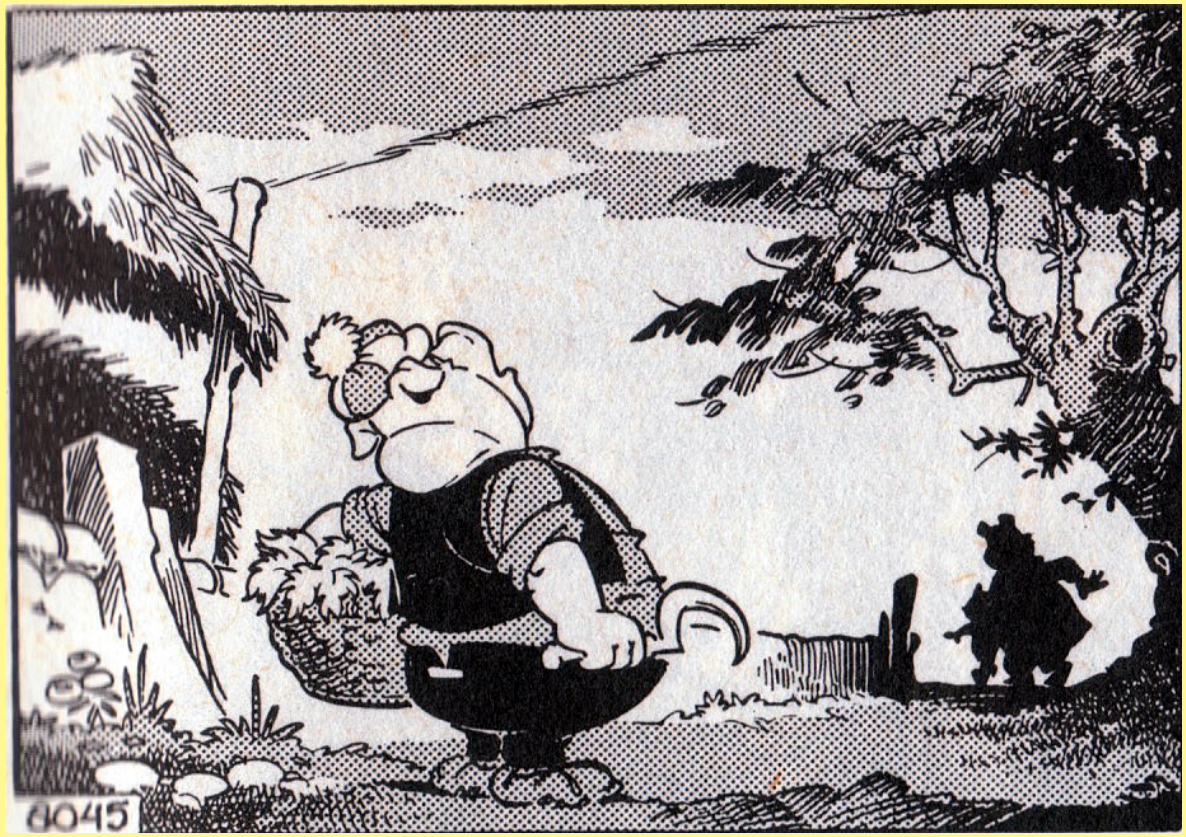
… AND THEN THINGS CHANGED

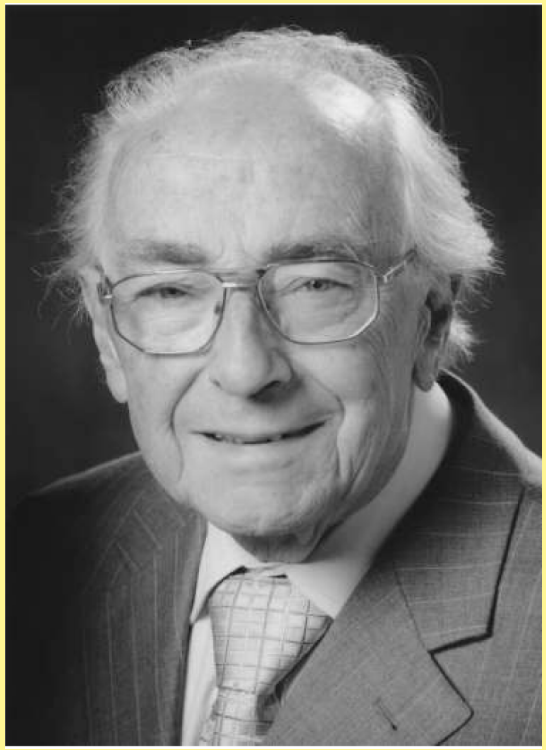


12 november 2015

1960-1980: views on numerical methods

(in Utrecht, professor A. van der Sluis, drs. Hans Zweerus)

- Wilkinson (1965)
- Linear systems: LU
- CG / Lanczos: finite methods
- All basic methods already invented
- New insights required for continous problems (pde's, quadrature, ode's) more mathematical skills necessary: Functional Analysis



The solution: Gerard Sleijpen

- Gerard's expertise before Utrecht:
- Thesis: Convolution measure algebras on semigroups
- Scary titles like: The support of the Wiener algebra on stips,
- And: emaciated sets and measures with continuous translations
- And: The action of a semigroup on a space of bounded Radon measures,
- And 10 more
- So, when did Gerard come to Utrecht?

Reconstruction of Gerard's CV

A simple NA-type of analysis:

1. Born in 1950 (since he is 65 now)

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1. Born in 1950 (since he is 65 now)
2. Clever person, hence after 17 years to Nijmegen
3. I guess he did his master in about 5 years

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This amounts to: $(1950+17+5+4+5)(1+4\xi)\approx 1981$

… and then things changed

- In 1982: his last paper on pure mathematics
- In 1983: first NA-paper, on parabolic pde's
- Later in the 1980's: 4 papers on Hopscotch methods (with and without Jan ter Maten)

Worked together with phd-students of van der Sluis

Intermezzo

Professor van der Sluis retired in 1988.

Two years of very hard work

All NA in Utrecht was done by Gerard

1990

- Workstations introduced in Utrecht (after 2 years of no-prof NA)

1990

- Workstations introduced in Utrecht (after 2 years of no-prof NA)
- Henk came from Delft to Utrecht

...and then things changed

- In 1991 first preprint on num lin alg (cg)
- 1993: 5 papers (4 with H)
- 1994: 8 papers (4 with H)
- 1995: 4 papers (with H)
- 1996: 11 papers (10 with H)
- 1997: 2 papers (1 with H) fatigue?
- 1998: 5 papers (with H)
- 1999: 4 papers (3 with H)
- 2000: 5 papers (with H)

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- 1995: 4 papers (with H)
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- 1998: 5 papers (with H)
- 1999: 4 papers (3 with H)
- 2000: 5 papers (with H)

- After 2000 some 25 papers, now with other co-authors, but still mainly on iterative methods (JD, IDR, multilevel)
- And many of my phd-students (piao's of Gerard)

highlights

Numerical Algorithms 7(1994)75–109

BiCGstab(l) and other hybrid Bi-CG methods

G.L.G. Sleijpen, H.A. van der Vorst and D.R. Fokkema

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Received 29 October 1993; revised 2 March 1994
Communicated by C. Brezinski

It is well-known that Bi-CG can be adapted so that the operations with A^T can be avoided, and hybrid methods can be constructed in which it is attempted to further improve the convergence behaviour. Examples of this are CGS, Bi-CGSTAB, and the more general BiCGstab(l) method. In this paper it is shown that BiCGstab(l) can be implemented in different ways. Each of the suggested approaches has its own advantages and disadvantages. Our implementations allow for combinations of Bi-CG with arbitrary polynomial methods. The choice for a specific implementation can also be made for reasons of numerical stability. This aspect receives much attention. Various effects have been illustrated by numerical examples.

Keywords: Bi-Conjugate gradients, non-symmetric linear systems, CGS, Bi-CGSTAB, iterative solvers, ORTHODIR, Krylov subspace.

AMS subject classification: 65F10.

1. Introduction and background

The Bi-CG algorithm [3,7] is an iterative solution method for linear systems

$$Ax = b \tag{1}$$

in which A is some given non-singular $n \times n$ matrix and b some given n-vector. Typically, n is large and A is sparse. For ease of presentation, we assume A and b to be real.

Starting with some initial approximation x_0 for x and some "shadow" residual $\tilde{r}_0$ Bi-CG produces iteratively sequences of approximations x_k, residuals r_k and search directions u_k by

$$u_k = r_k - \beta_k u_{k-1}, \quad x_{k+1} = x_k + \alpha_k u_k, \quad r_{k+1} = r_k - \alpha_k A u_k, \tag{2}$$

where α_k and β_k are appropriate scalars, $u_{-1} = 0$, and $r_0 = b - Ax_0$. The residual r_k and the search direction u_k are in the Krylov subspace $\mathcal{K}_{k+1}(A; r_0)$ of order $k+1$ generated by A and r_0. This implies that the residuals r_k can be written as $r_k = \phi_k(A) r_0$ where ϕ_k is a certain polynomial, the so-called Bi-CG polynomial, in the space $\mathcal{P}_k^1$ of all polynomials q of degree k for which $q(0) = 1$. We will use

highlights

SIAM REVIEW
Vol. 42, No. 2, pp. 267–293

A Jacobi–Davidson Iteration Method for Linear Eigenvalue Problems*

Gerard L. G. Sleijpen†
Henk A. Van der Vorst†

Abstract. In this paper we propose a new method for the iterative computation of a few of the extremal eigenvalues of a symmetric matrix and their associated eigenvectors. The method is based on an old and almost unknown method of Jacobi. Jacobi's approach, combined with Davidson's method, leads to a new method that has improved convergence properties and that may be used for general matrices. We also propose a variant of the new method that may be useful for the computation of nonextremal eigenvalues as well.

Key words. eigenvalues and eigenvectors, Davidson's method, Jacobi iterations, harmonic Ritz values

AMS subject classifications. 65F15, 65N25

PII. S0036144599363084

1. Introduction. Suppose we want to compute one or more eigenvalues and their corresponding eigenvectors of the $n \times n$ matrix A. Several iterative methods are available: Jacobi's diagonalization method [9], [23], the power method [9], the method of Lanczos [13], [23], Arnoldi's method [1], [26], and Davidson's method [4], [26], [3], [15], [18]. The latter method has been reported to be quite successful, most notably in connection with certain symmetric problems in computational chemistry [4], [5], [32]. The success of the method seems to depend quite heavily on the (strong) diagonal dominance of A.

The method of Davidson is commonly seen as an extension to Lanczos's method, but as Saad [26] points out, from the implementation point of view it is more related to Arnoldi's method. In spite of these relations, the success of the method is not well understood [26]. Some recent convergence results and improvements, as well as numerical experiments, are reported in [3], [15], [16], [18], [17], [19], [28].

Jacobi [12] proposed a method for eigenvalue approximation that essentially was a combination of (1) Jacobi rotations, (2) Gauss–Jacobi iterations, and (3) an almost forgotten method that we will refer to as Jacobi's orthogonal component correction (JOCC). Reinvestigation of Jacobi's ideas leads to another view of Davidson's method, and this not only helps us explain the behavior of the method, but it also leads to a new and robust method with superior convergence properties for nondiagonally dominant (unsymmetric) matrices as well. Special variants of this method are already known; see [19], [28], and our discussion in section 4.1.

*Published electronically April 24, 2000. This paper originally appeared in *SIAM Journal on Matrix Analysis and Applications*, Volume 17, Number 2, 1996, pages 401–425.
http://www.siam.org/journals/sirev/42-2/36308.html

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Computing 56, 141–163 (1996)

Computing

Reliable Updated Residuals in Hybrid Bi-CG Methods

G. L. G. Sleijpen and **H. A. van der Vorst**, Utrecht

Received February 1, 1995; revised May 29, 1995

Abstract — Zusammenfassung

Reliable Updated Residuals in Hybrid Bi-CG Methods. Many iterative methods for solving linear equations $Ax = b$ aim for accurate approximations to x, and they do so by updating residuals iteratively. In finite precision arithmetic, these computed residuals may be inaccurate, that is, they may differ significantly from the (true) residuals that correspond to the computed approximations. In this paper we will propose variants on Neumaier's strategy, originally proposed for CGS, and explain its success. In particular, we will propose a more restrictive strategy for accumulating groups of updates for updating the residual and the approximation, and we will show that this may improve the accuracy significantly, while maintaining speed of convergence. This approach avoids restarts and allows for more reliable stopping criteria. We will discuss updating conditions and strategies that are efficient, lead to accurate residuals, and are easy to implement. For CGS and Bi-CG these strategies are particularly attractive, but they may also be used to improve Bi-CGSTAB, BiCGstab(l), as well as other methods.

AMS Subject Classification: 65F10

Key words: Non-symmetric linear systems, iterative solver, CGS, Bi-CGSTAB, BiCGstab(l).

Zuverläßlich berechnete Residuen in hybriden Bi-CG Verfahren. Viele iterative Methoden zur Lösung linearer Gleichungssysteme berechnen die Iterierten über aufdatierte Residuen. In endlicher Arithmetik können diese Residuen sehr ungenau sein, d.h., sie können sich erheblich von den tatsächlichen unterscheiden. In dieser Arbeit stellen wir Varianten der Neumaier Strategie vor, die ursprünglich für das CGS-Verfahren vorgeschlagen wurde, und erklären deren Erfolge. Insbesondere werden wir eine Variante vorschlagen, bei der mehrere Aufdatierungsschritte zusammengefaßt werden. Wir zeigen, daß sich die Genauigkeit der berechneten Residuen dadurch erheblich verbessern läßt, ohne daß die Konvergenzgeschwindigkeit beeinträchtigt wird. Dieser Ansatz vermeidet Neustarts und ermöglicht zuverlässigere Abbruchkriterien. Wir diskutieren Aufdatierungsbedingungen und Strategien, die effizient und leicht zu implementieren sind. Diese Strategien führen zu genaueren Residuen und sind insbesondere für CGS und Bi-CG–aber auch für Bi-CGSTAB, BiCGstab(l) und andere Verfahren–sehr attraktiv.

1. Introduction

We will focus on the iterative solution of linear systems

$$Ax = b \tag{1}$$

in which A is a non-singular $n \times n$ matrix and b a given n-vector. Typically n is large and A is sparse. To simplify our presentation, we will assume A and b to be real. The class of iterative methods is characterized by the fact that the

highlights

SIAM J. SCI. COMPUT.
Vol. 20, No. 1, pp. 94–125

JACOBI–DAVIDSON STYLE QR AND QZ ALGORITHMS FOR THE REDUCTION OF MATRIX PENCILS*

DIEDERIK R. FOKKEMA†‡, GERARD L. G. SLEIJPEN†, AND HENK A. VAN DER VORST†

Abstract. Recently the Jacobi–Davidson subspace iteration method has been introduced as a new powerful technique for solving a variety of eigenproblems. In this paper we will further exploit this method and enhance it with several techniques so that practical and accurate algorithms are obtained. We will present two algorithms, JDQZ for the generalized eigenproblem and JDQR for the standard eigenproblem, that are based on the iterative construction of a (generalized) partial Schur form. The algorithms are suitable for the efficient computation of several (even multiple) eigenvalues and the corresponding eigenvectors near a user-specified target value in the complex plane. An attractive property of our algorithms is that explicit inversion of operators is avoided, which makes them potentially attractive for very large sparse matrix problems.

We will show how effective restarts can be incorporated in the Jacobi–Davidson methods, very similar to the implicit restart procedure for the Arnoldi process. Then we will discuss the use of preconditioning, and, finally, we will illustrate the behavior of our algorithms by a number of well-chosen numerical experiments.

Key words. linear eigenproblems, generalized eigenproblems, Schur form, generalized Schur form, QR-algorithm, QZ-algorithm, Jacobi–Davidson, iterative methods

AMS subject classifications. 65F15, 65N25

PII. S1064827596300073

1. Introduction.

In this paper we expand on the usage of the Jacobi–Davidson method [26], [24] for the computation of several solutions of the generalized eigenproblem[1]

$$(\beta \mathbf{A} - \alpha \mathbf{B})\,\mathbf{q} = \mathbf{0}, \tag{1}$$

where $\mathbf{A}$ and $\mathbf{B}$ are large and sparse $(n \times n)$-matrices, which may be complex and/or nonnormal. We will also discuss the standard eigenproblem

$$(\mathbf{A} - \lambda \mathbf{I})\,\mathbf{q} = \mathbf{0}. \tag{2}$$

Of course, with $\mathbf{B} = \mathbf{I}$ the generalized eigenproblem reduces to a standard eigenproblem, and we could have restricted ourselves to the generalized eigenproblem case. However, simplifications are possible when $\mathbf{B} = \mathbf{I}$ that help reduce the memory requirements and the computational complexity, and some phenomena are easier to explain.

Our algorithms are based on the Jacobi–Davidson method described in [26] and are adapted for generalized eigenproblems (and other polynomial eigenproblems) in [24]. We have modified the Jacobi–Davidson approach so that partial (generalized) Schur forms are computed. The partial Schur forms have been chosen mainly

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‡Current address: ISE Integrated Systems Engineering AG, Technopark Zürich, Technoparkstrasse 1, CH-8005 Zürich, Switzerland (fokkema@ise.ch).
[1]The family $\mathbf{A} - \lambda\mathbf{B}$ is called a *matrix pencil*, and the generalized eigenvalues $\langle \alpha, \beta \rangle$, solutions of (1), are also called eigenvalues of the matrix pencil (cf., e.g., [30]).

highlights

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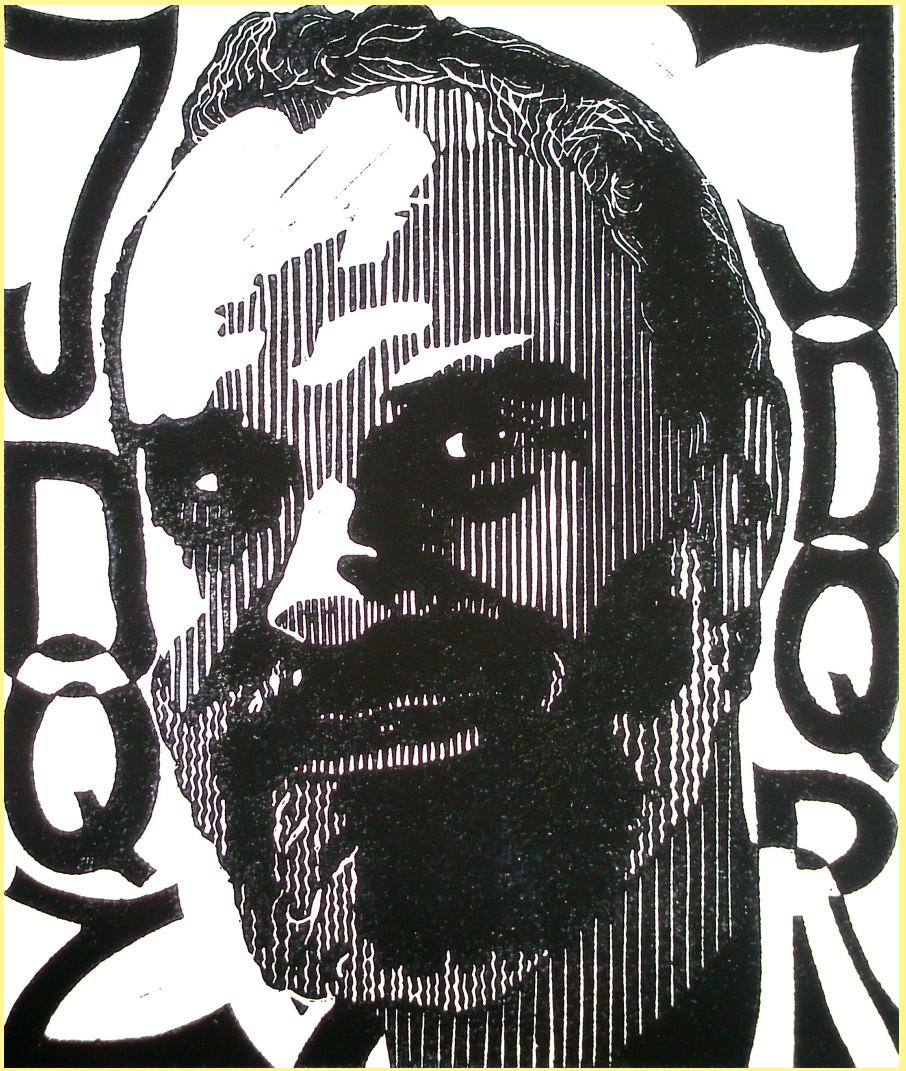
highlights



highlights

SIAM J. SCI. COMPUT.
Vol. 19, No. 2, pp. 657–674, March 1998

020

ACCELERATED INEXACT NEWTON SCHEMES FOR LARGE SYSTEMS OF NONLINEAR EQUATIONS*

DIEDERIK R. FOKKEMA†, GERARD L. G. SLEIJPEN‡, AND HENK A. VAN DER VORST‡

Abstract. Classical iteration methods for linear systems, such as Jacobi iteration, can be accelerated considerably by Krylov subspace methods like GMRES. In this paper, we describe how inexact Newton methods for nonlinear problems can be accelerated in a similar way and how this leads to a general framework that includes many well-known techniques for solving linear and nonlinear systems, as well as new ones. Inexact Newton methods are frequently used in practice to avoid the expensive exact solution of the large linear system arising in the (possibly also inexact) linearization step of Newton's process. Our framework includes acceleration techniques for the "linear steps" as well as for the "nonlinear steps" in Newton's process. The described class of methods, the accelerated inexact Newton (AIN) methods, contains methods like GMRES and GMRESR for linear systems, Arnoldi and Jacobi–Davidson for linear eigenproblems, and many variants of Newton's method, like damped Newton, for general nonlinear problems. As numerical experiments suggest, the AIN approach may be useful for the construction of efficient schemes for solving nonlinear problems.

Key words. nonlinear problems, Newton's method, inexact Newton, iterative methods

AMS subject classification. 65H10

PII. S1064827595296148

1. Introduction. Our goal in this paper is twofold. A number of iterative solvers for linear systems of equations, such as the full orthogonalization method (FOM) [23], the generalized minimal residual method (GMRES) [26], the generalized congruent residual method (GCR) [31], the flexible GMRES method [25], the GMRES recursive method (GMRESR) [29], and the GCR orthogonal method (GCRO) [7], are in structure very similar to iterative methods for linear eigenproblems, like shift and invert Arnoldi [1, 24], Davidson [6, 24], and Jacobi–Davidson [28]. We will show that all these algorithms can be viewed as instances of an accelerated inexact Newton (AIN) scheme (cf. Algorithm 3) when applied to either linear equations or linear eigenproblems. This observation may help us in the design and analysis of algorithms by "transporting" algorithmic approaches from one application area to another. Moreover, our aim is to identify efficient AIN schemes for nonlinear problems as well, and we will show how we can learn from the algorithms for linear problems.

To be more specific, we will be interested in the numerical approximation of the solution u of the nonlinear equation

$$F(u) = 0, \tag{1.1}$$

where F is some smooth (nonlinear) map from a domain in $\mathbb{R}^n$ (or $\mathbb{C}^n$) that contains the solution u, into $\mathbb{R}^n$ (or $\mathbb{C}^n$), where n is typically large.

Some special types of systems of equations will play an important motivating role in this paper.

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SIAM J. MATRIX ANAL. APPL.
Vol. 22, No. 3, pp. 726–751

DIFFERENCES IN THE EFFECTS OF ROUNDING ERRORS IN KRYLOV SOLVERS FOR SYMMETRIC INDEFINITE LINEAR SYSTEMS*

GERARD L. G. SLEIJPEN†, HENK A. VAN DER VORST†, AND JAN MODERSITZKI‡

Abstract. The three-term Lanczos process for a symmetric matrix leads to bases for Krylov subspaces of increasing dimension. The Lanczos basis, together with the recurrence coefficients, can be used for the solution of symmetric indefinite linear systems, by solving a reduced system in one way or another. This leads to well-known methods: MINRES (minimal residual), GMRES (generalized minimal residual), and SYMMLQ (symmetric LQ). We will discuss in what way and to what extent these approaches differ in their sensitivity to rounding errors.

In our analysis we will assume that the Lanczos basis is generated in exactly the same way for the different methods, and we will not consider the errors in the Lanczos process itself. We will show that the method of solution may lead, under certain circumstances, to large additional errors, which are not corrected by continuing the iteration process.

Our findings are supported and illustrated by numerical examples.

Key words. linear systems, iterative methods, MINRES, GMRES, SYMMLQ, stability

AMS subject classifications. 65F10, 65N12

PII. S0895479897323087

1. Introduction.

We consider iterative methods for the construction of approximations to the solution of a linear system $\mathbf{Ax} = \mathbf{b}$, where $\mathbf{A}$ is supposed to be a real symmetric n by n matrix. Without loss of generality, we assume $\mathbf{x}_0 = 0$. Let $\mathbf{r}_k = \mathbf{b} - \mathbf{A}\mathbf{x}_k$ (in particular, $\mathbf{r}_0 = \mathbf{b}$) and

$$\mathcal{K}_k(\mathbf{A};\mathbf{b}) \equiv \text{Span}\{\mathbf{b}, \mathbf{Ab}, \ldots, \mathbf{A}^{k-1}\mathbf{b}\},$$

the k-dimensional Krylov subspace. The methods to be analyzed build the iterates $\mathbf{x}_k$ such that

1. $\mathbf{x}_k \in \mathcal{K}_k(\mathbf{A};\mathbf{b})$ and $\|\mathbf{b} - \mathbf{A}\mathbf{x}_k\|_2 = \min$ (GMRES, MINRES),
2. $\mathbf{x}_k \in \mathbf{A}\mathcal{K}_k(\mathbf{A};\mathbf{b})$ and $\|\mathbf{A}^{-1}\mathbf{b} - \mathbf{x}_k\|_2 = \min$ (SYMMLQ).

With the standard three-term Lanczos process, we generate an orthonormal basis $\mathbf{v}_1, \ldots, \mathbf{v}_k$ for $\mathcal{K}_k(\mathbf{A};\mathbf{b})$, with $\mathbf{v}_1 \equiv \mathbf{b}/\|\mathbf{b}\|_2$. The three-term Lanczos process can be recast in matrix formulation as

$$\mathbf{AV}_k = \mathbf{V}_{k+1}\underline{T}_k, \tag{1}$$

in which $\mathbf{V}_j$ is defined as the n by j matrix with columns $\mathbf{v}_1, \ldots, \mathbf{v}_j$, and $\underline{T}_k$ is a $k+1$ by k tridiagonal matrix.

Paige [9] has shown that in finite precision arithmetic, the Lanczos process can be implemented so that the *computed* $\mathbf{V}_{k+1}$ and $\underline{T}_k$ satisfy

$$\mathbf{AV}_k = \mathbf{V}_{k+1}\underline{T}_k + \mathbf{F}_k, \tag{2}$$

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http://www.siam.org/journals/simax/22-3/32308.html
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highlights

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