Solving symmetric quadratic eigenvalue problems with SLEPc

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This work [?] is framed in the context of SLEPc, the Scalable Library for Eigenvalue Problem Computations [?]. SLEPc contains parallel implementations of various eigensolvers for different types of eigenproblems. The linear eigenvalue problem solver (`EPS`) contains basic methods as well as more advanced algorithms, including Krylov-Schur, Generalized Davidson, Jacobi-Davidson, Rayleigh-quotient conjugate gradient or the contour integral spectral slicing technique. Eigensolvers can be combined with spectral transformations (such as shift-and-invert) or preconditioners in the case of preconditioned eigensolvers. Linear solvers as well as data structures for matrices and vectors are provided by PETSc [?], on which SLEPc is based. Further functionality of SLEPc includes solvers for the partial singular value decomposition, as well as quadratic and general nonlinear eigenproblems.

For quadratic eigenvalue problems (`QEP`) we provide a solver based on linearization, as well as various memory-efficient solvers. The former explicitly builds the matrices of a companion linearization of the quadratic problem and then invokes a linear eigensolver from `EPS` to obtain the solution. The latter include the Q-Arnoldi and TOAR methods, that aim at exploiting the structure of the linearization in such a way that memory requirements for storing the Krylov basis are roughly divided by two.

In this work we investigate how to adapt the Q-Arnoldi method [?] for the case of symmetric quadratic eigenvalue problems, that is, we are interested in computing a few eigenpairs (λ, x) of $(\lambda^2 M + \lambda C + K)x = 0$ with M, C, K symmetric $n \times n$ matrices. This problem has no particular structure, in the sense that eigenvalues can be complex or even defective. Still, symmetry of the matrices can be exploited to some extent. For this, we perform a symmetric linearization $Ay = \lambda By$, where A, B are symmetric $2n \times 2n$ matrices but the pair (A, B) is indefinite and hence standard Lanczos methods are not applicable. We implement a symmetric-indefinite Lanczos method [?] and enrich it with a thick-restart technique [?]. This method uses pseudo inner products induced by matrix B for the orthogonalization of vectors (indefinite Gram-Schmidt). Restarting the pseudo-Lanczos recurrence requires special ways of solving the projected problems, using techniques such as those described in [?], that try to minimize the use of non-orthogonal transformation to try to elude instability.

The next step is to write a specialized, memory-efficient version that exploits the block structure of A and B, referring only to the original problem matrices M, C, K as in the Q-Arnoldi method. This results in what we have called the Q-Lanczos method. The Q-Arnoldi method may suffer from instability when the Hessenberg matrix of the Arnoldi relation has large norm, and so may Q-Lanczos. Therefore, we need to define a stabilized variant analog of the TOAR method, which represents the basis vectors of the pseudo-Lanczos recurrence as the product of two matrices that are orthogonal with respect to some non-standard inner product (STOAR). Restarting in this case is more complicated and involves computing the SVD of a small matrix.

We show results obtained with parallel implementations of all methods in SLEPc, when solving several problems from the NLEVP collection [**?**]. Although the methods relying on an indefinite inner product are not guaranteed to be stable, we observe reasonably good behaviour of the pseudo-Lanczos method operating on the explicit linearization as well as the STOAR variant.

References

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