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AN IMPLEMENTATION OF THE QMR METHOD BASED ON COUPLED TWO-TERM RECURRENCES*

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Abstract. Recently, the authors proposed a new Krylov subspace iteration, the quasi-minimal residual (QMR) algorithm, for solving non-Hermitian linear systems. In the original implementation of the QMR method, the Lanczos process with look-ahead is used to generate basis vectors for the underlying Krylov subspaces. In the Lanczos algorithm, these basis vectors are computed by means of three-term recurrences. It has been observed that, in finite-precision arithmetic, vector iterations based on three-term recursions are usually less robust than mathematically equivalent coupled two-term vector recurrences.

This paper presents a look-ahead algorithm that constructs the Lanczos basis vectors by means of coupled two-term recursions. Some implementation details are given, and the look-ahead strategy is described. A new implementation of the QMR method, based on this coupled two-term algorithm, is proposed. A simplified version of the QMR algorithm without look-ahead is also presented, and the special case of QMR for complex symmetric linear systems is considered. Results of numerical experiments comparing the original and the new implementations of the QMR method are reported.

Key words. Krylov subspace iteration, quasi-minimal residual method, non-Hermitian matrices, coupled two-term recurrences, look-ahead techniques, complex symmetric matrices

AMS subject classifications. 65F10, 65N22

1. Introduction.

Recently, we proposed a new Krylov subspace method, the quasi-minimal residual (QMR) algorithm [9], for the iterative solution of general nonsingular non-Hermitian systems of linear equations

$$Ax = b. \tag{1.1}$$

The QMR method is closely related to the classical biconjugate gradient (BCG) algorithm due to Lanczos [17]. The BCG method aims at generating approximate solutions for (1.1) that satisfy a Galerkin condition. Unfortunately, for non-Hermitian matrices A, such iterates need not always exist, and this is the source of one of the two possible breakdowns—triggered by division by 0—that can occur during each iteration step of BCG. The second breakdown is equivalent to the possible breakdown—also triggered by division by 0—of the nonsymmetric Lanczos process [16]. In finite-precision arithmetic, it is unlikely that one encounters exact breakdowns in the BCG algorithm. However, near-breakdowns can occur, which can cause a buildup of round-off in successive iterations. Another problem with BCG is the lack of a residual minimization property for its iterates, which leads to a typically erratic convergence behavior, with wild oscillations in the residual norm.

The QMR method offers remedies for these problems. It generates iterates that are defined by a quasi minimization of the residual norm, rather than a Galerkin condition. This eliminates the oscillations and leads to a smooth and nearly monotone convergence behavior. In contrast to BCG, a QMR iterate always exists at each iteration step, and this excludes breakdowns caused by nonexistent iterates. Moreover, possible breakdowns in the underlying Lanczos

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process are prevented by using look-ahead techniques. Therefore, except for the rare event of an incurable breakdown, breakdowns cannot occur in the QMR method.

In the original QMR algorithm [9], an implementation of the Lanczos method with look-ahead is used to generate basis vectors for the underlying Krylov subspaces. In the Lanczos process, these basis vectors are generated by means of three-term recurrences. It turns out that, in finite-precision arithmetic, these three-term vector iterations are usually less robust than mathematically equivalent coupled two-term vector recurrences. In this paper, we present a general look-ahead algorithm based on coupled two-term recursions for constructing basis vectors of Krylov subspaces. Based on this algorithm we then propose a new implementation of the QMR method.

We stress that the better numerical behavior of coupled two-term recurrences is not a characteristic of QMR only, and that this phenomenon was also observed for other Krylov subspace methods. For instance, Joubert [15] remarked that BCG, which is based on coupled two-term recurrences, is more robust than the mathematically equivalent Lanczos/Orthodir and Lanczos/Orthores algorithms, which are both based on three-term vector recursions. Indeed, Lanczos/Orthodir and Lanczos/Orthores often converge considerably slower than BCG, or they even diverge, while BCG converges; we refer the reader to [18] for numerical examples that illustrate this phenomenon. Finally, we remark that the standard implementation of the classical conjugate gradient (CG) method of Hestenes and Stiefel [14] is also based on coupled two-term recurrences. Reid [20] mentions that this version of CG is "preferable on computational grounds" to an equivalent three-term implementation of CG. Woźniakowski [24] presents numerical examples for which an implementation of CG based on two-term recurrences generates approximate solutions to a higher accuracy than does a three-term version of CG.

The remainder of the paper is organized as follows. In §2, we briefly review the Lanczos process and the original QMR algorithm. In §3, we present a sketch of the proposed look-ahead procedure for constructing Lanczos vectors by means of coupled two-term recurrences. In §4, we discuss the look-ahead strategy for this algorithm, and in §5, we give some implementation details. Next we combine the coupled two-term procedure with the QMR approach. In §6, we outline the resulting implementation for the general case of QMR with look-ahead. In §7, we present a simplified version of the QMR algorithm without look-ahead. In §8, we consider a variant of QMR for the special case of complex symmetric linear systems. In §9, we report results of numerical experiments comparing the original and the new implementations of the QMR method. Finally, in §10, we make some concluding remarks.

Throughout the paper, all vectors and matrices are allowed to have real or complex entries. As usual, $M^T = [m_{kj}]$ and $M^H = [\overline{m}_{kj}]$ denote the transpose and the conjugate transpose, respectively, of the matrix $M = [m_{jk}]$. We use $\sigma_{\max}(M)$ and $\sigma_{\min}(M)$ for the largest and smallest singular value of M, respectively. The vector norm $\|x\| := \sqrt{x^H x}$ is always the Euclidean norm and $\|M\| := \sigma_{\max}(M)$ is the corresponding matrix norm. We denote by

$$\mathcal{P}_n := \{\varphi(\lambda) \equiv \gamma_0 + \gamma_1\lambda + \cdots + \gamma_n\lambda^n \mid \gamma_0, \gamma_1, \ldots, \gamma_n \in \mathbb{C}\}$$

the set of all complex polynomials of degree at most n. The nth Krylov subspace of $\mathbb{C}^N$ generated by $c \in \mathbb{C}^N$ and the $N \times N$ matrix B is defined by

$$K_n(c, B) := \operatorname{span}\{c, Bc, \ldots, B^{n-1}c\},$$

and we will make use of the fact that

$$K_n(c, B) = \{\varphi(B)c \mid \varphi \in \mathcal{P}_{n-1}\}.$$

Furthermore, it is always assumed that A is an $N \times N$ matrix, singular or nonsingular.

Finally, we remark that, for complex matrices, there are two equivalent formulations of the Lanczos process, using either A^T or A^H. In this paper, we have chosen the formulation with A^T, for two reasons. First, it avoids complex conjugation of the scalars in some of the recurrence relations, and, second, the recursions reduce immediately for the special case of complex symmetric matrices.

2. The QMR algorithm. In this section, we briefly describe the QMR method and its original implementation [9]. We remark that, in [9], QMR was proposed for nonsingular linear systems (1.1). Freund and Hochbruck [8] showed that the QMR method can also be applied to singular square systems, and that it always generates well-defined iterates. However, as discussed in [8], these iterates converge to a meaningful solution of (1.1) only for consistent systems with coefficient matrices of index 1. An important special case for which these conditions are satisfied is consistent singular systems with a one-dimensional null space, i.e.,

$$b \in \{Ax \mid x \in \mathbb{C}^N\} \quad \text{and} \quad \dim\{x \in \mathbb{C}^N \mid Ax = 0\} = 1. \tag{2.1}$$

In this paper, we always consider the QMR method for the general case of $N \times N$ linear systems, with singular or nonsingular coefficient matrices A.

2.1. Krylov subspace methods. Let $x_0 \in \mathbb{C}^N$ be an arbitrary initial guess for the linear system (1.1), and denote by $r_0 := b - Ax_0$ the corresponding residual vector. An iterative scheme for solving (1.1) is called a *Krylov subspace method* if, for any choice of x_0, it produces approximate solutions of the form

$$x_n \in x_0 + K_n(r_0, A), \qquad n = 1, 2, \ldots . \tag{2.2}$$

Clearly, the design of a Krylov subspace algorithm consists of two main parts: the construction of suitable basis vectors for the Krylov subspaces $K_n(r_0, A)$ in (2.2) and the choice of the actual iterates x_n. The QMR method is an example of a Krylov subspace iteration, where the basis vectors are generated by means of the nonsymmetric Lanczos process, and the iterates are characterized by a QMR property. Next, we describe these two main ingredients of QMR.

2.2. The Lanczos process. The Lanczos method is started with two vectors

$$v_1 = r_0/\rho_1, \quad \text{where } \rho_1 = \|r_0\|, \tag{2.3}$$

and an arbitrary second starting vector

$$w_1 \in \mathbb{C}^N \quad \text{with } \|w_1\| = 1. \tag{2.4}$$

It then produces two sequences of vectors

$$\{v_j\}_{j=1}^n \quad \text{and} \quad \{w_j\}_{j=1}^n, \tag{2.5}$$

such that, for $n = 1, 2, \ldots,$

$$\begin{aligned} \operatorname{span}\{v_1, v_2, \ldots, v_n\} &= K_n(v_1, A), \\ \operatorname{span}\{w_1, w_2, \ldots, w_n\} &= K_n(w_1, A^T), \end{aligned} \tag{2.6}$$

and the two sets are biorthogonal or block biorthogonal, i.e.,

$$W_n^T V_n = D_n, \tag{2.7}$$

where D_n is a diagonal or block-diagonal matrix. Here, and in the sequel, we denote by

$$V_n := [\, v_1 \quad v_2 \quad \cdots \quad v_n \,] \quad \text{and} \quad W_n := [\, w_1 \quad w_2 \quad \cdots \quad w_n \,] \tag{2.8}$$

the matrices containing the Lanczos vectors $\{v_j\}_{j=1}^n$ and $\{w_j\}_{j=1}^n$ as columns. We remark that the conditions (2.6)–(2.7) determine the vectors (2.5) only up to scaling. Throughout this paper, we always scale the Lanczos vectors to have unit length

$$\|v_n\| = \|w_n\| = 1, \qquad n = 1, 2, \ldots . \tag{2.9}$$

The crucial point of the Lanczos process is that vectors satisfying (2.6)–(2.7) can be constructed by means of short vector recursions. In the classical Lanczos algorithm [16], the vectors are generated using simple three-term recurrences:

$$\begin{aligned} \tilde{v}_{n+1} &= A v_n - v_n \mu_n - v_{n-1} \nu_n, \\ \rho_{n+1} &= \|\tilde{v}_{n+1}\|, \qquad v_{n+1} = \tilde{v}_{n+1}/\rho_{n+1}, \end{aligned} \tag{2.10}$$

$$\begin{aligned} \tilde{w}_{n+1} &= A^T w_n - w_n \mu_n - w_{n-1}(\nu_n \rho_n / \xi_n), \\ \xi_{n+1} &= \|\tilde{w}_{n+1}\|, \qquad w_{n+1} = \tilde{w}_{n+1}/\xi_{n+1}, \end{aligned} \tag{2.11}$$

where

$$\mu_n = w_n^T A v_n / w_n^T v_n, \qquad \nu_n = \xi_n w_n^T v_n / w_{n-1}^T v_{n-1}. \tag{2.12}$$

In this case, the matrix D_n in (2.7) is diagonal and nonsingular:

$$D_n = \operatorname{diag}(\delta_1, \delta_2, \ldots, \delta_n), \quad \text{where } \delta_j := w_j^T v_j \neq 0. \tag{2.13}$$

Furthermore, we note that, by using the notation introduced in (2.8), the recurrence relations (2.10)–(2.11) for the first $n+1$ Lanczos vectors $\{v_j\}_{j=1}^{n+1}$ and $\{w_j\}_{j=1}^{n+1}$ can be written compactly in matrix form:

$$A V_n = V_{n+1} H_n, \tag{2.14}$$

$$A^T W_n = W_{n+1} \Gamma_{n+1}^{-1} H_n \Gamma_n. \tag{2.15}$$

Here, H_n is an $(n+1) \times n$ tridiagonal matrix, and

$$\Gamma_n := \operatorname{diag}(\gamma_1, \gamma_2, \ldots, \gamma_n), \quad \text{where } \gamma_j := \begin{cases} 1 & \text{if } j = 1, \\ \gamma_{j-1} \rho_j / \xi_j & \text{if } j > 1, \end{cases} \tag{2.16}$$

is a diagonal scaling matrix with positive diagonal entries. Finally, for later use, we note that all subdiagonal elements of H_n are nonzero, and therefore

$$\operatorname{rank} H_n = n. \tag{2.17}$$

Unfortunately, in the classical Lanczos algorithm, breakdowns cannot be excluded. Indeed, by (2.12), division by 0 will occur during the construction of v_{n+1} and w_{n+1} if $w_n^T v_n = 0$, but $w_n \neq 0$ and $v_n \neq 0$. Parlett, Taylor, and Liu [19] were the first to devise a practical modification of the Lanczos procedure that uses look-ahead to skip over possible *exact breakdowns* ($w_n^T v_n = 0$) or *near-breakdowns* ($w_n^T v_n$ is nonzero, but small in some sense). The QMR algorithm is based on a different implementation of the look-ahead Lanczos method, recently

developed by Freund, Gutknecht, and Nachtigal [7]. Next, we briefly sketch this look-ahead Lanczos procedure.

As in the classical Lanczos algorithm, two sequences of Lanczos vectors $\{v_j\}_{j=1}^n$ and $\{w_j\}_{j=1}^n$ are generated, starting with (2.3) and (2.4). Again, we will use the matrix notation V_n and W_n defined in (2.8). As before, these vectors satisfy (2.6)–(2.7), but now D_n is generally only a block-diagonal matrix, with $l := l(n)$ square blocks of dimension h_j, $j = 1, 2, \ldots, l$, on the diagonal. More precisely, we have

$$D_n = \operatorname{diag}(D^{(1)}, D^{(2)}, \ldots, D^{(l)}), \quad \text{where } D^{(j)} := (W^{(j)})^T V^{(j)}. \tag{2.18}$$

Here, the matrices $V^{(j)}$ and $W^{(j)}$, $j = 1, 2, \ldots, l$, are defined by partitioning V_n and W_n into blocks, according to the look-ahead steps taken:

$$V_n = \begin{bmatrix} V^{(1)} & V^{(2)} & \cdots & V^{(l)} \end{bmatrix} \quad \text{and} \quad W_n = \begin{bmatrix} W^{(1)} & W^{(2)} & \cdots & W^{(l)} \end{bmatrix}. \tag{2.19}$$

We remark that the matrices $V^{(j)}$ and $W^{(j)}$ are of size $N \times h_j$, and they contain as their columns the Lanczos vectors constructed in the jth look-ahead step. The integer h_j is called the length of the jth look-ahead step, and l in (2.18)–(2.19) is the number of look-ahead steps that were performed during the first n steps of the Lanczos process. For later use, we introduce some further notation. For $j = 1, 2, \ldots$, we denote by n_j the index of the first vectors of the blocks $V^{(j)}$ and $W^{(j)}$ in (2.19); hence, we have

$$V^{(j)} = \begin{bmatrix} v_{n_j} & v_{n_j+1} & \cdots \end{bmatrix} \quad \text{and} \quad W^{(j)} = \begin{bmatrix} w_{n_j} & w_{n_j+1} & \cdots \end{bmatrix}. \tag{2.20}$$

Note that the indices n_j satisfy

$$1 =: n_1 < n_2 < \cdots < n_l \leq n < n_{l+1}. \tag{2.21}$$

The vectors v_{n_j} and w_{n_j} are called *regular*, while the remaining vectors in the blocks $V^{(j)}$ and $W^{(j)}$ are called *inner*. We remark that, in view of (2.7) and (2.18), the regular vectors are biorthogonal to all previous Lanczos vectors, i.e.,

$$w_i^T v_{n_j} = w_{n_j}^T v_i = 0 \quad \text{for all } i = 1, 2, \ldots, n_j - 1, \tag{2.22}$$

while the inner vectors in the jth blocks $V^{(j)}$ and $W^{(j)}$ are biorthogonal to all Lanczos vectors from the previous blocks, but not necessarily to the Lanczos vectors in the jth blocks. Finally, we note that, in (2.18), the blocks $D^{(j)}$, $j = 1, 2, \ldots, l-1$, are all nonsingular, while the last block $D^{(l)}$ is nonsingular if $n_{l+1} = n + 1$, i.e., if v_{n+1} and w_{n+1} are constructed as regular vectors.

In the look-ahead algorithm, the Lanczos vectors (2.5) are again generated using only short vector recurrences, which now involve vectors from the last two blocks $V^{(l)}$, $V^{(l-1)}$ and $W^{(l)}$, $W^{(l-1)}$, instead of just v_n, v_{n-1} and w_n, w_{n-1}, as in the classical algorithm. For example, v_{n+1} is computed by means of the relations

$$\begin{aligned} \tilde{v}_{n+1} &= A v_n - V^{(l)} \mu_n - V^{(l-1)} \nu_n, \\ \rho_{n+1} &= \|\tilde{v}_{n+1}\|, \qquad v_{n+1} = \tilde{v}_{n+1}/\rho_{n+1}, \end{aligned} \tag{2.23}$$

where $\mu_n \in \mathbb{C}^{h_l}$ and $\nu_n \in \mathbb{C}^{h_{l-1}}$ are suitably chosen coefficient vectors. The second Lanczos vector w_{n+1} is obtained similarly. As before, the recurrence relations for the Lanczos vectors can be summarized in the form (2.14)–(2.15). Here, H_n is now a block-tridiagonal matrix with l square blocks on the diagonal, where the jth block has dimension $h_j \times h_j$, $j = 1, 2, \ldots, l$.

In addition, H_n is also an upper Hessenberg matrix. Furthermore, (2.16) and (2.17) remain valid, and ρ_j and ξ_j in (2.16) are scaling factors used to ensure the normalization (2.9) of the Lanczos vectors; see (2.23).

We would like to stress that the look-ahead strategy (see [7] and also §4 below) is such that the algorithm performs mostly standard Lanczos steps, i.e., look-ahead steps of length $h_j = 1$ with blocks $V^{(j)}$ and $W^{(j)}$ that consist of only single Lanczos vectors. True look-ahead steps, i.e., steps of size $h_j > 1$, are only used to avoid exact and near-breakdowns. Typically, except for contrived examples, only few true look-ahead steps occur, and their size is usually small, mostly $h_j = 2$. We note that, if only steps of length $h_j = 1$ are performed, then the look-ahead Lanczos algorithm reduces to the classical algorithm. Finally, we remark that so-called incurable breakdowns [23], [13] can occur in the Lanczos process. Such breakdowns cannot be remedied by look-ahead, and indeed, in such a case, the look-ahead Lanczos algorithm would build a block of size $h_l = \infty$. Fortunately, incurable breakdowns are extremely rare, and they do not present a problem in practice.

The look-ahead Lanczos algorithm is intimately connected with formally orthogonal polynomials; see, e.g., [13], [7]. In particular, we will use the fact that each pair of Lanczos vectors v_j and w_j can be expressed in the form

$$v_j = \phi_{j-1}(A)v_1 \quad \text{and} \quad w_j = \gamma_j \phi_{j-1}(A^T)w_1, \tag{2.24}$$

where $\phi_{j-1} \in \mathcal{P}_{j-1}$ is of exact degree $j-1$ and $\gamma_j > 0$ is defined in (2.16).

For further details and properties of the look-ahead Lanczos algorithm, we refer the reader to [7].

2.3. The QMR property. In the QMR method, the vectors $\{v_j\}_{j=1}^n$ generated by the look-ahead Lanczos algorithm are used as a basis for the Krylov subspace $K_n(r_0, A)$ in (2.2). The nth QMR iterate x_n is then defined by

$$x_n = x_0 + V_n z_n, \tag{2.25}$$

where $z_n \in \mathbb{C}^n$ is the unique solution of the least-squares problem

$$\| f_{n+1} - \Omega_{n+1} H_n z_n \| = \min_{z \in \mathbb{C}^n} \| f_{n+1} - \Omega_{n+1} H_n z \|. \tag{2.26}$$

Here

$$f_{n+1} := \omega_1 \rho_1 \cdot [1 \quad 0 \quad \cdots \quad 0]^T \in \mathbb{R}^{n+1}, \tag{2.27}$$

with ρ_1 given in (2.3), and

$$\Omega_{n+1} := \operatorname{diag}(\omega_1, \omega_2, \ldots, \omega_{n+1}), \quad \omega_j > 0, \quad j = 1, 2, \ldots, n+1, \tag{2.28}$$

is an arbitrary diagonal weighting matrix. Note that, in view of (2.17) and (2.28), the $(n+1) \times n$ matrix $\Omega_{n+1} H_n$ has full rank n. This guarantees that there always exists a unique solution of (2.26). Furthermore, we remark that the standard choice for the weights in (2.28) is

$$\omega_j = 1 \quad \text{for all } j. \tag{2.29}$$

However, there are instances (see [11]) where the use of different weights is crucial, and therefore we formulate the QMR method in the general setting (2.28).

From (2.25), (2.14), (2.27), and (2.3), it follows that the residual vector $r_n := b - Ax_n$ corresponding to x_n satisfies

$$r_n = V_{n+1} \Omega_{n+1}^{-1} \left(f_{n+1} - \Omega_{n+1} H_n z_n \right). \tag{2.30}$$

Hence, in view of (2.26), the nth QMR iterate x_n is characterized by a minimization of the second factor in (2.30); this is just the *quasi-minimal residual* property. The relation (2.30) shows that the scaling (2.29) is very natural, in the sense that all columns of $V_{n+1}\Omega_{n+1}^{-1}$ in the representation (2.30) of r_n are treated equally. We remark that the QMR iterates x_n can be easily updated from step to step. Due to the block-tridiagonal structure of H_n, this update can be implemented with only short recurrences; see [9] for details. Finally, we note that the QMR property can be used to derive convergence results for the QMR method; we refer the reader to [9] and [6].

3. A coupled two-term procedure with look-ahead. In this section, we consider a different approach to constructing the Lanczos vectors. The basic idea is to break up the three-term recurrences in the Lanczos process into coupled two-term recurrences, by using (in addition to the Lanczos vectors) a suitable second set of basis vectors for the underlying Krylov subspaces. In §9, we will illustrate that QMR based on this coupled two-term procedure has better numerical properties than the original implementation of QMR based on three-term recurrences.

3.1. The general setting. In the following, let $\{v_j\}_{j=1}^n$ and $\{w_j\}_{j=1}^n$ always denote the sequence of vectors generated by the look-ahead Lanczos algorithm as described in §2.2. We assume that we are also given a second set of basis vectors

$$\{p_j\}_{j=1}^n \quad \text{and} \quad \{q_j\}_{j=1}^n \tag{3.1}$$

for the Krylov subspaces $K_n(v_1, A)$ and $K_n(w_1, A^T)$. More precisely, we consider vectors (3.1) that, in analogy to (2.24), are of the form

$$p_j = \psi_{j-1}(A)v_1 \quad \text{and} \quad q_j = \gamma_j\psi_{j-1}(A^T)w_1, \tag{3.2}$$

where $\gamma_j > 0$ is given by (2.16), and $\psi_{j-1} \in \mathcal{P}_{j-1}$ is of exact degree $j-1$ with the same leading coefficient as the polynomial ϕ_{j-1} in (2.24). To distinguish between the two bases, we will often refer to the Lanczos vectors $\{v_j\}_{j=1}^n$ and $\{w_j\}_{j=1}^n$ as the *V–W sequence* and to the vectors (3.1) as the *P–Q sequence*.

From (2.24) and (3.2), we conclude that, for each $n = 1, 2, \ldots,$

$$p_n = v_n - \sum_{i=1}^{n-1} p_i u_{in}, \tag{3.3}$$

$$q_n = w_n - \sum_{i=1}^{n-1} q_i u_{in}(\gamma_n/\gamma_i), \tag{3.4}$$

with suitable coefficients $u_{in} \in \mathbb{C}$, $i = 1, 2, \ldots, n-1$. Similarly, in view of (2.23), (2.24), (3.2), and (2.16), we have

$$\tilde{v}_{n+1} = Ap_n - \sum_{i=1}^{n} v_i l_{in}, \quad \rho_{n+1} = \|\tilde{v}_{n+1}\|, \quad v_{n+1} = \tilde{v}_{n+1}/\rho_{n+1}, \tag{3.5}$$

$$\tilde{w}_{n+1} = A^T q_n - \sum_{i=1}^{n} w_i l_{in}(\gamma_n/\gamma_i), \quad \xi_{n+1} = \|\tilde{w}_{n+1}\|, \quad w_{n+1} = \tilde{w}_{n+1}/\xi_{n+1}, \tag{3.6}$$

with suitable coefficients $l_{in} \in \mathbb{C}$, $i = 1, 2, \ldots, n$. Note that (3.3)–(3.6) are coupled recurrences for generating the P–Q and V–W sequences: first, p_n and q_n are computed by means

of (3.3)–(3.4), and then, the next Lanczos pair v_{n+1} and w_{n+1} is obtained from (3.5)–(3.6). Of course, it remains to specify the actual choice of the P–Q sequence. In order to minimize work and storage of previous vectors, the goal here is to select these vectors such that the recurrences (3.3)–(3.6) are as short as possible.

In addition to (2.8), it will be convenient to use the notation

$$P_n := [\, p_1 \quad p_2 \quad \cdots \quad p_n \,] \quad \text{and} \quad Q_n := [\, q_1 \quad q_2 \quad \cdots \quad q_n \,].$$

The recurrences (3.3)–(3.6) for the vectors $\{p_j\}_{j=1}^{n}$, $\{q_j\}_{j=1}^{n}$, $\{v_j\}_{j=1}^{n+1}$, and $\{w_j\}_{j=1}^{n+1}$ can then be written compactly in matrix form:

$$V_n = P_n U_n, \qquad A P_n = V_{n+1} L_n, \tag{3.7}$$

$$W_n = Q_n \Gamma_n^{-1} U_n \Gamma_n, \qquad A^T Q_n = W_{n+1} \Gamma_{n+1}^{-1} L_n \Gamma_n. \tag{3.8}$$

Here, U_n is an upper triangular matrix and L_n is an upper Hessenberg matrix given by

$$U_n := \begin{bmatrix} 1 & u_{12} & \cdots & u_{1n} \\ 0 & 1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & u_{n-1,n} \\ 0 & \cdots & 0 & 1 \end{bmatrix} \quad \text{and} \quad L_n := \begin{bmatrix} l_{11} & l_{12} & \cdots & l_{1n} \\ \rho_2 & l_{22} & & \vdots \\ 0 & \rho_3 & \ddots & \vdots \\ \vdots & \ddots & \ddots & l_{nn} \\ 0 & \cdots & 0 & \rho_{n+1} \end{bmatrix}, \tag{3.9}$$

respectively, and Γ_n is the diagonal matrix defined in (2.16). Note that, by eliminating P_n in (3.7), we obtain

$$A V_n = V_{n+1} L_n U_n. \tag{3.10}$$

By comparing (3.10) with (2.14), it follows that

$$H_n = L_n U_n, \tag{3.11}$$

i.e., the matrices (3.9) define a factorization of the block-tridiagonal Hessenberg matrix H_n generated by the look-ahead Lanczos algorithm.

Recall from (2.7) and (2.18) that the Lanczos vectors are block biorthogonal. These biorthogonality relations determine the coefficients l_{in} in (3.5)–(3.6). For example, consider the case that v_{n+1} and w_{n+1} are constructed as regular vectors. Then, in view of (2.22), we have the condition $W_n^T v_{n+1} = 0$, which, by (3.5), is equivalent to

$$0 = W_n^T A p_n - \sum_{i=1}^{n} W_n^T v_i l_{in}. \tag{3.12}$$

Using (2.7), (2.8), and the first equation in (3.8), we deduce from (3.12) that

$$\begin{bmatrix} l_{1n} \\ \vdots \\ l_{nn} \end{bmatrix} = D_n^{-1} \Gamma_n U_n^T \Gamma_n^{-1} Q_n^T A p_n. \tag{3.13}$$

Recall from (2.18), (2.16), and (3.9) that the matrices D_n^{-1}, Γ_n, and U_n^T are block diagonal, diagonal, and lower triangular, respectively. Hence the relation (3.13) implies that the vector $Q_n^T A p_n$ determines the length of the recurrences (3.5)–(3.6). In particular, in order to obtain recursions that are as short as possible, the P–Q sequence should be chosen such that the vector

$Q_n^T A p_n$ has as many leading zeros as possible. The same conclusion also holds for the case that v_{n+1} and w_{n+1} are constructed as inner vectors.

Motivated by this discussion, we require that the vectors in the P–Q sequence be A-biorthogonal or block A-biorthogonal, in the sense that the matrix

$$E_n := Q_n^T A P_n \tag{3.14}$$

should be diagonal or block diagonal. Note that the vector $Q_n^T A p_n$ is just the nth column of E_n. Furthermore, we remark that $q_n^T A P_n$, the nth row of E_n, has the same zero structure as $Q_n^T A p_n$. This is a consequence of relation (3.16) in the following lemma, which we will also need later on.

LEMMA 3.1. *Let* $\{v_i\}_{i=1}^n$, $\{w_i\}_{i=1}^n$ *and* $\{p_i\}_{i=1}^n$, $\{q_i\}_{i=1}^n$ *be vectors satisfying* (2.24) *and* (3.2), *respectively, and let* $\Gamma_n = \operatorname{diag}(\gamma_1, \gamma_2, \ldots, \gamma_n)$. *Let* D_n *and* E_n *be the matrices given by* (2.7) *and* (3.14), *respectively. Then*

$$D_n \Gamma_n = (D_n \Gamma_n)^T, \tag{3.15}$$

$$E_n \Gamma_n = (E_n \Gamma_n)^T. \tag{3.16}$$

Proof. Using the polynomial representation (2.24) for the V–W vectors and the fact that polynomials in a matrix commute, we obtain

$$w_i^T v_j \gamma_j = \gamma_i w_1^T \phi_{i-1}(A) \phi_{j-1}(A) v_1 \gamma_j = \gamma_j w_1^T \phi_{j-1}(A) \phi_{i-1}(A) v_1 \gamma_i = w_j^T v_i \gamma_i$$

and thus (3.15). The relation (3.16) follows similarly. □

3.2. The coupled algorithm without look-ahead. Next, we briefly consider the case that the V–W sequence consists of the vectors generated by the classical Lanczos algorithm without look-ahead. Recall from (2.13) that here the matrix D_n in (2.7) is diagonal, and that the Lanczos vectors are biorthogonal:

$$w_j^T v_n = \begin{cases} 0 & \text{if } j \neq n, \\ \delta_n \neq 0 & \text{if } j = n. \end{cases} \tag{3.17}$$

Suppose that it is possible to construct the vectors in the P–Q sequence such that the matrix E_n in (3.14) is also diagonal:

$$E_n = \operatorname{diag}(\epsilon_1, \epsilon_2, \ldots, \epsilon_n), \quad \text{where } \epsilon_j := q_j^T A p_j \neq 0. \tag{3.18}$$

By (3.14) and (3.18), the P–Q vectors are then A-biorthogonal:

$$q_j^T A p_n = \begin{cases} 0 & \text{if } j \neq n, \\ \epsilon_n \neq 0 & \text{if } j = n. \end{cases} \tag{3.19}$$

With (2.13), (3.9), and (3.19), we deduce from (3.13) that

$$l_{in} = 0, \quad i = 1, 2, \ldots, n-1, \quad \text{and} \quad l_{nn} = \beta_n := \epsilon_n / \delta_n. \tag{3.20}$$

Furthermore, by multiplying (3.3) from the left by $q_j^T A$ and by using (3.19), (3.6), and (3.17), we obtain that, for $j = 1, 2, \ldots, n-1$,

$$\begin{aligned} 0 = q_j^T A p_n &= q_j^T A v_n - \epsilon_j u_{jn} \\ &= (A^T q_j)^T v_n - \epsilon_j u_{jn} \\ &= \xi_{j+1} w_{j+1}^T v_n - \epsilon_j u_{jn}. \end{aligned} \tag{3.21}$$

With (3.17), it follows from (3.21) that

$$u_{in} = 0, \quad i = 1, 2, \ldots, n-2, \quad \text{and} \quad u_{n-1,n} = \xi_n \delta_n / \epsilon_{n-1}. \tag{3.22}$$

In view of (3.20) and (3.22), all but the last terms vanish in each of the sums in (3.3)–(3.6), and hence (3.3)–(3.6) reduces to a coupled two-term procedure for generating the P–Q and V–W sequences.

The nth iteration of the resulting algorithm can be summarized as follows.

ALGORITHM 3.2 (nth iteration of the coupled algorithm without look-ahead).

1. If $\epsilon_{n-1} = 0$, then stop.
   Otherwise, compute $\delta_n = w_n^T v_n$.
   If $\delta_n = 0$, then stop.
2. Compute

$$\begin{aligned} p_n &= v_n - p_{n-1}(\xi_n \delta_n / \epsilon_{n-1}), \\ q_n &= w_n - q_{n-1}(\rho_n \delta_n / \epsilon_{n-1}). \end{aligned}$$

3. Compute $\epsilon_n = q_n^T A p_n$, $\beta_n = \epsilon_n / \delta_n$, and set

$$\begin{aligned} \tilde{v}_{n+1} &= A p_n - v_n \beta_n, \quad \rho_{n+1} = \|\tilde{v}_{n+1}\|, \\ \tilde{w}_{n+1} &= A^T q_n - w_n \beta_n, \quad \xi_{n+1} = \|\tilde{w}_{n+1}\|. \end{aligned}$$

4. If $\rho_{n+1} = 0$ or $\xi_{n+1} = 0$, then stop.
   Otherwise, set

$$v_{n+1} = \tilde{v}_{n+1} / \rho_{n+1}, \quad w_{n+1} = \tilde{w}_{n+1} / \xi_{n+1}.$$

We remark that the vectors in the P–Q and V–W sequences are, up to scaling, just the search directions and the residual vectors generated by the BCG method [17], [4]. In particular, Algorithm 3.2 can be viewed as the nth iteration of a rescaled version of BCG, where the computation of the BCG iterates is omitted.

In exact arithmetic, one of the termination checks in steps 1 or 4 of the coupled two-term procedure will be satisfied after at most N iterations. Normally, the algorithm stops due to $\rho_{n+1} = 0$ or $\xi_{n+1} = 0$, and then the procedure has constructed a basis for the invariant subspaces $K_n(v_1, A)$ or $K_n(w_1, A^T)$, respectively. This is called regular termination. If $\epsilon_{n-1} = 0$ or $\delta_n = 0$ occurs, then the algorithm has to be stopped to avoid division by 0. This is referred to as an exact breakdown. Recall from §2.2 that $\delta_n = 0$ signals a breakdown in the classical Lanczos algorithm. Note that, like BCG, the coupled two-term procedure now has a second source of breakdown, namely, the case $\epsilon_{n-1} = 0$. It can be shown that the condition $\epsilon_{n-1} = 0$ corresponds to a breakdown in the BCG algorithm due to an nth iterate not being defined by the Galerkin condition.

In finite-precision arithmetic, exact breakdowns are rather unlikely. However, near-breakdowns, where δ_n or ϵ_{n-1} is nonzero, but small in some sense, may occur, leading to numerical instabilities in subsequent iterations. Next, we sketch a coupled two-term procedure that uses look-ahead in the construction of both the V–W and P–Q sequences to avoid exact and near-breakdowns.

3.3. The general algorithm with look-ahead. For describing the look-ahead in the V–W sequence, we will use the notations (2.18)–(2.21) introduced in §2.2. In particular, the integer $l := l(n)$ denotes the number of look-ahead steps that were performed during the construction of the first n vectors $\{v_i\}_{i=1}^n$ and $\{w_i\}_{i=1}^n$ in the V–W sequence, and the n_j's in (2.21) are the indices of the regular vectors. Recall that, by (2.7) and (2.18), the V–W vectors satisfy the block-biorthogonality conditions

$$(W^{(i)})^T V^{(j)} = \begin{cases} 0 & \text{if } i \neq j, \\ D^{(j)} & \text{if } i = j, \end{cases} \qquad i, j = 1, 2, \ldots, l. \tag{3.23}$$

Here, the blocks $D^{(j)}$ are all nonsingular, except for possibly $D^{(l)}$. However, we have that necessarily

$$D^{(l)} \text{ is nonsingular, if } n_{l+1} = n + 1. \tag{3.24}$$

Next, we introduce similar notations for describing the look-ahead in the P–Q sequence. We denote by $k := k(n)$ the number of look-ahead steps that were performed during the construction of the first $n-1$ vectors $\{p_i\}_{i=1}^{n-1}$ and $\{q_i\}_{i=1}^{n-1}$ in the P–Q sequence. In analogy to (2.19), we partition these vectors into blocks, according to the look-ahead steps taken:

$$P_{n-1} = \left[P^{(1)} \quad P^{(2)} \quad \cdots \quad P^{(k)} \right] \quad \text{and} \quad Q_{n-1} = \left[Q^{(1)} \quad Q^{(2)} \quad \cdots \quad Q^{(k)} \right]. \tag{3.25}$$

Recall from (3.14) that the P–Q vectors are constructed to be block A-biorthogonal. More precisely, we have

$$E_{n-1} = \operatorname{diag}(E^{(1)}, E^{(2)}, \ldots, E^{(k)}),$$

or, equivalently,

$$(Q^{(i)})^T A P^{(j)} = \begin{cases} 0 & \text{if } i \neq j, \\ E^{(j)} & \text{if } i = j, \end{cases} \qquad i, j = 1, 2, \ldots, k. \tag{3.26}$$

Here, the blocks $E^{(j)}$ are nonsingular, except for possibly the last block $E^{(k)}$. In analogy to (2.21), we denote by m_j the indices of the first vectors of the blocks $P^{(j)}$ and $Q^{(j)}$ in (3.25). Hence, for $j = 1, 2, \ldots, k$, we have

$$P^{(j)} = \left[p_{m_j} \quad p_{m_j+1} \quad \cdots \quad \right] \quad \text{and} \quad Q^{(j)} = \left[q_{m_j} \quad q_{m_j+1} \quad \cdots \quad \right]. \tag{3.27}$$

Furthermore, the indices m_j satisfy

$$1 =: m_1 < m_2 < \cdots < m_k < n \leq m_{k+1}. \tag{3.28}$$

We remark that, by (3.26) and (3.27), the vectors p_{m_j} and q_{m_j} are A-biorthogonal to all previous P–Q vectors, i.e.,

$$q_i^T A p_{m_j} = q_{m_j}^T A p_i = 0 \quad \text{for all } i = 1, 2, \ldots, m_j - 1.$$

Therefore, using the same notation as for the V–W sequence, we refer to the vectors p_{m_j} and q_{m_j} as *regular* vectors, while the remaining vectors in (3.27) are called *inner*. Finally, it turns out that, in (3.26), the last block $E^{(k)}$ has to be nonsingular, if p_n and q_n are constructed as regular vectors. This means that, in analogy to (3.24),

$$E^{(k)} \text{ is nonsingular, if } m_{k+1} = n. \tag{3.29}$$

After these preliminaries, we can now sketch the actual algorithm. Let $n \geq 1$, and assume that we have already generated the first $n-1$ vectors $\{p_i\}_{i=1}^{n-1}$ and $\{q_i\}_{i=1}^{n-1}$ of the P–Q sequence, and the first n vectors $\{v_i\}_{i=1}^{n}$ and $\{w_i\}_{i=1}^{n}$ of the V–W sequence.

First, the next pair of P–Q vectors, p_n and q_n, is constructed, using the recurrences (3.3)–(3.4). Here, the coefficients u_{in} need to be chosen such that p_n satisfies the corresponding A-biorthogonality conditions (3.26). We note that, in view of (3.16), the A-biorthogonality relations for the vector q_n are then also fulfilled. With (3.6) and (3.23), one readily verifies that

$$q_i^T A v_n = (A^T q_i)^T v_n = 0 \quad \text{for all } i = 1, 2, \ldots, n_l - 2.$$

By rewriting this in terms of the blocks $Q^{(j)}$, we obtain that

$$(Q^{(j)})^T A v_n = 0 \quad \text{for all } j = 1, 2, \ldots, k^\star - 1, \tag{3.30}$$

where $k^\star := k^\star(n)$ is given by

$$k^\star = \max\left\{ j \;\middle|\; 1 \leq j \leq k \text{ and } m_j \leq \max\{1, n_l - 1\} \right\}. \tag{3.31}$$

The orthogonality conditions (3.30), together with (3.26), imply that, in (3.3), we have $u_{in} = 0$ for all $i < m_{k^\star}$. Thus the recurrences (3.3)–(3.4) reduce to

$$p_n = v_n - \sum_{i=m_{k^\star}}^{n-1} p_i u_{in}, \tag{3.32}$$

$$q_n = w_n - \sum_{i=m_{k^\star}}^{n-1} q_i u_{in} (\gamma_n / \gamma_i). \tag{3.33}$$

Now we need to determine the coefficients u_{in} for $m_{k^\star} \leq i \leq n-1$. This is done by enforcing the remaining A-biorthogonality conditions (3.26) for p_n and the vectors q_i, namely,

$$q_i^T A p_n = 0 \quad \text{for all } i = m_{k^\star}, m_{k^\star} + 1, \ldots, m^\star. \tag{3.34}$$

Here, $m^\star := n-1$ if p_n and q_n are constructed as regular vectors, and $m^\star := m_k - 1$ otherwise. Note that, in view of (3.28), we always have $m_k - 1 \leq m^\star$. First, we consider (3.34) for the indices i in the range $m_{k^\star} \leq i \leq m_k - 1$. Using (3.32) and (3.26), we deduce from (3.34) that

$$U_{m_{k^\star}:m_k-1,n} = (\operatorname{diag}(E^{(k^\star)}, \ldots, E^{(k-1)}))^{-1} \left[Q^{(k^\star)} \quad \cdots \quad Q^{(k-1)} \right]^T A v_n. \tag{3.35}$$

Here, and in the sequel, we use the notation

$$M_{i:j,n} := [\, m_{in} \quad m_{i+1,n} \quad \cdots \quad m_{jn} \,]^T$$

for vectors consisting of successive elements of the nth column of the matrix $M = [\, m_{ij} \,]$. If p_n and q_n are constructed as regular vectors, then we also have to ensure that (3.34) holds for i with $m_k \leq i \leq n-1$, and this gives

$$U_{m_k:n-1,n} = (E^{(k)})^{-1} (Q^{(k)})^T A v_n. \tag{3.36}$$

We remark that, by (3.29), the matrix $E^{(k)}$ in (3.36) is necessarily nonsingular since the vectors p_n and q_n are regular. If p_n and q_n are constructed as inner vectors, then $m^\star = m_k - 1$,

and (3.34) yields no conditions for the choice of the coefficients u_{in} with $m_k \le i < n-1$. In this case, we set

$$u_{in} = \zeta_{in} \quad \text{for } i = m_k, m_k+1, \ldots, n-1, \tag{3.37}$$

where $\zeta_{in} \in \mathbb{C}$ can be chosen arbitrarily. Finally, if p_n and q_n are regular, we update the "regular" indices (3.28) by setting $m_{k+1} := n$ and $k := k+1$. This completes the construction of the p_n and q_n vectors.

In a second step, we now compute the next pair of V–W vectors, v_{n+1} and w_{n+1}, using the recurrences (3.5)–(3.6). Here, we have to determine the coefficients l_{in} such that v_{n+1} satisfies the corresponding biorthogonality conditions (3.23). Note that, in view of (3.15), the relations (3.23) for w_{n+1} are then fulfilled automatically. We proceed similar to the construction of p_n and q_n. By using (3.26) and the fact that the columns of the matrices Q_i and W_i span the same space, it is easily verified that

$$(W^{(j)})^T A p_n = 0 \quad \text{for all } j = 1, 2, \ldots, l^\star - 1, \tag{3.38}$$

where $l^\star := l^\star(n)$ is given by

$$l^\star = \max\left\{ j \;\middle|\; 1 \le j \le l \text{ and } n_j \le m_k \right\}. \tag{3.39}$$

From (3.38), we conclude that the recurrences (3.5)–(3.6) reduce as follows:

$$\tilde{v}_{n+1} = A p_n - \sum_{i=n_{l^\star}}^{n} v_i l_{in}, \tag{3.40}$$

$$\tilde{w}_{n+1} = A^T q_n - \sum_{i=n_{l^\star}}^{n} w_i l_{in} (\gamma_n/\gamma_i). \tag{3.41}$$

The recurrence coefficients l_{in} in (3.40)–(3.41) are determined by enforcing the remaining biorthogonality conditions (3.23) for the vectors v_{n+1} and w_i, $n_{l^\star} \le i \le n$. This gives

$$L_{n_{l^\star}:n_l-1,n} = (\operatorname{diag}(D^{(l^\star)}, \ldots, D^{(l-1)}))^{-1} \left[W^{(l^\star)} \quad \ldots \quad W^{(l-1)} \right]^T A p_n. \tag{3.42}$$

Moreover, if v_{n+1} and w_{n+1} are constructed as regular vectors, then

$$L_{n_l:n,n} = (D^{(l)})^{-1} (W^{(l)})^T A p_n. \tag{3.43}$$

Note that, by (3.24), the matrix $D^{(l)}$ in (3.43) is necessarily nonsingular since v_{n+1} and w_{n+1} are regular. If v_{n+1} and w_{n+1} are built as inner vectors, then we set

$$l_{in} = \eta_{in} \quad \text{for } i = n_l, n_l+1, \ldots, n, \tag{3.44}$$

where $\eta_{in} \in \mathbb{C}$ can be chosen arbitrarily. Finally, if v_{n+1} and w_{n+1} are regular, then we update the indices (2.21) by setting $n_{l+1} := n+1$ and $l := l+1$.

The resulting coupled procedure for generating the P–Q and V–W sequences can be sketched as follows.

ALGORITHM 3.3 (Coupled algorithm with look-ahead).

0. Choose $v_1, w_1 \in \mathbb{C}^N$ with $\|v_1\| = \|w_1\| = 1$.
   Set $V^{(1)} = v_1$, $W^{(1)} = w_1$, $D^{(1)} = w_1^T v_1$.
   Set $k = 1, m_k = 1, l = 1, n_l = 1$.

For $n = 1, 2, \ldots,$ do:

1. Determine $k^\star$ from (3.31).
2. Decide whether to construct p_n and q_n as regular or inner vectors and go to step 3 or 4, respectively.
3. Compute p_n and q_n by means of (3.35)–(3.36) and (3.32)–(3.33).
   Set $m_{k+1} = n$, $k = k + 1$, $P^{(k)} = Q^{(k)} = \emptyset$ and go to step 5.
4. Compute p_n and q_n by means of (3.35), (3.37), and (3.32)–(3.33).
5. Set
$$P^{(k)} = \left[P^{(k)} \quad p_n \right], \quad Q^{(k)} = \left[Q^{(k)} \quad q_n \right], \quad E^{(k)} = (Q^{(k)})^T A P^{(k)}.$$
6. Determine $l^\star$ from (3.39).
7. Decide whether to construct v_{n+1} and w_{n+1} as regular or inner vectors and go to step 8 or 9, respectively.
8. Compute $\tilde{v}_{n+1}$ and $\tilde{w}_{n+1}$ by means of (3.42)–(3.43) and (3.40)–(3.41).
   Set $n_{l+1} = n + 1$, $l = l + 1$, $V^{(l)} = W^{(l)} = \emptyset$ and go to step 10.
9. Compute $\tilde{v}_{n+1}$ and $\tilde{w}_{n+1}$ by means of (3.42), (3.44), and (3.40)–(3.41).
10. Compute $\rho_{n+1} = \|\tilde{v}_{n+1}\|$ and $\xi_{n+1} = \|\tilde{w}_{n+1}\|$.
    If $\rho_{n+1} = 0$ or $\xi_{n+1} = 0$, then stop.
    Otherwise, set
$$v_{n+1} = \tilde{v}_{n+1}/\rho_{n+1}, \quad w_{n+1} = \tilde{w}_{n+1}/\xi_{n+1},$$
$$V^{(l)} = \left[V^{(l)} \quad v_{n+1} \right], \quad W^{(l)} = \left[W^{(l)} \quad w_{n+1} \right], \quad D^{(l)} = (W^{(l)})^T V^{(l)}.$$

We remark that Algorithm 3.3 reduces to the coupled two-term procedure described in § 3.2 if all vectors in the P–Q and V–W sequences are built as regular vectors. Note that in this case, we have $k(n) = n - 1$, $n_{k^\star} = n - 1$, $l(n) = n$, and $n_{l^\star} = n$ for all n.

4. The look-ahead strategy. As described in §3.2, there are two possible breakdowns in the coupled two-term procedure without look-ahead: one associated with the V–W sequence, and another associated with the P–Q sequence. In particular, Algorithm 3.2 will encounter an exact breakdown in the V–W sequence if $w_n^T v_n = 0$, or in the P–Q sequence if $q_{n-1}^T A p_{n-1} = 0$. The exact breakdowns of the two sequences are not independent of each other, as was pointed out by Gutknecht in [12]. For a full description of the structure and coupling of the exact breakdowns, we refer the reader to [12] and [2], and the references given there. However, in practice one is also concerned with avoiding near-breakdowns; that is, situations when $w_n^T v_n$ or $q_{n-1}^T A p_{n-1}$ are not exactly zero, but are small in some sense.

In the coupled procedure with look-ahead, which we sketched in §3.3, exact and near-breakdowns in the P–Q, respectively V–W, sequence are prevented by building the next pair of vectors p_n and q_n, respectively v_{n+1} and w_{n+1}, as inner vectors. In this section, we describe the look-ahead strategy that is used to decide in steps 2 and 7 of Algorithm 3.3 whether vectors are constructed as regular or inner vectors.

Recall from §2.2 that the vectors $\{v_i\}_{i=1}^{n+1}$ and $\{w_i\}_{i=1}^{n+1}$ in the look-ahead Lanczos algorithm satisfy a block three-term recurrence that can be written compactly as (2.14)–(2.15). By eliminating V_n and W_n in (3.7) and (3.8), one obtains a similar recurrence relation for the vectors $\{p_i\}_{i=1}^{n}$ and $\{q_i\}_{i=1}^{n}$ of the P–Q sequence:

$$A P_{n-1} = P_n U_n L_{n-1} \quad \text{and} \quad A^T Q_{n-1} = Q_n \Gamma_n^{-1} U_n L_{n-1} \Gamma_{n-1}. \tag{4.1}$$

By using the A-biorthogonality of p_n and q_n, it is easy to show that the recurrences for the P–Q sequence are also three-term recurrences, or, in the general case, block three-term recurrences. We note that, in (4.1), the matrix $U_n L_{n-1}$ of recurrence coefficients is obtained by multiplying the factors L_{n-1} and U_n from the decompositions (3.11) of H_{n-1} and H_n, respectively, in reverse order. This was first remarked by Rutishauser [21] for the special case of no look-ahead, and recently by Gutknecht [12], for the general case.

The look-ahead strategy consists of monitoring breakdowns in the two sequences independently. For the V–W sequence, the criteria used are the same as those proposed in [7]:

$$\sigma_{\min}(D^{(l)}) \geq \text{eps}, \tag{4.2}$$

$$n(A) \geq \sum_i \left|(L_n U_n)_{in}\right|, \tag{4.3}$$

$$n(A) \geq \sum_i \frac{\gamma_n}{\gamma_i} \left|(L_n U_n)_{in}\right|, \tag{4.4}$$

where eps is machine epsilon, and $n(A)$ is an estimate for the norm of A. The Lanczos vectors v_{n+1} and w_{n+1} are built as regular vectors only if all three of the above checks are satisfied. The check (4.2) ensures that the diagonal blocks $D^{(j)}$ are nonsingular, while the checks (4.3)–(4.4) ensure that the size of the coefficients μ_n and ν_n in (2.23) and in the corresponding relation for $\tilde{w}_{n+1}$ do not exceed an estimate $n(A)$ for the norm of A. The first condition is needed since the inverse of $D^{(l)}$ appears in μ_n, while the second and third conditions attempt to ensure that the components from $K_n(r_0, A)$ and from $K_n(w_1, A^T)$ do not dominate the Av_n and $A^T w_n$ terms, respectively. Another motivation for these checks is as follows. The symmetric Lanczos process for Hermitian matrices A generates tridiagonal matrices H_n that satisfy

$$\|H_n\| \leq \|A\| \quad \text{for all } n. \tag{4.5}$$

For the classical nonsymmetric Lanczos algorithm, the relation (4.5) does not hold in general. Indeed, formally, we have $\|H_n\| = \infty$ if a breakdown occurs. As David Day has pointed out to us,[1] an "ideal" look-ahead Lanczos procedure would ensure that (4.5) also holds for non-Hermitian matrices. The criteria (4.3)–(4.4) can be viewed as a cheap way of modeling the conditions (4.5). We remark that the checks (4.3)–(4.4) take advantage of the normalization (2.9) of the Lanczos vectors.

For the P–Q sequence, the criteria are similar: the diagonal blocks $E^{(j)}$ must be nonsingular, and the size of the last columns of $U_n L_{n-1}$ and of $\Gamma_n^{-1} U_n L_{n-1} \Gamma_{n-1}$ must not exceed the estimate $n(A)$ for the norm of A. Singularity of $E^{(k)}$ is once again checked from its smallest singular value:

$$\sigma_{\min}(E^{(k)}) \geq \text{eps}.$$

However, for the second and third checks, it is no longer sufficient to compute just the norm of the last column of the matrices of recurrence coefficients, as the vectors p_n and q_n are not normalized to unit length. Instead, one must check

$$n(A)\|p_n\| \geq \sum_i \left|(U_n L_{n-1})_{i,n-1}\right| \|p_i\| \tag{4.6}$$

and

$$n(A)\|q_n\| \geq \sum_i \frac{\gamma_{n-1}}{\gamma_i} \left|(U_n L_{n-1})_{i,n-1}\right| \|q_i\|. \tag{4.7}$$

[1] Private communication, Berkeley, March 1992.

This means that the look-ahead strategy for the P–Q sequence requires the computation of the two norms $\|p_n\|$ and $\|q_n\|$ at each step, work that would otherwise not be needed by the algorithm. Once again, the vectors p_n and q_n are built as regular vectors only if all three of the above checks are satisfied. We remark that the look-ahead strategy presented here builds regular vectors in preference to inner vectors and will therefore build as few inner vectors as possible.

Finally, we note that other look-ahead strategies are also possible. For example, Gutknecht [12] proposed a look-ahead strategy that assumes that the near-breakdowns encountered in the two sequences have the same structure as the exact breakdowns. We have chosen to monitor the two sequences independently; nevertheless, our strategy will recover the exact-breakdown structure if only exact breakdowns are considered.

5. Implementation details. In this section, we discuss some of the details of an implementation of Algorithm 3.3. The nth iteration of Algorithm 3.3 updates the matrices E_{n-1}, L_{n-1}, U_{n-1}, P_{n-1}, Q_{n-1}, V_n, W_n, and D_n, to E_n, L_n, U_n, P_n, Q_n, V_{n+1}, W_{n+1}, and D_{n+1}, respectively. We are interested in obtaining an implementation that requires only two inner products per iteration to compute all the coefficients of the recurrence formulas. Recall that the look-ahead strategy (4.6)–(4.7) for the P–Q sequence and the normalization (2.9) require a total of four norm computations, so that the implementation will require two inner products and four norms per iteration.

Let us introduce the auxiliary matrices

$$F_n = W_n^T A P_n \quad \text{and} \quad \tilde{F}_n = Q_n^T A V_n,$$

whose columns are needed in (3.42)–(3.43) and (3.35)–(3.36). It turns out that these two matrices are essentially the transpose of each other.

LEMMA 5.1. *The matrices F_n and $\tilde{F}_n$ satisfy $F_n \Gamma_n = (\tilde{F}_n \Gamma_n)^T$.*

Proof. The proof is similar to the proof of Lemma 3.1. □

At the beginning of each iteration, we will have available the $n \times (n-1)$ matrix $F_{1:n,1:n-1}$, which we will update to $F_{1:n+1,1:n}$.

To compute the coefficients u_{in} needed in (3.32)–(3.33), $\tilde{F}_{1:n-1,n}$ is obtained by Lemma 5.1. The vectors p_n and q_n are then computed from (3.32)–(3.33). To obtain E_n from E_{n-1}, the diagonal term $q_n^T A p_n$ is computed directly, requiring one inner product. Then, using

$$F_n = W_n^T A P_n = \Gamma_n U_n^T \Gamma_n^{-1} Q_n^T A P_n = \Gamma_n U_n^T \Gamma_n^{-1} E_n, \tag{5.1}$$

the remainder of the last row of E_n is computed from E_{n-1}, $F_{n,1:n-1}$, and U_{n-1}. The last column of E_n is obtained by symmetry, using (3.16) from Lemma 3.1. One then computes $F_{1:n,n}$, using (5.1) and the new column $E_{1:n,n}$. The vectors v_{n+1} and w_{n+1} are then computed from (3.40)–(3.41).

Next, we consider the update of D_{n+1} from D_n. The diagonal term $w_{n+1}^T v_{n+1}$ is once again computed directly, thus requiring the second inner product per iteration. Next, using

$$\begin{aligned} F_n &= W_n^T A P_n = W_n^T V_{n+1} L_n \\ &= D_n L_{1:n,1:n} + l_{n+1,n} D_{1:n,n+1} [\,0 \quad \cdots \quad 0 \quad 1\,], \end{aligned} \tag{5.2}$$

the remainder of the last column of D_{n+1} is computed from D_n, F_n, and L_n. The last row of D_{n+1} is obtained by symmetry, using (3.15) from Lemma 3.1. One then computes $F_{n+1,1:n}$, using (5.2) and the new row $D_{n+1,1:n+1}$.

Thus, the coupled Lanczos Algorithm 3.3 requires the computation of two inner products and four vector norms per iteration. We conclude this section by noting that, in Algorithm 3.3,

the choice of the inner recurrence coefficients (3.37) and (3.44) is arbitrary. In our implementation of the algorithm, we used

$$\begin{aligned} u_{n-1,n} &= 1, \\ u_{n-2,n} &= 1 \quad \text{when } m_k \le n-2, \\ u_{in} &= 0 \quad \text{for } i = m_k, \ldots, n-3, \\ l_{nn} &= 1, \\ l_{n-1,n} &= 1 \quad \text{when } n_l \le n-1, \\ l_{in} &= 0 \quad \text{for } i = n_l, \ldots, n-2, \end{aligned}$$

for the inner-vector recurrence coefficients.

6. An implementation of QMR with look-ahead. We now return to linear systems (1.1) and the QMR method. In this section, we propose an implementation of the QMR method based on the coupled two-term look-ahead Algorithm 3.3.

Recall that the nth QMR iterate x_n is defined by (2.25)–(2.26) in terms of the matrices V_n and H_n generated by the look-ahead Lanczos algorithm. In the original implementation of QMR, the solution z_n of the least-squares problem (2.26) is computed by means of a QR decomposition of the matrix $\Omega_{n+1}H_n$.

Here we consider the case that the Lanczos vectors are constructed using the coupled two-term Algorithm 3.3. Recall that Algorithm 3.3 yields as a by-product the factors L_n and U_n in the decomposition (3.11) of H_n. Using the factorization (3.11) and setting $y_n := U_n z_n$, we can rewrite the definition (2.25)–(2.26) of x_n as follows:

$$x_n = x_0 + V_n U_n^{-1} y_n, \tag{6.1}$$

where y_n is the unique solution of the least-squares problem

$$\| f_{n+1} - \Omega_{n+1} L_n y_n \| = \min_{y \in \mathbb{C}^n} \| f_{n+1} - \Omega_{n+1} L_n y \|. \tag{6.2}$$

Here, as before, f_{n+1} is given by (2.27) and Ω_{n+1} is defined in (2.28). We remark that the least-squares problem (6.2) is actually cheaper to solve than the original one (2.26). The reason is that the matrix L_n in (6.2) has fewer nonzero elements than H_n in (2.26). For example, if no look-ahead steps are taken, then H_n is tridiagonal, while L_n is a lower bidiagonal matrix. This special case will be considered in more detail in §7. We remark that, typically, the coefficient matrix $\Omega_{n+1}L_n$ of (6.2) is better conditioned than the matrix $\Omega_{n+1}H_n$ in (2.26). Consequently, the least-squares problem (6.2) usually can be solved to higher accuracy than the original one (2.26); see the examples in §9. This is another advantage of the coupled two-term implementation of QMR.

As discussed in [9], solutions of least-squares problems of the type (6.2) can be easily updated from step to step, using the QR decomposition of $\Omega_{n+1}L_n$,

$$\Omega_{n+1} L_n = Q_n^H \begin{bmatrix} R_n \\ 0 \end{bmatrix}, \tag{6.3}$$

where Q_n is a unitary $(n+1) \times (n+1)$ matrix, and R_n is a nonsingular upper triangular $n \times n$ matrix. With this, the least-squares problem (6.2) becomes

$$\begin{aligned} \min_{y \in \mathbb{C}^n} \| f_{n+1} - \Omega_{n+1} L_n y \| &= \min_{y \in \mathbb{C}^n} \left\| Q_n^H \left(Q_n f_{n+1} - \begin{bmatrix} R_n \\ 0 \end{bmatrix} y \right) \right\| \\ &= \min_{y \in \mathbb{C}^n} \left\| Q_n f_{n+1} - \begin{bmatrix} R_n \\ 0 \end{bmatrix} y \right\|. \end{aligned}$$

For y_n this gives:

$$y_n = R_n^{-1} t_n, \quad \text{where } t_n = \begin{bmatrix} \tau_1 \\ \vdots \\ \tau_n \end{bmatrix}, \quad \begin{bmatrix} t_n \\ \tilde{\tau}_{n+1} \end{bmatrix} := Q_n f_{n+1}. \tag{6.4}$$

Finally, we note that it is possible to update the QMR iterate at each step, as was done in the original QMR algorithm. Full implementation details were given in [9, §4], and we will not repeat them here. The point is that the QMR iterates have an update formula of the form

$$x_n = x_{n-1} + d_n \tau_n. \tag{6.5}$$

Here, τ_n is given by (6.4), and d_n is an auxiliary search direction defined as the last column of the matrix $V_n U_n^{-1} R_n^{-1} = P_n R_n^{-1}$, which appears in (6.1) after inserting y_n from (6.4). The vectors d_n are also updated with short recurrences: the recurrence for d_n involves only as many vectors as the recurrence for v_{n+1}. For full details of the update procedure for d_n, we refer the reader to [9].

The basic outline of the resulting implementation of QMR based on the coupled two-term Algorithm 3.3 is then as follows.

ALGORITHM 6.1 (QMR based on coupled recurrences).

0. Choose $x_0 \in \mathbb{C}^N$ and set $r_0 = b - Ax_0$, $\rho_1 = \|r_0\|$, $v_1 = r_0/\rho_1$.
   Choose $w_1 \in \mathbb{C}^N$ with $\|w_1\| = 1$.

For $n = 1, 2, \ldots$, do:

1. Perform the nth iteration of the coupled two-term Algorithm 3.3.
   This yields matrices L_n, P_n, U_n, and V_{n+1}, which satisfy (3.7).
2. Update the QR factorization (6.3) of $\Omega_{n+1} L_n$ and the vector t_n in (6.4).
3. Update the QMR iterate x_n by means of (6.5).
4. If x_n has converged, then stop.

In [9], various properties of the QMR method are given. For example, it is shown how existing BCG iterates can be easily recovered from the QMR process and how estimates for the QMR residual norms can be obtained at no extra costs. We would like to stress that these properties also hold true for the particular implementation of QMR sketched in Algorithm 6.1. Finally, recall from (2.29) that we recommend the use of unit weights $\omega_j = 1$ in $\Omega_{n+1} = \text{diag}(\omega_1, \omega_2, \ldots, \omega_{n+1})$.

7. An implementation of QMR without look-ahead. In this section, we present the simplification of Algorithm 6.1 to the case where no look-ahead is used. We also briefly address the issue of preconditioning.

Let M be a given nonsingular $N \times N$ matrix that approximates in some sense the coefficient matrix A of (1.1). Suppose further that M is decomposed as

$$M = M_1 M_2. \tag{7.1}$$

Then, one applies the QMR algorithm to the system

$$A' y' = b', \tag{7.2}$$

where $A' = M_1^{-1} A M_2^{-1}$, $b' = M_1^{-1} b$, and $x' = M_2 x$. It is easy to see that the linear systems (1.1) and (7.2) are equivalent, and that one can transform back from the iterates x'_n and the

residuals r'_n of the system (7.2) to the iterates x_n and the residuals r_n of the system (1.1). For example, while applying QMR to the preconditioned system (7.2), it is possible to write the resulting algorithm in terms of the quantities corresponding to the original system (1.1); this is what is done below.

We now present a version of the QMR algorithm based on the coupled Algorithm 3.2, which does not have look-ahead. We remark that in this case, by (3.22) and (3.20), the matrix U_n in (3.9) is upper bidiagonal, and L_n is a lower bidiagonal matrix. We also implement preconditioning, as discussed above. The resulting QMR algorithm is as follows.

ALGORITHM 7.1 (QMR based on coupled recurrences without look-ahead).

0. Choose $x_0 \in \mathbb{C}^N$ and set $r_0 = b - Ax_0$.
   Compute $\rho_1 = \|M_1^{-1} r_0\|$ and set $v_1 = r_0/\rho_1$.
   Choose $w_1 \in \mathbb{C}^N$ with $\|M_2^{-T} w_1\| = 1$.
   Set $p_0 = q_0 = d_0 = 0$, $c_0 = \epsilon_0 = \xi_1 = 1$, $\vartheta_0 = 0$, $\eta_0 = -1$.

For $n = 1, 2, \ldots,$ do:

1. If $\epsilon_{n-1} = 0$, then stop.
   Compute $\delta_n = w_n^T M^{-1} v_n$. If $\delta_n = 0$, then stop.

2. Compute

$$p_n = M^{-1} v_n - p_{n-1}(\xi_n \delta_n / \epsilon_{n-1}),$$
$$q_n = M^{-T} w_n - q_{n-1}(\rho_n \delta_n / \epsilon_{n-1}).$$

3. Compute $\epsilon_n = q_n^T A p_n$, $\beta_n = \epsilon_n / \delta_n$, and set

$$\tilde{v}_{n+1} = A p_n - v_n \beta_n, \qquad \rho_{n+1} = \|M_1^{-1} \tilde{v}_{n+1}\|,$$
$$\tilde{w}_{n+1} = A^T q_n - w_n \beta_n, \qquad \xi_{n+1} = \|M_2^{-T} \tilde{w}_{n+1}\|.$$

4. Compute

$$\vartheta_n = \frac{\omega_{n+1} \rho_{n+1}}{\omega_n c_{n-1} |\beta_n|}, \quad c_n = \frac{1}{\sqrt{1 + \vartheta_n^2}}, \quad \eta_n = -\eta_{n-1} \frac{\rho_n c_n^2}{\beta_n c_{n-1}^2},$$
$$d_n = p_n \eta_n + d_{n-1} (\vartheta_{n-1} c_n)^2, \quad x_n = x_{n-1} + d_n.$$

5. If $\rho_{n+1} = 0$ or $\xi_{n+1} = 0$, then stop.
   Otherwise, set

$$v_{n+1} = \tilde{v}_{n+1} / \rho_{n+1}, \quad w_{n+1} = \tilde{w}_{n+1} / \xi_{n+1}.$$

As pointed out in §3.2, the vectors computed in steps 2 and 3 of Algorithm 7.1 are rescaled versions of vectors used in BCG. Freund and Szeto [11] used this connection to derive an implementation of QMR without look-ahead that is directly based on BCG. Their Algorithm 3.1 in [11] and Algorithm 7.1 are mathematically equivalent.

8. QMR for complex symmetric matrices. In this section, we briefly discuss the application of the QMR Algorithm 7.1 to the solution of complex symmetric linear systems, i.e., systems with

$$A = A^T \in \mathbb{C}^{N \times N}.$$

We note that the QMR approach was originally proposed by Freund in [5] for exactly this class of linear systems. We stress that the implementation of complex symmetric QMR in [5] is based on the three-term Lanczos recurrence. Here we present a different implementation based on coupled two-term recursions.

The benefit of applying a Lanczos method to complex symmetric systems is that the underlying Lanczos algorithm simplifies naturally. Recall that in the coupled Algorithm 3.3, the second starting vector w_1 is arbitrary. In the case of a symmetric matrix, if w_1 is chosen equal to v_1, then it is easy to show that $w_n = v_n$ and $q_n = p_n$ for all n. Thus, the recurrences for w_n and q_n can be eliminated, saving roughly half the amount of work and storage.

However, we remark that, in contrast to the Lanczos algorithm for Hermitian matrices where breakdowns are excluded, the Lanczos process for complex symmetric also requires look-ahead to avoid exact and near-breakdowns. This is discussed in detail in [5].

The only other issue in the case of complex symmetric systems is that the preconditioner M in (7.1) must also be symmetric, i.e.,

$$M = M_1 M_2 = (M_1 M_2)^T = M^T. \tag{8.1}$$

For example, this is always guaranteed if the decomposition (7.1) is "symmetric" in the sense that

$$M_2 = M_1^T. \tag{8.2}$$

However, we stress that the condition (8.2) is not necessary, and M_1 and M_2 can be arbitrary matrices satisfying (8.1). We remark that standard preconditioning techniques, such as incomplete factorization, yield symmetric preconditioners (8.1) when applied to symmetric matrices A.

In this case, one can apply the QMR Algorithm 7.1 to the resulting preconditioned system. Once again writing everything in terms of the quantities corresponding to the original system (1.1), one obtains the following iteration.

ALGORITHM 8.1 (QMR without look-ahead for complex symmetric systems).

0. Choose $x_0 \in \mathbb{C}^N$ and set $r_0 = b - Ax_0$.
   Compute $\rho_1 = \|M_1^{-1} r_0\|$ and set $v_1 = r_0/\rho_1$.
   Set $p_0 = d_0 = 0$, $c_0 = \epsilon_0 = 1$, $\vartheta_0 = 0$, $\eta_0 = -1$.

For $n = 1, 2, \ldots$, do:

1. If $\epsilon_{n-1} = 0$, then stop.
   Compute $\delta_n = v_n^T M^{-1} v_n$. If $\delta_n = 0$, then stop.

2. Compute

$$p_n = M^{-1} v_n - p_{n-1}(\rho_n \delta_n / \epsilon_{n-1}).$$

3. Compute $\epsilon_n = p_n^T A p_n$, $\beta_n = \epsilon_n/\delta_n$, and

$$\tilde{v}_{n+1} = Ap_n - v_n \beta_n, \quad \rho_{n+1} = \|M_1^{-1} \tilde{v}_{n+1}\|.$$

4. Compute

$$\vartheta_n = \frac{\omega_{n+1}\rho_{n+1}}{\omega_n c_{n-1} |\beta_n|}, \quad c_n = \frac{1}{\sqrt{1+\vartheta_n^2}}, \quad \eta_n = -\eta_{n-1} \frac{\rho_n c_n^2}{\beta_n c_{n-1}^2},$$

$$d_n = p_n \eta_n + d_{n-1}(\vartheta_{n-1} c_n)^2, \quad x_n = x_{n-1} + d_n.$$

5. If $\rho_{n+1} = 0$, then stop.
   Otherwise, set

$$v_{n+1} = \tilde{v}_{n+1}/\rho_{n+1}.$$

9. Numerical experiments. In this section, we present a few numerical examples. We compare the original and the new implementation of the QMR algorithm, as well as illustrate an application of the coupled QMR algorithm to the solution of complex symmetric linear systems.

In Figs. 9.1–9.3 below, we always show the true relative residual norm $\|r_n\|/\|r_0\|$ plotted versus the iteration index n. All examples were run on a Sun SparcStation 2 using double precision, with machine epsilon of order $\mathcal{O}(10^{-16})$. In all cases, we used unit weights $\omega_j = 1$ for all j in the least-squares problems (6.2), respectively (2.26).

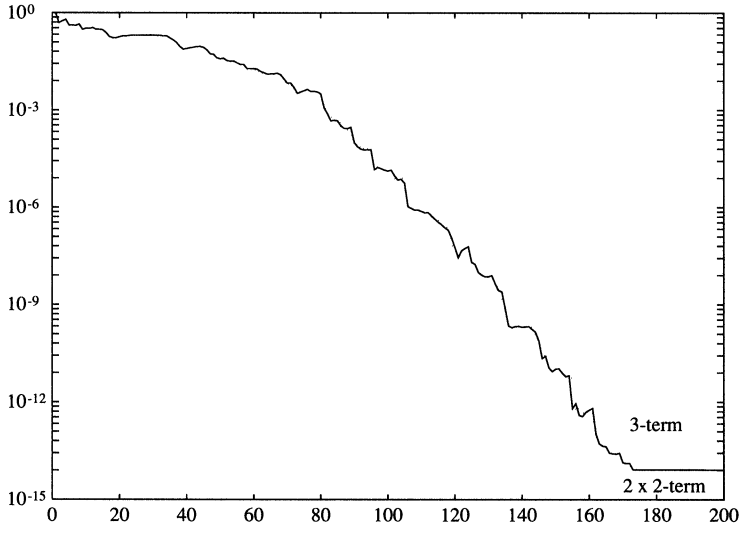

FIG. 9.1. *Convergence curves for Example* 9.1.

Example 9.1. This example is taken from [1] and is meant to illustrate the typical behavior that can be expected from the new implementation of QMR when compared to the original implementation. We consider the partial differential equation

$$Lu = f \quad \text{on } (0, 1) \times (0, 1), \tag{9.1}$$

where

$$Lu := -\frac{\partial}{\partial x}\left(e^{-xy}\frac{\partial u}{\partial x}\right) - \frac{\partial}{\partial y}\left(e^{xy}\frac{\partial u}{\partial y}\right)$$
$$+20(x+y)\frac{\partial u}{\partial x} + 20\frac{\partial}{\partial x}((x+y)u) + \frac{1}{1+x+y}u,$$

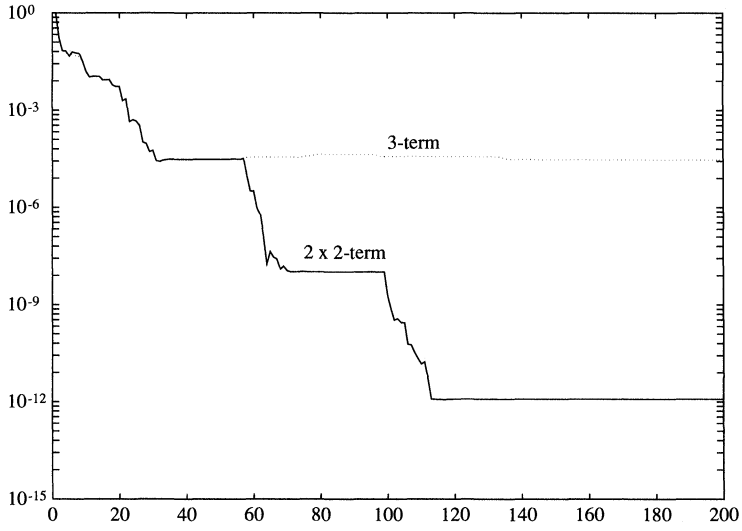

FIG. 9.2. *Convergence curves for Example* 9.2.

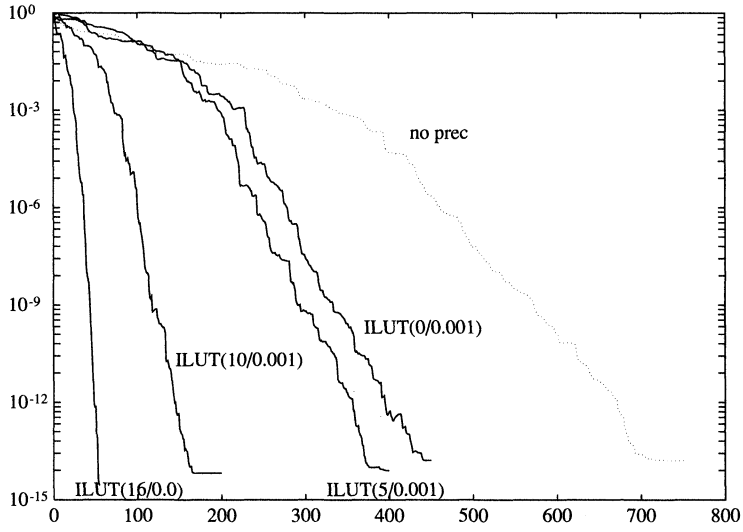

FIG. 9.3. *Convergence curves for Example* 9.3.

with Dirichlet boundary conditions $u = 0$. We discretized (9.1) using centered differences on a 30×30 grid with mesh size $h = \frac{1}{31}$. This leads to a linear system $Ax = b$, where A is a nonsymmetric matrix of order $N = 900$ with 4380 nonzero entries. We ran the original and the new implementations of QMR, both with look-ahead and with the same starting conditions, until the true residual norm $\|r_n\|$ was not reduced any further. The vectors b and w_1 were

random vectors, the initial guess x_0 was zero, and the example was run without preconditioning. The original QMR algorithm is plotted in Fig. 9.1 with a dotted line; it stagnated at `6.7e-14`, and it built six look-ahead blocks of size 2. The coupled QMR algorithm is plotted in Fig. 9.1 with a solid line; it stagnated at `8.3e-15`, and it built four blocks of size 2 in the V–W sequence and seven blocks of size 2 in the P–Q sequence. Recall from §6 that the coupled two-term QMR algorithm solves the least-squares problem (6.2) with coefficient matrix L_n, while the original three-term implementation is based on the least-squares problem (2.26) with coefficient matrix H_n. The Euclidean condition numbers of these matrices at step $n = 165$, respectively $n = 173$, when the original QMR algorithm, respectively the coupled QMR algorithm, begins to stagnate, are $\text{cond}(L_n) =$ `5.2e+03` and $\text{cond}(H_n) =$ `7.3e+03` for both $n = 165$ and $n = 173$. Thus the least-squares problem (6.2) is slightly better conditioned than (2.26).

The behavior in Example 9.1 seems to be fairly typical, in that usually the new implementation is better than the original implementation, but the difference is not very large. However, there are cases where the coupled implementation is significantly better than the original QMR implementation. The next example is of this type.

Example 9.2. This is a linear system that arises in performance modeling of multiprocessor systems, using Petri-net analysis. In such applications, one obtains large sparse singular matrices A with null spaces of dimension 1, and one needs to compute a nontrivial basis vector for this null space. This leads to a linear system of the form $Ax = 0$, and thus condition (2.1) is satisfied. We used a matrix A of size $N = 3663$ with 23397 nonzero elements. The vector b was zero, while the initial guess x_0 and the starting vector w_1 were both random. The linear system is a difficult one, and iterative methods do not converge easily without preconditioning. We used the variant described in [9] of Saad's ILUT preconditioner [22], with no additional fill-in allowed and a drop tolerance of `0.001`, which generated a preconditioning matrix M with 23397 elements. The original QMR algorithm is plotted in Fig. 9.2 with a dotted line; it stagnated at `2.9e-05`, and it built two blocks of size 2. On the other hand, the new implementation, plotted in Fig. 9.2 with a solid line, stagnated at `1.2e-12`, and it built one block of size 2 in the V–W sequence and three blocks of size 2 in the P–Q sequence. The Euclidean condition numbers of the coefficient matrices L_n and H_n of the least-squares problems (6.2) and (2.26) at step $n = 58$, when the original QMR algorithm begins to stagnate, are $\text{cond}(L_{58}) =$ `4.5e+06` and $\text{cond}(H_{58}) =$ `2.4e+10`. At step $n = 113$, when the coupled QMR algorithm begins to stagnate, we have $\text{cond}(L_{113}) =$ `4.9e+06` and $\text{cond}(H_{113}) =$ `3.8e+10`. Thus the least-squares problem (6.2) is considerably better conditioned than (2.26).

Example 9.3. Here A is the complex symmetric YOUNG1C matrix from the Harwell–Boeing test collection of sparse matrices [3]. The matrix arises in a scattering problem in aerodynamics research; it is of dimension $N = 841$ with 4089 nonzero elements. We ran Algorithm 8.1 without look-ahead, with various complex symmetric ILUT preconditioners. In all cases, the iteration was started with the same random vector for b and zero initial guess x_0. This system is also a difficult one, and, if not preconditioned, the QMR algorithm requires around 700 iterations to reach the stagnation level of `2.5e-14`; the corresponding convergence curve is plotted in Fig. 9.3 with a dotted line. However, the ILUT preconditioner is quite effective in this example, especially at higher levels of allowed fill-in and/or drop tolerance. In Fig. 9.3, we show, in order of solid lines from right to left, ILUT with no additional fill-in and `0.001` drop tolerance (2375 nonzero elements), ILUT with five additional fill-in and `0.001` drop tolerance (5171 nonzero elements), ILUT with 10 additional fill-in and `0.001` drop tolerance (9320 nonzero elements), and finally ILUT with 16 additional fill-in and `0.0` drop tolerance (13329 nonzero elements). As can be seen, all variants reach roughly the same stagnation level, around `1.0e-14`. However, as shown in Table 9.1, they do so in

TABLE 9.1
Total execution times (secs) for Example 9.3, average of five runs.

Preconditioner	no prec	ILUT 0/0.001	ILUT 5/0.001	ILUT 10/0.001	ILUT 16/0.0
Iterations	750	450	400	200	55
Time (secs)	144.5	111.4	123.3	75.9	44.4

fewer and fewer iterations, and, in fact, for this example, the additional time spent computing the denser preconditioners was almost always made up by faster convergence.

10. Concluding remarks. We presented a new look-ahead algorithm for constructing Lanczos vectors based on coupled two-term recurrences instead of the usual three-term recurrences. We then discussed a new implementation of the QMR algorithm, using the coupled process to build the basis for the Krylov space. While the theoretical results derived for the original algorithm carry over to the new one, the latter was shown in examples to have better numerical properties. We also briefly covered an implementation of the new QMR method without look-ahead, as well as the application of the QMR algorithm to the solution of complex symmetric linear systems, where the underlying Lanczos process naturally simplifies. Finally, an extended version of this paper, with a more detailed implementation section, is available as a RIACS Technical Report [10].

FORTRAN 77 codes for the proposed coupled-two term look-ahead procedure and the resulting new implementation of the QMR algorithm can be obtained electronically from the authors (freund@research.att.com and na.nachtigal@na-net.ornl.gov). We note that FORTRAN 77 codes for the original implementation of QMR and the underlying look-ahead Lanczos algorithm are available from netlib by sending an email message consisting of the single line "send lalqmr from linalg" to netlib@ornl.gov or netlib@research.att.com.

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