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I Introduction

The computation of spectra can boldly be considered the 'fundamental problem of operator theory' [1]. The spectrum of an operator holds the same key to the entire structure as eigenvalues do for linear algebra, however (as often occurs when passing from the finite- to infinite-dimensional case) we lose the ease of representation that allows the creation of such algorithms and formulae as those used for matrices.

We must first define our quantity of interest: the spectrum of an operator.

Definition. ***(Resolvent and spectrum)*** *(Adapted from [2]) Let T be a linear operator on a Banach space.*

- *The resolvent of T is the set $\rho(T) := \{\eta \in \mathbb{C} : (T - \eta I) \text{ is bijective}\}$, where I is the identity operator.*
- *The spectrum of T, denoted $Spec(T)$, is $\mathbb{C} \setminus \rho(T)$, i.e. the set of all complex numbers λ such that the operator $(T - \lambda I)$ does not have a bounded inverse.*

One can see that this concept generalises the eigenvalues of a matrix to any Banach space, and that for a finite-dimensional Banach space (of which $\mathbb{R}^n$ and $\mathbb{C}^n$ are major examples) we can recover the eigenvector equation. For an operator on an infinite-dimensional space, values which satisfy the eigenvector equation *are* in the spectrum of the operator, but they do not comprise the entire spectrum - nor do we necessarily have a spectrum made up of a discrete set of values.

Example 1. *Let S be the 'right-shift' operator on the sequence space $\ell^2(\mathbb{N})$, which has the following action: $S(x_1, x_2, x_3, ...) = (0, x_1, x_2, x_3, ...)$; that is, for a sequence u we map u_n to u_{n+1}, and pad the vector with a zero in u_1's place. S has no eigenvalues, and its spectrum is the open unit disc $D = \{z \in \mathbb{C} : |z| = 1\}$.*

As we have alluded to, there is no universal algorithm for the calculation of operator spectra in the way that there is the QR algorithm ([3]) for matrices. To devise a formula for the spectrum of even a specific class of operators is a mathematical feat, and varieties of operators important to fields such as still withhold the structure of their spectra from decades-long attempts at discovery. To this end, we must employ numerical methods. We shall find that even approximating spectra computationally is not so easy.

Definition. ***(Compressions, truncations, and Ritz matrices)*** *(Adapted from [**davies2004spectral**]) Let T be an operator on a Hilbert space H, $\mathcal{L} \subseteq Dom(T)$ a closed linear subspace, and $P_{\mathcal{L}}$ the orthogonal projection of H onto $\mathcal{L}$.*

- *The **compression** of the operator T, which we will often denote $T_{\mathcal{L}}$, is defined*
$$T_{\mathcal{L}} := P_{\mathcal{L}} T\big|_{\mathcal{L}}$$
where $\big|_{\mathcal{L}}$ denotes domain restriction to $\mathcal{L}$.
- *If $\{\phi_n\}_{n\in\mathbb{N}}$ is an orthonormal basis for H, the n'th **truncation** of T is the compression of T to $Span\{\phi_1, \phi_2, ..., \phi_n\}$.*
- *We will call the matrix representation of T truncated to $Span\{\phi_1, \phi_2, ..., \phi_n\}$ the **Ritz matrix** of T, and denote it T_n when the context is obvious. T_n is an $n \times n$ matrix with entries*
$$(T_n)_{i,j} := (T\phi_i, \phi_j) \quad \forall i, j \leq n.$$

This definition raises a natural question; do the eigenvalues of the matrices T_n converge to the spectrum of the operator T? This question was investigated by Walther H. W. Ritz for whom we name our matrices, as well as by Boris Galerkin; the method of approximating the spectrum of an operator by the eigenvalues of its truncations is often called the Ritz method, Galerkin method, or indeed the Ritz-Galerkin method. We will formulate answers to these questions in due course, but for our introduction it suffices to say that the answer is "not quite". What can go wrong?

Definition. ***(Spectral pollution)*** *(Adapted from [**davies2004spectral**]) Let $(T_n)_{n\in\mathbb{N}}$ be an increasing sequence of truncations of an operator T. A value $\lambda \in \mathbb{C}$ is said to be a point of **spectral pollution** if there is a sequence $\lambda_n \in Spec(T_n)$ such that $\lambda_n \to \lambda$ but $\lambda \notin Spec(A)$.*

Points of spectral pollution are, intuitively, artefacts of the approximation which will never converge to a point in the actual spectrum. We will see that they exist, that they are relatively common, and that they *get worse* as the approximation goes to higher iterations. Unless we already know what the spectrum of the operator is, it can be incredibly hard for us to decide whether a point is actually in the spectrum or whether it is spurious. In applications of spectral theory, this difference can be beyond a simple 'error bar' nuisance - rather, a confounding problem.

Example 2.

References

[1] William Arveson, FW Gehring, and KA Ribet. *A short course on spectral theory*. Vol. 209. Springer, 2002.

[2] Lawrence C Evans. *Partial differential equations*. 2nd ed. Vol. 19. American Mathematical Society, 2010.

[3] John GF Francis. “The QR transformation a unitary analogue to the LR transformation—Part 1”. In: *The Computer Journal* 4.3 (1961), pp. 265–271.

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