ of problem (5), when the RB space is spanned by the first three singular vectors of S_3.

for each $j = 1, \dots, m_i$, we want to find the value of $\ell \in \{1, \dots, m_k\}$ such that $\lambda_j(\mu_i)$ and $\lambda_\ell(\mu_k)$ belong to the same eigenvalue curve $\lambda^\star \colon \mathcal{M} \to [\lambda_{min}, \lambda_{max}]$, i.e.,

$$\lambda^\star(\mu_i) = \lambda_j(\mu_i), \qquad \lambda^\star(\mu_k) = \lambda_\ell(\mu_k). \tag{8}$$

Notice that this problem may have no solutions if some curve $\lambda^\star$ is entering or exiting the window $[\lambda_{min}, \lambda_{max}]$ in the interval identified by μ_i and μ_k. For the same reason, in general, m_i may be different from m_k.

For this purpose, we adapt to our setting the following idea from [17]. Under the assumption $m_i = m_k = m$, we construct the cost matrix $D \in \mathbb{R}^{m \times m}$

$$D^{i,k}_{j,\ell} = |\lambda_j(\mu_i) - \lambda_\ell(\mu_k)| + w \min(\|u_j(\mu_i) - u_\ell(\mu_k)\|, \|u_j(\mu_i) + u_\ell(\mu_k)\|) \tag{9}$$

where w is a suitable positive weight. We aim at finding one value per row and one value per column of D so that the sum of the selected matrix entries is minimized. In other words, we look for a permutation $\boldsymbol{\sigma} = (\sigma_1, \dots, \sigma_m) \colon \{1, \dots, m\} \to \{1, \dots, m\}$ such that $\lambda_j(\mu_i)$ and $\lambda_{\sigma_j}(\mu_k)$ belong to the same eigenvalue curve in the sense of equation (8), for $j = 1, \dots, m$. This is an optimization problem for which various solutions methods are available; for instance, a quite convenient solution strategy involves the use of the Hungarian algorithm.

We make a couple of observations.

- Each entry of the cost matrix (9) has two ingredients: the first measures the distance between the two sets of eigenvalues, and the second measures the distance between the two sets of eigenfunctions. The weight w express the relative importance of the second term with respect to the first one. Even though one might be tempted to consider the first term, only, i.e., taking $w = 0$, in the majority of the cases this might lead to the wrong matching.

- In applications we often get $m_i \neq m_k$, leading to a rectangular cost matrix D. Typically, this happens when an eigenvalue curve $\lambda^\star(\mu)$, $\mu \in \mathcal{M}$, attains values that are out of the window of interest $[\lambda_{min}, \lambda_{max}]$. In this situation, the cost matrix is rectangular, and the output of the Hungarian matrix is a permutation matching $m = \min\{m_i, m_k\}$ eigenpairs.

Preliminary computations show that the a priori matching performs generally well with some exceptions. In particular, in some cases the matching strategy described above might fail, delivering the wrong eigenpair matching and, moreover, it might not be able to deal with clusters of eigenvalues, namely, when two or more eigenvalues are close to each other, even if not multiple. For these reasons, a novel a posteriori matching strategy is under development which is able to resolve these issues. Starting from an initial discretization $\mathcal{M}_0$ of the parameter set $\mathcal{M}$, and employing the a posteriori indicator, we will be able to build up a greedy algorithm that selects the areas of $\mathcal{M}$ where refinement is needed, delivering a problem-adapted discretization $\mathcal{M}_1$ of $\mathcal{M}$.

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