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Contents

- 1 A preconditioner for a FETI-DP method for mortar element discretization of a 4th order problem in 2D. *Leszek Marcinkowski.*

Abstract.

In this paper a parallel preconditioner for a FETI-DP formulation for a mortar discretization of a fourth order problem is presented and analyzed. We show that the condition number of the preconditioned FETI-DP operator is proportional to $(1 + \log(H/h))^2$, where H and h are mesh sizes.

Key Words.

FETI-DP, mortar, nonmatching meshes, finite element, preconditioner

AMS Subject Classifications.

65N30, 65N55

- 17 On an SVD-based algorithm for identifying meta-stable states of Markov chains. *Ryan M. Tifenbach.*

Abstract.

A Markov chain is a sequence of random variables $X = \{x_t\}$ that take on values in a state space \mathcal{S} . A meta-stable state with respect to X is a collection of states $\mathcal{E} \subseteq \mathcal{S}$ such that transitions of the form $x_t \in \mathcal{E}$ and $x_{t+1} \notin \mathcal{E}$ are exceedingly rare. In Fritzsche et al. [Electron. Trans. Numer. Anal., 29 (2008), pp. 46–69], an algorithm is presented that attempts to construct the meta-stable states of a given Markov chain. We supplement the discussion contained therein concerning the two main results.

Key Words.

Markov chains; conformation dynamics; singular value decomposition

AMS Subject Classifications.

15A18, 15A51, 60J10, 60J20, 65F15

- 34 Applications of a nonnegatively constrained iterative method with statistically based stopping rules to CT, PET, and SPECT imaging. *Johnathan M. Bardsley.*

Abstract.

In this paper, we extend a nonnegatively constrained iterative method and three stopping rules for its iteration to the medical imaging inverse problems of computed tomography (CT), positron emission tomography (PET), and single photon emission computed tomography (SPECT); the iterative method and stopping rules were

introduced for the use in astronomical imaging. The paper begins with a brief introduction to the CT, PET, and SPECT mathematical and statistical models.

Key Words.

nonnegatively constrained iterative methods, inverse problems, statistical methods, medical imaging

AMS Subject Classifications.

65J22, 65K10, 65F22

- 44 Error estimates for general fidelities. *Martin Benning and Martin Burger.*

Abstract.

Appropriate error estimation for regularization methods in imaging and inverse problems is of enormous importance for controlling approximation properties and understanding types of solutions that are particularly favoured. In the case of linear problems, i.e., variational methods with quadratic fidelity and quadratic regularization, the error estimation is well-understood under so-called source conditions. Significant progress for nonquadratic regularization functionals has been made recently after the introduction of the Bregman distance as an appropriate error measure. The other important generalization, namely for nonquadratic fidelities, has not been analyzed so far.

In this paper we develop a framework for the derivation of error estimates in the case of rather general fidelities and highlight the importance of duality for the shape of the estimates. We then specialize the approach for several important fidelities in imaging (L^1 , Kullback-Leibler).

Key Words.

error estimation, Bregman distance, discrepancy principle, imaging, image processing, sparsity

AMS Subject Classifications.

47A52, 65J20, 49M30

- 69 Steady-state analysis of Google-like stochastic matrices with block iterative methods. *Tuğrul Dayar and Gökçe N. Noyan.*

Abstract.

A Google-like matrix is a positive stochastic matrix given by a convex combination of a sparse, nonnegative matrix and a particular rank one matrix. Google itself uses the steady-state vector of a large matrix of this form to help order web pages in a search engine. We investigate the computation of the steady-state vectors of such matrices using block iterative methods. The block partitionings considered include those based on block triangular form and those having triangular diagonal blocks obtained using cutsets. Numerical results show that block Gauss-Seidel with partitionings based on block triangular form is most often the best approach. However, there are cases in which a block partitioning with triangular diagonal blocks is better, and the Gauss-Seidel method is usually competitive.

Key Words.

Google, PageRank, stochastic matrices, power method, block iterative methods, partitionings, cutsets, triangular blocks

AMS Subject Classifications.

60J10, 65F10, 65F50, 65B99

- 98 Fields of values and inclusion regions for matrix pencils. *Michiel E. Hochstenbach.*

Abstract.

We are interested in (approximate) eigenvalue inclusion regions for matrix pencils (A, B) , in particular of large dimension, based on certain fields of values. We show how the usual field of values may be efficiently approximated for large Hermitian positive definite B , but also point out limitations of this set. We introduce four field of values based inclusion regions, which may effectively be approximated, also for large pencils. Furthermore, we show that these four sets are special members of two families of inclusion regions, of which we study several properties. Connections with the usual harmonic Rayleigh–Ritz method and a new variant are shown, and we propose an automated algorithm which gives an approximated inclusion region. The results are illustrated by several numerical examples.

Key Words.

inclusion region, exclusion region, matrix pencil, numerical range, field of values, generalized eigenvalue problem, large sparse matrix, harmonic Rayleigh–Ritz, harmonic Ritz values, Krylov space

AMS Subject Classifications.

65F15, 65F50, 65F30, 65F35, 47A12

- 113 Two efficient SVD/Krylov algorithms for model order reduction of large scale systems. *Younès Chahlaoui.*

Abstract.

We present two efficient algorithms to produce a reduced order model of a time-invariant linear dynamical system by approximate balanced truncation. Attention is focused on the use of the structure and the iterative construction via Krylov subspaces of both controllability and observability matrices to compute low-rank approximations of the Gramians or the Hankel operator. This allows us to take advantage of any sparsity in the system matrices and indeed the cost of our two algorithms is only linear in the system dimension. Both algorithms efficiently produce good low-rank approximations (in the least square sense) of the Cholesky factor of each Gramian and the Hankel operator. The first algorithm computes low-rank approximation of each Gramian independently. The second algorithm works directly on the Hankel operator, and it has the advantage that it is independent of the chosen realization. Moreover, it is also an approximate Hankel norm method. The two reduced order models produced by our methods are guaranteed to be stable and balanced. We study the convergence of our iterative algorithms and the properties of the fixed point iteration. We also discuss the stopping criteria and the choice of the reduced order.

Key Words.

model order reduction, approximate balanced truncation, Stein equations, Hankel map, Krylov subspaces, approximate Hankel norm method, low-rank approximations

AMS Subject Classifications.

15A24, 65P99, 93B40, 93C55, 93D99

- 146 Robust rational interpolation and least-squares. *Pedro Gonnet, Ricardo Pachón, and Lloyd N. Trefethen.*

Abstract.

An efficient and robust algorithm and a Matlab code `ratdisk` are presented for rational interpolation or linearized least-squares approximation of a function based on its values at points equally spaced on a circle. The use of the singular value decomposition enables the detection and elimination of spurious poles or Froissart doublets that commonly complicate such fits without contributing to the quality of the approximation. As an application, the algorithm leads to a method for the stable computation of certain radial basis function interpolants in the difficult case of smoothness parameter ε close to zero.

Key Words.

rational interpolation, spurious poles, Froissart doublets, Padé approximation, radial basis functions, `ratdisk`, singular value decomposition

AMS Subject Classifications.

41A20, 41A21, 65D05

- 168 Pseudospectral mapping theorem II. *S. H. Lui.*

Abstract.

The pseudospectrum has become an important quantity for analyzing stability of non-normal systems. This paper is a continuation of an earlier paper of this author where a mapping theorem for pseudospectra was given, generalizing the spectral mapping theorem for eigenvalues. The main contribution of this paper consists of asymptotic expansions of quantities which determine the sizes of components of pseudospectral sets. As an application of this theory, we solve the eigenvalue perturbation problem for an analytic function of a matrix. Some numerical examples illustrate the theory.

Key Words.

eigenvalues, pseudospectra, spectral mapping theorem, condition number, eigenvalue perturbation of function of matrices

AMS Subject Classifications.

15A18, 15A60, 65F15

- 184 Positivity of dLV and mdLVs algorithms for computing singular values. *Masashi Iwasaki and Yoshimasa Nakamura.*

Abstract.

The discrete Lotka-Volterra (dLV) and the modified dLV with shift (mdLVs) algorithms for computing bidiagonal matrix singular values are considered. Positivity of the variables of the dLV algorithm is shown with the help of the Favard theorem and the Christoffel-Darboux formula of symmetric orthogonal polynomials. A suitable shift of origin also guarantees positivity of the mdLVs algorithm which results in a higher relative accuracy of the computed singular values.

Key Words.

dLV algorithm, mdLVs algorithm, singular values, relative accuracy

AMS Subject Classifications.

64F15, 33C45, 15A18, 37K10

- 202 Evaluating the Fréchet derivative of the matrix p th root. *João R. Cardoso.*

Abstract.

This paper shows that computing the Fréchet derivative of the matrix p th root is equivalent to solve a sequence of p Sylvester equations. This provides the theoretical support to design an algorithm for the effective computation of the Fréchet derivative. The conditioning of the Sylvester sequence is addressed and some numerical experiments are carried out to illustrate the results.

Key Words.

conditioning, matrix p th root, Sylvester equation, Fréchet derivative, Kronecker products, perturbation theory

- 218 A linear constructive approximation for integrable functions and a parametric quadrature model based on a generalization of Ostrowski-Grüss type inequalities. *Mohammad Masjed-Jamei.*

Abstract.

A new generalization of Ostrowski-Grüss type inequalities, depending on a parameter λ , is introduced in order to construct a specific linear approximation for integrable functions. Some important subclasses of this inequality such as $\lambda = 1/2, 1$, and $\sqrt{2}/2$ are studied separately. The generalized inequality is employed to establish a parametric quadrature model and obtain its error bounds.

Key Words.

Ostrowski-Grüss type inequalities, linear constructive approximation, numerical quadrature rules, Chebyshev functional, kernel function

AMS Subject Classifications.

26D15, 65D30, 26D20, 65D32

- 233 Convergence analysis of minimization-based noise level-free parameter choice rules for linear ill-posed problems. *Stefan Kindermann.*

Abstract.

Minimization-based noise level-free parameter choice rules for the selection of the regularization parameter in linear ill-posed problems are studied. Abstract convergence results for spectral filter regularization operators using a qualitative condition on the (deterministic) data noise are proven. Furthermore, under source conditions on the exact solution, suboptimal convergence rates and, under certain additional regularity conditions, optimal order convergence rates are shown. The abstract results are examined in more detail for several known parameter choice rules: the quasi-optimality rules (both continuous and discrete) and the Hanke-Raus rules, together with some specific regularization methods: Tikhonov regularization, Landweber iteration, and spectral cutoff.

Key Words.

regularization, heuristic parameter choice rule, Hanke-Raus rule, quasi-optimality rule, L-curve method

AMS Subject Classifications.

65J20, 47A52, 65J22

- 258 Application of barycenter refined meshes in linear elasticity and incompressible fluid dynamics. *Maxim A. Olshanskii and Leo G. Rebholz.*

Abstract.

The paper demonstrates that enhanced stability properties of some finite element methods on barycenter refined meshes enables efficient numerical treatment of problems involving incompressible or nearly incompressible media. One example is the linear elasticity problem in a pure displacement formulation, where a lower order finite element method is studied which is optimal order accurate and robust with respect to the Poisson ratio parameter. Another example is a penalty method for incompressible viscous flows. In this case, we show that barycenter refined meshes prompt a “first penalize, then discretize” approach, avoiding locking phenomena, and leading to a method with optimal convergence rates independent of the penalty parameter, and resulting in discrete systems with advantageous algebraic properties.

Key Words.

finite element method, barycenter-mesh refinement, locking-free penalty method, Navier-Stokes equations, linear elasticity

AMS Subject Classifications.

65F05, 65M60, 65M12, 76D05, 74B05

- 275 Perturbation analysis for complex symmetric, skew symmetric, even and odd matrix polynomials. *Sk. Safique Ahmad and Volker Mehrmann.*

Abstract.

In this work we propose a general framework for the structured perturbation analysis of several classes of structured matrix polynomials in homogeneous form, including complex symmetric, skew-symmetric, even and odd matrix polynomials. We introduce structured backward errors for approximate eigenvalues and eigenvectors and we construct minimal structured perturbations such that an approximate eigenpair is an exact eigenpair of an appropriately perturbed matrix polynomial. This work extends previous work of Adhikari and Alam for the non-homogeneous case (we include infinite eigenvalues), and we show that the structured backward errors improve the known unstructured backward errors.

Key Words.

polynomial eigenvalue problem, even matrix polynomial, odd matrix polynomial, complex symmetric matrix polynomial, complex skew-symmetric matrix polynomial, perturbation theory, backward error

AMS Subject Classifications.

65F15, 15A18, 65F35, 15A12

- 303 Computation of the torsional modes in an axisymmetric elastic layer. *Mohamed Kara, Boubakeur Merouani, and Lahcène Chorfi.*

Abstract.

This paper is devoted to the numerical study of an eigenvalue problem modeling the torsional modes in an infinite and axisymmetric elastic layer. In the cylindrical coordinates (r, z) , without θ , the problem is posed in a semi-infinite strip $\Omega = \mathbb{R}_+^* \times]0, L[$. For the numerical approximation, we formulate the problem in the bounded domain $\Omega_R =]0, R[\times]0, L[$. To this end, we use the localized

finite element method, which links two representations of the solution: the analytic solution in the exterior domain $\Omega'_R =]R, +\infty[\times]0, L[$ and the numerical solution in the interior domain Ω_R .

Key Words.

torsional modes, spectra, localized finite elements

AMS Subject Classifications.

35P15, 65N30, 47A70

- 317** Stieltjes interlacing of zeros of Jacobi polynomials from different sequences. *K. Driver, A. Jooste, and K. Jordaan.*

Abstract.

A theorem of Stieltjes proves that, given any sequence $\{p_n\}_{n=0}^\infty$ of orthogonal polynomials, there is at least one zero of p_n between any two consecutive zeros of p_k if $k < n$, a property called Stieltjes interlacing. We show that Stieltjes interlacing extends, under certain conditions, to the zeros of Jacobi polynomials from different sequences. In particular, we prove that the zeros of $P_{n+1}^{\alpha,\beta}$ interlace with the zeros of $P_{n-1}^{\alpha+k,\beta}$ and with the zeros of $P_{n-1}^{\alpha,\beta+k}$ for $k \in \{1, 2, 3, 4\}$ as well as with the zeros of $P_{n-1}^{\alpha+t,\beta+k}$ for $t, k \in \{1, 2\}$; and, in each case, we identify a point that completes the interlacing process. More generally, we prove that the zeros of the k th derivative of $P_n^{\alpha,\beta}$, together with the zeros of an associated polynomial of degree k , interlace with the zeros of $P_{n+1}^{\alpha,\beta}$, $k, n \in \mathbb{N}$, $k < n$.

Key Words.

interlacing of zeros; Stieltjes' Theorem; Jacobi polynomials

AMS Subject Classifications.

33C45, 42C05

- 327** A posteriori error estimation for the Legendre collocation method applied to integral-algebraic Volterra equations. *S. Pishbin, F. Ghoreishi, and M. Hadizadeh.*

Abstract.

In this work, we analyze the Legendre collocation method for a mixed system of Volterra integral equations of the first and second kind which is known as Integral Algebraic Equations (IAEs). In order to obtain the approximate solution, the kernels in the system of integral equations are approximated by using the discrete Legendre expansion. A posteriori error estimate is obtained which is based on the Lebesgue constants corresponding to the Lagrange interpolation polynomials and some well-known results of orthogonal polynomials theory. The spectral rate of convergence for the described method applied to linear and nonlinear IAEs is also established in the L^2 -norm. Finally, the proposed method is illustrated by several test problems which confirm the theoretical prediction of the error estimation.

Key Words.

integral algebraic equations, system of Volterra integral equations, Legendre collocation method, error analysis, numerical treatments

AMS Subject Classifications.

65R20, 34A05

- 347 Reduced rank extrapolation applied to electronic structure computations.
Sébastien Duminil and Hassane Sadok.

Abstract.

This paper presents a new approach for accelerating the convergence of a method for solving a nonlinear eigenvalue problem that arises in electronic structure computations. Specifically, we seek to solve the Schrödinger equation using the Kohn-Sham formulation. This requires the solution of a nonlinear eigenvalue problem. The currently prevailing method for determining an approximate solution is the Self-Consistent Field (SCF) method accelerated by Anderson's iterative procedure or a Broyden-type method. We propose to formulate the nonlinear eigenvalue problem as a nonlinear fixed point problem and to accelerate the convergence of fixed-point iteration by vector extrapolation. We revisit the reduced rank extrapolation method, a polynomial-type vector extrapolation method, and apply it in the RSDFT (real-space density functional theory) software.

Key Words.

nonlinear eigenvalue problem, vector extrapolation, Kohn-Sham equation, Anderson's method, Broyden's method, reduced rank extrapolation

AMS Subject Classifications.

65H10, 65F10

- 363 Block factorizations and qd-type transformations for the MR^3 algorithm.
Paul R. Willems and Bruno Lang.

Abstract.

Factorizing symmetric tridiagonal matrices and propagating the factorizations to shifted matrices are central tasks in the MR^3 algorithm for computing partial eigen-systems. In this paper we propose block bidiagonal factorizations LDL^* with 1×1 and 2×2 blocks in D as an alternative to the bidiagonal and twisted factorizations used hitherto. With block factorizations, the element growth can be reduced (or avoided altogether), which is essential for the success of the MR^3 algorithm, in particular, if the latter is used to determine the singular value decomposition of bidiagonal matrices. We show that the qd algorithm used for shifting bidiagonal factorizations, e.g., $LDL^* - \tau I =: L^+ D^+ (L^+)^*$ can be extended to work with blocks in a mixed stable way, including criteria for determining a suitable block structure dynamically.

Key Words.

symmetric tridiagonal matrix, eigensystem, MRRR algorithm, block bidiagonal factorizations, qd algorithm, theory and implementation

AMS Subject Classifications.

65F15, 65G50, 15A18