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Two-sided harmonic subspace extractions for the generalized eigenvalue problem

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One crucial step of the solution of large-scale generalized eigenvalue problems with iterative subspace methods, e.g. Arnoldi, Jacobi-Davidson, is a projection of the original large-scale problem onto a low dimensional subspaces. Here we investigate two-sided methods, where approximate eigenvalues together with their right and left eigenvectors of the full-size problem are extracted from the resulting small eigenproblem. The two-sided Ritz-Galerkin projection can be seen as the most basic form of this approach. It usually provides a good convergence towards the extremal eigenvalues of the spectrum. For improving the convergence towards interior eigenvalues, we investigate two approaches based on harmonic subspace extractions for the generalized eigenvalue problem.

1 Introduction

We investigate the solution of two-sided generalized eigenvalue problems

$$\begin{cases} Ax &= \lambda Bx \\ y^H A &= \lambda y^H B \end{cases}, \text{ where } A,\ B \in \mathbb{C}^{n\times n}, \lambda \in \mathbb{C} \text{ and } 0 \neq x, y \in \mathbb{C}^n.$$

A tuple $(\lambda,\ x,\ y)$ consisting of an *eigenvalue* λ as well as the corresponding *right* and *left eigenvectors* $x,\ y$ is an *eigentriple* of the *matrix pair* $(A,\ B)$. We assume that $(A,\ B)$ is a regular, but non-normal pair consisting of two large but sparse matrices. We are interested in a few eigentriples, in particular in the ones whose eigenvalues lie in the vicinity of a *target* $\tau \in \mathbb{C}\backslash\Lambda(A,\ B)$. One important application, where also the left eigenvectors are needed, is modal truncation, which is an eigenvalue based model order reduction approach for linear time-invariant systems [2]. The large size of $(A,\ B)$ prohibits an efficient application of the QZ algorithm and hence the usage of iterative, projection based eigenvalue solvers instead is advised. For the two-sided problem, such methods can be partitioned into the two subsequent parts:

1. Generate a suitable approximate eigentriple by projecting $(A,\ B)$ onto low-dimensional subspaces and computing eigentriples of the resulting small eigenproblem, e.g, with the QZ algorithm.
2. If the eigentriple is accurate enough, the method stops or proceeds to find another one. Otherwise, each subspace is expanded by a new basis vector and the overall process is repeated with increasing subspace dimensions.

In the paper we merely focus on the first step and assume that the subspace expansion in the second part is carried out via the two-sided Jacobi-Davidson method (BiJD). There, new basis vectors are obtained from linear systems, which can, e.g., be solved approximately by applying a few steps of a Krylov subspace method for linear systems (GMRES, BiCG, ...). This makes the algorithm very efficient, since basically only a limited number of matrix-vector products and no exact linear system solves are needed in each BiJD iteration. We refer to [2, 3, 5] for more information on this method.

2 Two-sided subspace extractions for generalized eigenvalue problems

Let in the following $(\theta,\ v,\ w) \approx (\lambda,\ x,\ y)$ denote an approximate eigentriple of $(A,\ B)$, and let $\mathcal{V},\ \mathcal{W} \subset \mathbb{C}^n$ be two k-dimensional subspaces with basis matrices $V,\ W \in \mathbb{C}^{n\times k},\ k \ll n$. One approach for extracting approximate eigentriples from $\mathcal{V},\ \mathcal{W}$ is the *two-sided Ritz-Galerkin extraction* [6, Ch. 7.8], where for $v \in \mathcal{V},\ w \in \mathcal{W}$ the orthogonality conditions on the residuals $r_1 := Av - \theta Bv \perp \mathcal{W}$, $r_2 := A^H w - \overline{\theta} B^H w \perp \mathcal{V}$ are imposed. With $q,\ z \in \mathbb{C}^k$, this is equivalent to

$$W^H AVq = \theta W^H BVq,\ z^H W^H AV = \theta z^H W^H BV.$$

The approximate eigentriples $(\theta,\ v := Vq,\ w := Wz)$ are called *two-sided Ritz triples* and are obtained from the eigentriples of the small matrix pair $(S := W^H AV \in \mathbb{C}^{k\times k},\ T := W^H BV \in \mathbb{C}^{k\times k})$. This approach works usually well for the approximation of exterior eigenvalues and is therefore applied in a wide range of two-sided eigenvalue methods.

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Now suppose we want to compute eigenvalues close to the target τ. A straightforward modification of the *two-sided harmonic Ritz extraction* for the standard eigenproblem from [1,5] leads to

$$\begin{array}{rcl} (A-\tau B)^{-1}Bv-(\theta-\tau)^{-1}v & \perp & \left((A-\tau B)^H\right)^2\mathcal{W}, \\ (A-\tau B)^{-H}B^Hw-(\overline{\theta-\tau})^{-1}w & \perp & (A-\tau B)^2\mathcal{V}. \end{array}$$

$$\iff \begin{cases} W^H(A-\tau B)^2Vq = \xi_1 W^H(A-\tau B)BVq, \\ z^HW^H(A-\tau B)^2V = \xi_2 z^HW^HB(A-\tau B)V, \end{cases}$$

with $\xi_j=\theta_j-\tau,\ j=1,2$. This approach turns out to be problematic, since the matrices on the right hand side are different from each other. Therefore, we get two sets of eigenpairs from two distinct small matrix pairs: (ξ_1,q) of the matrix pair $(S:=W^H(A-\tau B)^2V\in\mathbb{C}^{k\times k}, T_1:=W^H(A-\tau B)BV\in\mathbb{C}^{k\times k})$, and, respectively, $(\xi_2,\ z)$ of the pair $(S^H,\ T_2^H:=V^H(A-\tau B)^HB^HW\in\mathbb{C}^{k\times k})$. To get an approximate triple of $(A,\ B)$ we propose to choose the eigenvectors $q,\ z$ associated to $\xi_{1,2}$ with the smallest magnitude. These values correspond to the values of $\theta_{1,2}$ closest to τ. As final approximate eigentriple of $(A,\ B)$, we choose then $(\theta:=\frac{w^HAv}{w^HBv},\ v:=Vq,\ w:=Wz)$ and call this approach *two-sided harmonic extraction for the GEP*. Note that taking the generalized Rayleigh quotient as eigenvalue approximation ensures a higher accuracy and is a common strategy for harmonic subspace extractions. Another approach for the generalized eigenproblem is imposing orthogonaly conditions for right and left eigenvectors separately. We thus obtain the one-sided, harmonic Ritz extractions:

$$\begin{array}{rcl} (A-\tau B)Vq-(\theta-\tau)BVq & \perp & (A-\tau B)\mathcal{V}, \\ (A-\tau B)^HWz-(\overline{\theta-\tau})B^HWz & \perp & (A-\tau B)^H\mathcal{W} \end{array}$$

$$\iff \begin{cases} V^H(A-\tau B)^H(A-\tau B)Vq = \xi_1 V^H(A-\tau B)^HBVq, \\ z^HW^H(A-\tau B)(A-\tau B)^HW = \xi_2 z^HW^HB(A-\tau B)^HW. \end{cases}$$

As before, we obtain two sets of eigenpairs of two different matrix pairs: (ξ_1,q) of $(S_1:=V^H(A-\tau B)^H(A-\tau B)V\in\mathbb{C}^{k\times k}$, $T_1:=V^H(A-\tau B)^HBV\in\mathbb{C}^{k\times k})$, and, respectively, (ξ_2,z) of $(S_2:=W^H(A-\tau B)(A-\tau B)^HW\in\mathbb{C}^{k\times k},\ T_2:=W^H(A-\tau B)B^HW\in\mathbb{C}^{k\times k})$. The advantage of this approach is that for both harmonic Ritz pairs $(\theta_1=\xi_1+\tau,\ v:=Vq)$ and $(\theta_2=\xi_2+\tau,\ w:=Wz)$ it holds [4, Ch. 4.4.]: $\|(A-\tau B)v\|\le|\theta_1-\tau|\|Bv\|$ and $\|(A-\tau B)^Hw\|\le|\theta_2-\tau|\|B^Hw\|$. Hence we choose $q,\ z$ as before and take $(\theta:=\frac{w^HAv}{w^HBv},\ v:=Vq,\ w:=Wz)$ as approximate eigentriple. Due to its nature, we call this strategy *double one-sided harmonic extraction for the GEP*.

3 Numerical Experiment

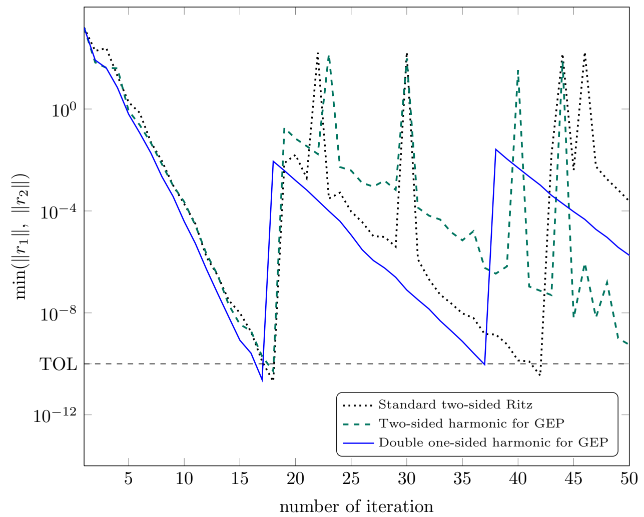

Fig. 1 Convergence history of BiJD using different subspace extractions with target 3i.

To illustrate the behavior of the discussed subspace extractions within BiJD, we compare both proposed harmonic strategies with the standard two-sided Ritz extraction. The generalized eigenproblem RBS480a/b[1] with $n=480$ serves as text example and we look for the eigenvalues closest to $\tau=3\mathrm{i}$. An eigentriple is said to be converged if $\min(\|r_1\|,\ \|r_2\|)<10^{-10}$. The correction equations of BiJD are solved inexactly by (at most) 10 steps of GMRES with an incomplete LU factorization $LU\approx A-\tau B$ with drop tolerance 10^{-3} as preconditioner. In Figure 1 the residual norms are plotted against the iteration number. Each time a residual curve falls below 10^{-10}, the found eigentriple is deflated and the algorithm tries to find another eigentriple. One observes that the double one-sided approach leads to the fastest convergence, which appears to be also monotonic, whereas with the double harmonic and standard Ritz extraction, BiJD shows an erratic and non monotonic performance.

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