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Cluster-robust accuracy bounds for Ritz subspaces

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ABSTRACT

Given an approximating subspace for a Hermitian matrix A, the Rayleigh–Ritz procedure is commonly used to compute a few approximate eigenvalues (called Ritz values) and corresponding approximate eigenvectors (called Ritz vectors). In this paper, new bounds on the canonical angles between the invariant subspace of A associated with its few extreme (smallest or largest) eigenvalues and its approximating Ritz subspace in terms of the differences between Ritz values and the targeted eigenvalues are obtained. From this result, various bounds are readily available to estimate how accurate the Ritz vectors computed from the approximating subspace may be, based on information on approximation accuracies in the Ritz values. The result is helpful in understanding how Ritz vectors move towards eigenvectors while Ritz values are made to move towards eigenvalues.

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1. Introduction

The Rayleigh–Ritz procedure [1, p. 234] is widely used to find approximate eigenpairs of a Hermitian matrix $A \in \mathbb{C}^{N\times N}$, given a subspace $\mathcal{X}$ of $\mathbb{C}^N$ with $\dim(\mathcal{X}) = \ell$. Let X be an orthonormal basis matrix of $\mathcal{X}$. The basic idea of the procedure goes as follows. Compute the eigen-decomposition of $X^{\mathrm{H}}AX$:

$$X^{\mathrm{H}}AX = W\widetilde{\Lambda}W^{\mathrm{H}}, \quad \widetilde{\Lambda} = \operatorname{diag}(\tilde{\lambda}_1, \ldots, \tilde{\lambda}_\ell),$$

where $W = [w_1, \ldots, w_\ell] \in \mathbb{C}^{\ell\times\ell}$ is unitary, and then take each pair $(\tilde{\lambda}_i, Xw_i)$, called a *Rayleigh–Ritz pair*, as an approximate eigenpair of A. The number $\tilde{\lambda}_i$ is called a *Ritz value* and Xw_i a corresponding *Ritz vector*.

In the case when $\mathcal{X}$ is an accurate approximate invariant subspace of A, each Rayleigh–Ritz pair should be a good approximate eigenpair of A. If $\mathcal{X}$ itself does not well approximate any invariant subspace of A, but contains a subspace that is a good approximation to some invariant subspace of A, then some, but not all, of the Rayleigh–Ritz pairs are expected to approximate well eigenpairs of A. The latter case is more common than the former in eigenvalue computations, where often a subspace is built to contain another subspace that approximates an invariant subspace of A well, e.g., in the Lanczos method a Krylov subspace is built and usually the Krylov subspace as a whole is not close to any invariant subspace (of the same dimension) but more likely contains a subspace that is a good approximation to an invariant subspace of A.

There are existing results to quantify how good the approximate eigenpairs are. Most results are bounds in terms of the norms of the residual

$$R(X) := AX - X(X^{\mathrm{H}}AX).$$

The interested reader is referred to a short summary at the end of [2] for bounds of this kind. The main result of [3] can be interpreted as one of this kind, too. Note $R(X) = 0$ if $\mathcal{X}$ is an exact invariant subspace.

Other results are bounds in terms of the canonical angles between $\mathcal{X}$ and the invariant subspace which $\mathcal{X}$ is supposed to approximate. In this regard, Knyazev and Argentati [4] presented the most comprehensive study so far. They obtained several beautiful results in terms of how the vector of eigenvalue differences between the exact eigenvalues and their approximations is *weakly majorized* by the canonical angles between/from the invariant subspace of interest and/to $\mathcal{X}$. We will state some of their results to motivate what we will do in Section 3. The results in [4] are basically about estimating the approximation accuracy of (some of) the Ritz values, given information on the approximate accuracy in $\mathcal{X}$ to an invariant subspace of A. In this paper, we are interested in the converses to these results, i.e., estimating the approximate accuracy in $\mathcal{X}$, given information on the approximation accuracy of (some of) the Ritz values. Our motivation is from eigenvector computations in Principal Component Analysis in image processing [5,6], where eigenvectors may be computed by optimizing Rayleigh quotients with conjugate gradient type