

# Electronic Transactions on Numerical Analysis

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### Contents

- 1 Error estimation of the Padé approximation of transfer functions via the Lanczos process. *Zhaojun Bai and Qiang Ye.*

**Abstract.** Krylov subspace based moment matching algorithms, such as PVL (Padé approximation Via the Lanczos process), have emerged as popular tools for efficient analyses of the impulse response in a large linear circuit. In this work, a new derivation of the PVL algorithm is presented from the matrix point of view. This approach simplifies the mathematical theory and derivation of the algorithm. Moreover, an explicit formulation of the approximation error of the PVL algorithm is given. With this error expression, one may implement the PVL algorithm that adaptively determines the number of Lanczos steps required to satisfy a prescribed error tolerance. A number of implementation issues of the PVL algorithm and its error estimation are also addressed in this paper. A generalization to a multiple-input-multiple-output circuit system via a block Lanczos process is also given.

**Key words.** transfer function, Padé approximation, Lanczos process, linear system.

**AMS(MOS) subject classification.** 41A21, 65F15, 65F10.

**Files.** vol.7.1998/pp1-17.dir/pp1-17.ps; vol.7.1998/pp1-17.dir/pp1-17.pdf.

**Forward References.**

- 18 Harmonic Ritz and Lehmann bounds. *Christopher Beattie.*

**Abstract.** This article reviews a variety of results related to optimal bounds for matrix eigenvalues — some results presented here are well-known; others are less known; and a few are new. The focus rests especially on Ritz and harmonic Ritz values, and right- and left-definite variants of Lehmann's optimal bounds. Two new computationally advantageous reformulations of left-definite Lehmann bounds are introduced, together with a discussion indicating why they might be preferable to the cheaper right-definite bounds.

**Key words.** optimal eigenvalue bounds, Lehmann intervals, harmonic Ritz values.

**AMS(MOS) subject classification.** 65F15, 49R05.

**Files.** vol.7.1998/pp18-39.dir/pp18-39.ps; vol.7.1998/pp18-39.dir/pp18-39.pdf.

**Forward References.**

- 40 Convergence analysis of an inexact truncated RQ-iteration. *Chao Yang.*

**Abstract.** The Truncated RQ-iteration (TRQ) can be used to calculate interior or clustered eigenvalues of a large sparse and/or structured matrix  $A$ . This method requires solving a sequence of linear equations. When these equations can be solved accurately by a direct solver, the convergence of each eigenvalue is quadratic in general and cubic if  $A$  is hermitian. An important question is whether the TRQ iteration will still converge if these equations are approximately solved by a preconditioned

iterative solver. If it does converge, how fast is the convergence rate? In this paper, we analyze the convergence of an inexact TRQ iteration in which linear systems are solved iteratively with some error. We show that under some appropriate conditions, the convergence rate of the inexact TRQ is at least linear with a small convergence factor.

**Key words.** Arnoldi method, Lanczos method, eigenvalues, truncated RQ-iteration.

**AMS(MOS) subject classification.** 65F15, 65G05.

**Files.** vol.7.1998/pp40-55.dir/pp40-55.ps; vol.7.1998/pp40-55.dir/pp40-55.pdf.

**Forward References.**

- 56 A block Rayleigh quotient iteration with local quadratic convergence. *Jean-Luc Fattebert.*

**Abstract.** We present an iterative method, based on a block generalization of the Rayleigh Quotient Iteration method, to search for the  $p$  lowest eigenpairs of the generalized matrix eigenvalue problem  $Au = \lambda Bu$ . We prove its local quadratic convergence when  $B^{-1}A$  is symmetric. The benefits of this method are the well-conditioned linear systems produced and the ability to treat multiple or nearly degenerate eigenvalues.

**Key words.** subspace iteration, Rayleigh quotient iteration, Rayleigh-Ritz procedure.

**AMS(MOS) subject classification.** 65F15.

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**Forward References.**

- 75 Efficient expansion of subspaces in the Jacobi-Davidson method for standard and generalized eigenproblems. *Gerard L.G. Sleijpen, Henk A. van der Vorst and Ellen Meijerink.*

**Abstract.** We discuss approaches for an efficient handling of the correction equation in the Jacobi-Davidson method. The correction equation is effective in a subspace orthogonal to the current eigenvector approximation. The operator in the correction equation is a dense matrix, but it is composed from three factors that allow for a sparse representation. If the given matrix eigenproblem is sparse then one often aims for the construction of a preconditioner for that matrix. We discuss how to restrict this preconditioner effectively to the subspace orthogonal to the current eigenvector. The correction equation itself is formulated in terms of approximations for an eigenpair. In order to avoid misconvergence one has to make the right selection for the approximations, and this aspect will be discussed as well.

**Key words.** linear eigenproblems, generalized eigenproblems, Jacobi-Davidson, harmonic Ritz values, preconditioning.

**AMS(MOS) subject classification.** 65F15.

**Files.** vol.7.1998/pp75-89.dir/pp75-89.ps; vol.7.1998/pp75-89.dir/pp75-89.pdf.

**Forward References.**

- 90 A theoretical comparison between inner products in the shift-invert Arnoldi method and the spectral transformation Lanczos method. *Karl Meerbergen.*

**Abstract.** The spectral transformation Lanczos method and the shift-invert Arnoldi method are probably the most popular methods for the solution of linear generalized eigenvalue problems originating from engineering applications, including structural and acoustic analyses and fluid dynamics. The orthogonalization of the Krylov vectors requires inner products. Often, one employs the standard inner product, but in many engineering applications one uses the inner product using the mass matrix. In this paper, we make a theoretical comparison between these inner products in the framework of the shift-invert Arnoldi method. The conclusion is that when the square-root of the condition number of the mass matrix is small, the convergence behavior does not strongly depend on the choice of inner product. The theory is illustrated by numerical examples arising from structural and acoustic analyses. The theory is extended to the discretized Navier-Stokes equations.

**Key words.** Lanczos method, Arnoldi's method, generalized eigenvalue problem, shift-invert.

**AMS(MOS) subject classification.** 65F15.

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**Forward References.**

- 104 Preconditioned eigensolvers—an oxymoron? *Andrew V. Knyazev.*

**Abstract.** A short survey of some results on preconditioned iterative methods for symmetric eigenvalue problems is presented. The survey is by no means complete and reflects the author's personal interests and biases, with emphasis on author's own contributions. The author surveys most of the important theoretical results and ideas which have appeared in the Soviet literature, adding references to work published in the western literature mainly to preserve the integrity of the topic. The aim of this paper is to introduce a systematic classification of preconditioned eigensolvers, separating the choice of a preconditioner from the choice of an iterative method. A formal definition of a preconditioned eigensolver is given. Recent developments in the area are mainly ignored, in particular, on Davidson's method. Domain decomposition methods for eigenproblems are included in the framework of preconditioned eigensolvers.

**Key words.** eigenvalue, eigenvector, iterative methods, preconditioner, eigensolver, conjugate gradient, Davidson's method, domain decomposition.

**AMS(MOS) subject classification.** 65F15, 65F50, 65N25.

**Files.** vol.7.1998/pp104-123.dir/pp104-123.ps; vol.7.1998/pp104-123.dir/pp104-123.pdf.■

**Forward References.**

- 124 Fast Leja points. *J. Baglama, D. Calvetti and L. Reichel.*

**Abstract.** Leja points are used in several areas of scientific computing, including polynomial approximation and eigenvalue computation. Their determination requires the maximization of a sequence of polynomials over a compact set in the complex plane. These computations can be quite time consuming when the number

of Leja points to be determined is large. This paper introduces a new set of points, referred to as fast Leja points, that are simpler and faster to compute. Interactive computations of fast Leja points can be found at <http://etna.mcs.kent.edu/vol.7.1998/pp124-140.html>

**Key words.** Leja points, polynomial interpolation, iterative methods, eigenvalue computation.

**AMS(MOS) subject classification.** 65D05, 65E05, 65F15, 65N25.

**Files.** vol.7.1998/pp124-140.dir/pp124-140.ps; vol.7.1998/pp124-140.dir/pp124-140.pdf.

**Forward References.**

- 141 Truncated  $QZ$  methods for large scale generalized eigenvalue problems. *D. C. Sorensen.*

**Abstract.** This paper presents three methods for the large scale generalized eigenvalue problem  $\mathbf{Ax} = \mathbf{Bx}\lambda$ . These methods are developed within a subspace projection framework as a truncation and modification of the  $QZ$ -algorithm for dense problems, that is suitable for computing partial generalized Schur decompositions of the pair  $(\mathbf{A}, \mathbf{B})$ . A generalized partial reduction to condensed form is developed by analogy with the Arnoldi process. Then truncated forward and backward  $QZ$  iterations are introduced to derive generalizations of the Implicitly Restarted Arnoldi Method and the Truncated  $RQ$  method for the large scale generalized eigenvalue problem. These two methods require the accurate solution of linear systems at each step of the iteration. Relaxing these accuracy requirements forces us to introduce non-Krylov projection spaces that lead most naturally to block variants of the  $QZ$  iterations. A two-block method is developed that incorporates  $k$  approximate Newton corrections at each iteration. An important feature is the potential to utilize  $k$  matrix vector products for each access of the matrix pair  $(\mathbf{A}, \mathbf{B})$ . Preliminary computational experience is presented to compare the three new methods.

**Key words.** generalized eigenvalue problem, Krylov projection methods, Arnoldi method, Lanczos method,  $QZ$  method, block methods, preconditioning, implicit restarting.

**AMS(MOS) subject classification.** 65F15, 65G05.

**Files.** vol.7.1998/pp141-162.dir/pp141-162.ps; vol.7.1997/pp141-162.dir/pp141-162.pdf.

**Forward References.**

- 163 Restarting techniques for the (Jacobi-)Davidson symmetric eigenvalue methods. *Andreas Stathopoulos and Yousef Saad.*

**Abstract.** The (Jacobi-)Davidson method, which is a popular preconditioned extension to the Arnoldi method for solving large eigenvalue problems, is often used with restarting. This has significant performance shortcomings, since important components of the invariant subspace may be discarded. One way of saving more information at restart is through “thick” restarting, a technique that involves keeping more Ritz vectors than needed. This technique and especially its dynamic version have proved very efficient for symmetric cases. A different restarting strategy for the Davidson method has been proposed in [14], motivated by the similarity between the spaces built by the Davidson and Conjugate Gradient methods. For the latter method, a three term recurrence implicitly maintains all required information.

In this paper, we consider the effects of preconditioning on the dynamic thick restarting strategy, and we analyze both theoretically and experimentally the strategy based on Conjugate Gradient. Our analysis shows that, in some sense, the two schemes are complementary, and that their combination provides an even more powerful technique. We also describe a way to implement this scheme without additional orthogonalizations or matrix multiplications.

**Key words.** Davidson, Jacobi-Davidson, Lanczos, conjugate gradient methods, eigenvalue, implicit restarting, deflation, preconditioning.

**AMS(MOS) subject classification.** 65F15.

**Files.** vol.7.1998/pp163-181.dir/pp163-181.ps; vol.7.1998/pp163-181.dir/pp163-181.pdf.■

**Forward References.**

- 182** On the Convergence of a new Rayleigh quotient method with applications to large eigenproblems. *D. P. O'leary and G. W. Stewart.*

**Abstract.** In this paper we propose a variant of the Rayleigh quotient method to compute an eigenvalue and corresponding eigenvectors of a matrix. It is based on the observation that eigenvectors of a matrix with eigenvalue zero are also singular vectors corresponding to zero singular values. Instead of computing eigenvector approximations by the inverse power method, we take them to be the singular vectors corresponding to the smallest singular value of the shifted matrix. If these singular vectors are computed exactly the method is quadratically convergent. However, exact singular vectors are not required for convergence, and the resulting method combined with Golub–Kahan–Krylov bidiagonalization looks promising for enhancement/refinement methods for large eigenvalue problems.

**Key words.** Rayleigh quotient method, singular value decomposition, large eigenproblem.

**AMS(MOS) subject classification.** 15A42, 65F15, 65H15.

**Files.** vol.7.1998/pp182-189.dir/pp182-189.ps; vol.7.1997/pp182-189.dir/pp182-189.pdf.■

**Forward References.**

- 190** Transfer functions and resolvent norm approximation of large matrices. *V. Simoncini and E. Gallopoulos.*

**Abstract.** A unifying framework for methods employed in the approximation of the resolvent norm of nonnormal matrices is presented. This formulation uses specific transfer functions, and it provides new information about the approximation properties of these methods and their application in computing the pseudospectrum of matrices.

**Key words.** resolvent norm, transfer function, Arnoldi iteration, pseudospectrum.

**AMS(MOS) subject classification.** 65F15.

**Files.** vol.7.1998/pp190-201.dir/pp190-201.ps; vol.7.1998/pp190-201.dir/pp190-201.pdf.■

**Forward References.**

- 202** Inexact Newton preconditioning techniques for large symmetric eigenvalue problems. *Kesheng Wu, Yousef Saad and Andreas Stathopoulos.*

**Abstract.** This paper studies a number of Newton methods and use them to define new secondary linear systems of equations for the Davidson eigenvalue method. The new secondary equations avoid some common pitfalls of the existing ones such as the correction equation and the Jacobi-Davidson preconditioning. We will also demonstrate that the new schemes can be used efficiently in test problems.

**Key words.** sparse matrix eigenvalue problem, Newton method, preconditioning for eigenvalue method.

**AMS(MOS) subject classification.** 65F50, 65F15.

**Files.** vol.7.1998/pp202-214.dir/pp202-214.ps; vol.7.1998/pp202-214.dir/pp202-214.pdf.■

**Forward References.**