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Spectral pollution and eigenvalue bounds

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A B S T R A C T

The Galerkin method can fail dramatically when applied to eigenvalues in gaps of the extended essential spectrum. This phenomenon, called spectral pollution, is notoriously difficult to predict and it can occur in models from relativistic quantum mechanics, solid state physics, magnetohydrodynamics and elasticity theory. The purpose of this survey paper is two-fold. On the one hand, it describes a rigorous mathematical framework for spectral pollution. On the other hand, it gives an account on two complementary state-of-the-art Galerkin-type methods for eigenvalue computation which prevent spectral pollution completely.

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1. Introduction

The Galerkin method can fail dramatically when applied to eigenvalues in gaps of the extended essential spectrum. This phenomenon, called spectral pollution, is notoriously difficult to predict and it can occur in models from relativistic quantum mechanics, solid state physics, magnetohydrodynamics, electromagnetism and elasticity theory. This survey paper has two specific purposes. On the one hand, it describes a rigorous framework for spectral pollution. On the other hand, it gives an account on two complementary state-of-the-art Galerkin-type methods for eigenvalue computation which prevent spectral pollution completely.

Introductory material is to be found in Section 2 and Section 3. The former is devoted to the basic notation around the classical Galerkin method. The latter includes a few canonical examples which illustrate the many subtleties of spectral pollution.

The main body of the text is Sections 4–6. In Section 4 a generalisation of the well-known theorem by H. Weyl on the stability of the essential spectrum is closely examined. This result implies a striking fact: the spectral pollution set is stable under compact perturbations.

The text then turns to the formulation of two complementary pollution-free techniques for computation of bounds for eigenvalues. One of these techniques is related to the classical Temple–Lehmann inequality and is considered in Section 5. It has a local character, meaning that it just allows determination of eigenvalue bounds in the vicinity of a given parameter. These bounds are optimal in a suitable setting.

The other technique, discussed in Section 6, does not lead to optimal spectral bounds but it has a global character. Given any trial subspace of the domain, it always renders true information about the spectrum. Moreover, it converges under fairly general conditions.

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These two approaches have recently been tested in various practical settings with successful outcomes. In order to show their implementation and range of applicability, various numerical experiments are included. These experiments are performed on two benchmark models, the two-dimensional Dirichlet Laplacian and the three-dimensional isotropic resonant cavity. They illustrate a few new features of the theory which have not been reported elsewhere. They are mostly elementary, however they may serve as a motivation for more serious investigations.

The exposition is intentionally made short and concise. It only includes the very basic aspects of both theory and applications. The material is fairly self-contained, so it must be accessible to non-specialist and PhD students in Analytical and Computational Spectral Theory. A guide for further reading is found in Section 7.

This survey paper began as notes from a four-weeks lecture course which I delivered at the Université de Franche-Comté Besançon in the Spring of 2012. I am duly grateful to Nabile Boussaïd and colleagues from the Laboratoire de Mathématiques for countless stimulating discussions during my visit. Financial support was provided by the Université de Franche-Comté, and the British Engineering and Physical Sciences Research Council (grant EP/I00761X/1).

2. The spectrum and the Galerkin method

The classical setting around the notions of discrete and essential spectra for self-adjoint operators, leads naturally to the framework of the Galerkin method. In this classical setting the Weyl Theorem on the stability of the essential spectrum plays a prominent role.

2.1. Nature of the spectrum for self-adjoint operators

Let $A : \operatorname{dom} A \longrightarrow \mathcal{H}$ be a densely defined self-adjoint operator on the infinite-dimensional separable Hilbert space $\mathcal{H}$. The *spectrum* of A,

$$\operatorname{spec} A = \{\lambda \in \mathbb{R} : (A - \lambda) \text{ does not have a bounded inverse}\} \quad ,$$

can be characterised by Weyl's criterion:

$$\lambda \in \operatorname{spec} A \iff \exists \{u_j\}_{j\in\mathbb{N}} \subset \operatorname{dom} A,\ \|u_j\| = 1,\ \|(A-\lambda)u_j\| \to 0 \quad .$$

The sequence of vectors $(u_j) \equiv (u_j)_{j=1}^{\infty}$ is called a *Weyl sequence (associated to λ)*. The *singular Weyl sequences* are the ones such that in addition are weakly convergent to zero,[1] $u_j \rightharpoonup 0$. They determine the classical decomposition of the spectrum into two disjoint components,

$$\operatorname{spec} A = [\operatorname{spec}_{\mathrm{dsc}} A] \cup [\operatorname{spec}_{\mathrm{ess}} A] \quad .$$

The *essential spectrum* are those λ for which there is a singular Weyl sequence,

$$\lambda \in \operatorname{spec}_{\mathrm{ess}} A \iff \begin{cases} \exists \{u_j\}_{j\in\mathbb{N}} \subset \operatorname{dom} A,\ \|u_j\| = 1, \\ u_j \rightharpoonup 0 \ \&\ \|(A-\lambda)u_j\| \to 0 \quad . \end{cases}$$

The *discrete spectrum* is then defined as the complementary set

$$\operatorname{spec}_{\mathrm{dsc}} A = [\operatorname{spec} A] \setminus [\operatorname{spec}_{\mathrm{ess}} A] \quad .$$

The latter comprises only those $\lambda \in \mathbb{R}$ which are eigenvalues of A of finite multiplicity,

$$1 \le \dim \ker(A - \lambda) < \infty \quad ,$$

and are isolated from the rest of the spectrum. See for example [38, §VII.3].

From the above classification of the spectrum, it is readily seen that if $B = B^*$ is another self-adjoint operator such that[2] $(A - B) \in \mathcal{K}(\mathcal{H})$, then

$$\operatorname{spec}_{\mathrm{ess}} B = \operatorname{spec}_{\mathrm{ess}} A \quad . \tag{1}$$

This observation highlights a fundamental property: the essential spectrum is a stable part of the spectrum. More generally, if A and B are *relatively compact perturbations of each other*, that is

$$(A-c)^{-1} - (B-c)^{-1} \in \mathcal{K}(\mathcal{H}) \tag{2}$$

for at least one[3] $c \notin \mathbb{R}$, then once again (1) holds true. This stability character of the essential spectrum, and other further generalisations, are usually identified in the literature as Weyl's Theorems, see [39, Theorem XIII.14].

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[1] Meaning $\langle u_j, v\rangle \to 0$ for all $v \in \mathcal{H}$.

[2] Here and everywhere below $\mathcal{K}(\mathcal{H})$ is the algebra of compact operators in $\mathcal{H}$.

[3] Hence for all $c \notin (\operatorname{spec} A) \cup (\operatorname{spec} B)$.

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