

Electronic Transactions on Numerical Analysis

Volume 20, 2005

Contents

- 1 Fast Givens transformation for quaternion valued matrices applied to Hessenberg reductions. *Drahoslava Janovská and Gerhard Opfer.*

Abstract.

In a previous paper we investigated Givens transformations applied to quaternion valued matrices. Since arithmetic operations with quaternions are very costly it is desirable to reduce the number of arithmetic operations with quaternions. We show that the Fast Givens transformation, known for the real case, can also be defined for quaternion valued matrices, and we apply this technique to the reduction of an arbitrary quaternion valued matrix to upper Hessenberg form and also include a numerical example. We offer two algorithms. One is based on the classical real case using dynamically two transformation matrices, while the other is based on four transformation matrices where in each step that matrix is selected that has the smallest condition number. For the first algorithm we show that the essential information (namely the two numbers s and c which define the Givens transformation) can be stored in only one variable. This is apparently even new for the real case. We include, necessarily, some investigations on the determination of the relevant condition numbers. We show that in general the application of the Fast Givens transformation in the quaternion case is not as favorable as in the real case with respect to (relative) savings in arithmetic operations. We begin with some introduction into the field of quaternions. In the end in an appendix we present some results concerning the computation of roots of quaternions which in some cases are needed.

Key Words.

fast Givens rotation, quaternions, quaternion valued matrices, Hessenberg form for quaternion valued matrices, roots of quaternions

AMS(MOS) Subject Classifications.

11R52, 12E15, 15A66, 65F30, 70Exx

- 27 Stability of numerical methods for ordinary stochastic differential equations along Lyapunov-type and other functions with variable step sizes. *Henri Schurz.*

Abstract.

Some general concepts and theorems on the stability of numerical methods for ordinary stochastic differential equations (SDEs) along Lyapunov-type and other Borel-measurable, nonnegative functions are presented. In particular, we deal with almost sure, moment and weak V -stability, exponential and asymptotic stability of related stochastic difference equations with nonrandom, variable step sizes. The applicability of the main results is explained with the class of balanced implicit methods (i.e. certain stochastic linear-implicit methods with appropriate weights). It is shown that, they are rich enough to provide asymptotically, exponentially and polynomially stable numerical methods discretizing stable continuous time SDEs by controlling the choice of their weights.

Key Words.

stochastic-numerical approximation, stochastic stability, ordinary stochastic differential equations, numerical methods, drift-implicit Euler methods, balanced implicit methods, Lyapunov-type functions, numerical weak V -stability, stability of moments, a.s. stability, asymptotic stability

AMS(MOS) Subject Classifications.

65C20, 65C30, 65C50, 60H10, 37H10, 34F05

- 50** On the use of larger bulges in the QR algorithm. *Daniel Kressner.*

Abstract.

The role of larger bulges in the QR algorithm is controversial. Large bulges are infamous for having a strong, negative influence on the convergence of the implicitly shifted QR algorithm. This paper provides a new explanation of this shift blurring effect, by connecting the computation of the first column of the shift polynomial to the notoriously ill-conditioned pole placement problem. To avoid shift blurring, modern variants of the QR algorithm employ chains of tightly coupled tiny bulges instead of one large bulge. It turns out that larger bulges still play a positive role in these variants; a slight increase of the bulge sizes often results in considerable performance improvements.

Key Words.

QR algorithm, bulges, shift blurring, pole placement

AMS(MOS) Subject Classifications.

65F15, 15A18

- 64** Fractal trigonometric approximation. *M. A. Navascues.*

Abstract.

A general procedure to define nonsmooth fractal versions of classical trigonometric approximants is proposed. The systems of trigonometric polynomials in the space of continuous and periodic functions $\mathcal{C}(2\pi)$ are extended to bases of fractal analogues. As a consequence of the process, the density of trigonometric fractal functions in $\mathcal{C}(2\pi)$ is deduced. We generalize also some classical results (Dini-Lipschitz's Theorem, for instance) concerning the convergence of the Fourier series of a function of $\mathcal{C}(2\pi)$. Furthermore, a method for real data fitting is proposed, by means of the construction of a fractal function proceeding from a classical approximant.

Key Words.

iterated function systems, fractal interpolation functions, trigonometric approximation

AMS(MOS) Subject Classifications.

37M10, 58C05

- 75** Crout versions of ILU factorization with pivoting for sparse symmetric matrices. *Na Li and Yousef Saad.*

Abstract.

The Crout variant of ILU preconditioner (ILUC) developed recently has been shown

to be generally advantageous over ILU with Threshold (ILUT), a conventional row-based ILU preconditioner. This paper explores pivoting strategies for sparse symmetric matrices to improve the robustness of ILUC. We integrate two symmetry-preserving pivoting strategies, the diagonal pivoting and the Bunch-Kaufman pivoting, into ILUC without significant overheads. The performances of the pivoting methods are compared with ILUC and ILUTP ([20]) on a set of problems, including a few arising from saddle-point (KKT) problems.

Key Words.

incomplete LU factorization, ILU, ILUC, sparse Gaussian elimination, crout factorization, preconditioning, diagonal pivoting, Bunch-Kaufman pivoting, ILU with threshold, iterative methods, sparse symmetric matrices

AMS(MOS) Subject Classifications.

65F10, 65F50

- 86** Uniform convergence of monotone iterative methods for semilinear singularly perturbed problems of elliptic and parabolic types. *Igor Boglaev.*

Abstract.

This paper deals with discrete monotone iterative methods for solving semilinear singularly perturbed problems of elliptic and parabolic types. The monotone iterative methods solve only linear discrete systems at each iterative step of the iterative process. Uniform convergence of the monotone iterative methods are investigated and rates of convergence are estimated. Numerical experiments complement the theoretical results.

Key Words.

singular perturbation, reaction-diffusion problem, convection-diffusion problem, discrete monotone iterative method, uniform convergence

AMS(MOS) Subject Classifications.

65M06, 65N06

- 104** Quadrature over the sphere. *Kendall Atkinson and Alvise Sommariva.*

Abstract.

Consider integration over the unit sphere in \mathbb{R}^3 , especially when the integrand has singular behaviour in a polar region. In an earlier paper [4], a numerical integration method was proposed that uses a transformation that leads to an integration problem over the unit sphere with an integrand that is much smoother in the polar regions of the sphere. The transformation uses a *grading parameter* q . The trapezoidal rule is applied to the spherical coordinates representation of the transformed problem. The method is simple to apply, and it was shown in [4] to have convergence $O(h^{2q})$ or better for integer values of $2q$. In this paper, we extend those results to non-integral values of $2q$. We also examine superconvergence that was observed when $2q$ is an odd integer. The overall results agree with those of [11], although the latter is for a different, but related, class of transformations.

Key Words.

spherical integration, trapezoidal rule, Euler-MacLaurin expansion

AMS(MOS) Subject Classifications.

65D32

- 119 Oblique projection methods for linear systems with multiple right-hand sides. *K. Jbilou, H. Sadok, and A. Tinzefté.*

Abstract.

In the present paper, we describe new Lanczos-based methods for solving nonsymmetric linear systems of equations with multiple right-hand sides. These methods are based on global oblique projections of the initial residual onto a matrix Krylov subspace. We first derive the global Lanczos process to construct biorthonormal bases and we give some of its properties. Then we introduce new methods such as the global BCG and the global BiCGSTAB algorithms. Look-ahead versions of these algorithms are also given. Finally numerical examples will be given.

Key Words.

global Lanczos, matrix Krylov subspace, block methods, iterative methods, non-symmetric linear systems, multiple right-hand sides

AMS(MOS) Subject Classifications.

65F10, 65F25

- 139 A nonnegatively constrained trust region algorithm for the restoration of images with an unknown blur. *Johnathan M. Bardsley.*

Abstract.

We consider a large-scale optimization problem with nonnegativity constraints that arises in an application of phase diversity to astronomical imaging. We develop a cost function that incorporates information about the statistics of atmospheric turbulence, and we use Tikhonov regularization to induce stability. We introduce an efficient and easily implementable algorithm that intersperses gradient projection iterations with iterations from a well-known, unconstrained Newton/trust region method. Due to the large size of our problem and to the fact that our cost function is not convex, we approximately solve the trust region subproblem via the Steihaug-Toint truncated CG iteration. Iterations from the trust region algorithm are restricted to the inactive variables. We also present a highly effective preconditioner that dramatically speeds up the convergence of our algorithm. A numerical comparison using real data between our method and another standard large-scale, bound constrained optimization algorithm is presented.

Key Words.

constrained optimization, phase diversity, astronomical imaging

AMS(MOS) Subject Classifications.

65K10, 65F22

- 154 Convergence analysis of the rotated Q_1 element on anisotropic rectangular meshes. *Shipeng Mao and Shaochun Chen.*

Abstract.

The main aim of this paper is to study the convergence of the well-known nonconforming rotated Q_1 element for the second order elliptic problems on anisotropic rectangular meshes, i.e., the meshes considered in our work do not satisfy the regular assumption. Lastly, a numerical test is carried out, which coincides with our theoretical analysis.

Key Words.

anisotropic, interpolation error, nonconforming, the rotated Q_1 element

AMS(MOS) Subject Classifications.

65N30, 65N15

- 164** A BDDC algorithm for a mixed formulation of flow in porous media. *Xuemin Tu.*

Abstract.

The BDDC (balancing domain decomposition by constraints) algorithms are similar to the balancing Neumann-Neumann methods, with a small number of continuity constraints enforced across the interface throughout the iterations. These constraints form a coarse, global component of the preconditioner. The BDDC methods are powerful for solving large sparse linear algebraic systems arising from discretizations of elliptic boundary value problems. In this paper, the BDDC algorithm is extended to saddle point problems generated from the mixed finite element methods used to approximate the scalar elliptic problems for flow in porous media. Edge/face average constraints are enforced and the same rate of convergence is obtained as for simple elliptic cases. The condition number bound is estimated and numerical experiments are discussed. In addition, a comparison of the BDDC method with an edge/face-based iterative substructuring method is provided.

Key Words.

BDDC, domain decomposition, saddle point problem, condition number, benign space, edge/face-based iterative substructuring method

AMS(MOS) Subject Classifications.

65N30, 65N55, 65F10

- 180** On the worst-case convergence of MR and CG for symmetric positive definite tridiagonal Toeplitz matrices. *Jörg Liesen and Petr Tichý.*

Abstract.

We study the convergence of the minimal residual (MR) and the conjugate gradient (CG) method when applied to linear algebraic systems with symmetric positive definite tridiagonal Toeplitz matrices. Such systems arise, for example, from the discretization of one-dimensional reaction-diffusion equations with Dirichlet boundary conditions. Based on our previous results in [J. Liesen and P. Tichý, *BIT*, 44 (2004), pp. 79–98], we concentrate on the next-to-last iteration step, and determine the initial residuals and initial errors for the MR and CG method, respectively, that lead to the slowest possible convergence. By this we mean that the methods have made the least possible progress in the next-to-last iteration step. Using these worst-case initial vectors, we discuss which source term and boundary condition in the underlying reaction-diffusion equation are the worst in the sense that they lead to the worst-case initial vectors for the MR and CG methods. Moreover, we determine (or very tightly estimate) the worst-case convergence quantities in the next-to-last step, and compare these to the convergence quantities obtained from average (or unbiased) initial vectors. The spectral structure of the considered matrices allows us to apply our worst-case results for the next-to-last step to derive worst-case bounds also for other iteration steps. We present a comparison of the worst-case convergence quantities with the classical convergence bound based on the condition number of A , and finally we discuss the MR and CG convergence for the special case of the one-dimensional Poisson equation with Dirichlet boundary conditions.

Key Words.

Krylov subspace methods, conjugate gradient method, minimal residual method, convergence analysis, tridiagonal Toeplitz matrices, Poisson equation

AMS(MOS) Subject Classifications.

15A09, 65F10, 65F20

- 198** Recursive computation of certain integrals of elliptic type. *P. G. Novario.*

Abstract.

An algorithm for the numerical calculation of the integral function

$$N_n(x) = \int_0^{\pi/2} \frac{\cos^{2n}(\Phi)}{\sqrt{1-x \cdot \sin^2(\Phi)}} \cdot d\Phi \quad (0 \leq x < 1; n = 0, 1, 2, \dots),$$

distinguished solution of the second-order difference equation

$$(2n + 1) \cdot x \cdot N_{n+1}(x) + 2n \cdot (1 - 2x) \cdot N_n(x) = (2n - 1) \cdot (1 - x) \cdot N_{n-1}(x) \quad (n = 1, 2, \dots),$$

that uses the recurrence relation and its related continued fraction expansion, is described and discussed. The numerical efficiency of the algorithm is analysed for various x values of the interval $(0 \leq x < 1)$. A twelve digits tabulation of $N_n(x)$ for $n = 1(1)20$ and $x = 0(0.02)1$ is presented as example of the algorithm utilization.

Key Words.

recurrence relations, elliptic integrals, continued fractions

AMS(MOS) Subject Classifications.

65Q05, 33E05, 11A55

- 212** Krylov subspace spectral methods for variable-coefficient initial-boundary value problems. *James V. Lambers.*

Abstract.

This paper presents an alternative approach to the solution of diffusion problems in the variable-coefficient case that leads to a new numerical method, called a Krylov subspace spectral method. The basic idea behind the method is to use Gaussian quadrature in the spectral domain to compute components of the solution, rather than in the spatial domain as in traditional spectral methods. For each component, a different approximation of the solution operator by a restriction to a low-dimensional Krylov subspace is employed, and each approximation is optimal in some sense for computing the corresponding component. This strategy allows accurate resolution of all desired frequency components without having to resort to smoothing techniques to ensure stability.

Key Words.

spectral methods, Gaussian quadrature, variable-coefficient, Lanczos method

AMS(MOS) Subject Classifications.

65M12, 65M70, 65D32

- 235** Generalizations of harmonic and refined Rayleigh–Ritz. *Michiel E. Hochstenbach.*

Abstract.

We investigate several generalizations of the harmonic and refined Rayleigh–Ritz method. These may be practical when one is interested in eigenvalues close to one of two targets (for instance, when the eigenproblem has Hamiltonian structure such

that eigenvalues come in pairs or quadruples), or in rightmost eigenvalues close to (for instance) the imaginary axis. Our goal is to develop new methods to extract promising approximate eigenpairs from a search space, for instance one generated by the Arnoldi or Jacobi–Davidson method. We give theoretical as well as numerical results of the methods, and recommendations for their use.

AMS(MOS) Subject Classifications.

65F15, 65F50

Key Words.

rational harmonic Rayleigh–Ritz, rightmost eigenvalue, structured eigenproblem, Hamiltonian matrix, Rayleigh–Ritz, harmonic Rayleigh–Ritz, refined Rayleigh–Ritz, subspace method, subspace extraction, Jacobi–Davidson

253 A linear acceleration row action method for projecting onto subspaces. *Glenn Appleby and Dennis C. Smolarski.*

Abstract.

This article describes an extension of projection or “row action” methods proposed first by Kaczmarz and by Cimmino. The method of this article constructs a line through two centroids computed by a modified Cimmino procedure and uses the actual or approximate intersection of this line with one of the hyperplanes associated with rows of the system matrix as an approximation to the solution. Comparisons are made with similar methods described by Pierra and Dax.

Key Words.

linear systems, projection methods, row action methods, iterative methods, Kaczmarz, Cimmino, Pierra, Dax

AMS(MOS) Subject Classifications.

15A06, 65F10, 65J05, 90C25, 90C55