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Contents

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

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

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

202 Evaluating the Fréchet derivative of the matrix pth root. *João R. Cardoso*.

Abstract.
This paper shows that computing the Fréchet derivative of the matrix pth 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 pth 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

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 kth derivative of $P_n^{\alpha,\beta}$, together with the zeros of an associated polynomial of degree k, interlace with the zeros of $P_{n+1}^{\alpha,\beta}, k, n \in N, k < n$.

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 eigensystems. 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., $\mathsf{LDL}^* - \tau\mathsf{I} =: \mathsf{L}^+\mathsf{D}^+(\mathsf{L}^+)^*$ 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