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KRYLOV SUBSPACE METHODS FOR SOLVING LARGE LYAPUNOV EQUATIONS*

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Abstract. This paper considers several methods for calculating low-rank approximate solutions to large-scale Lyapunov equations of the form $AP+PA'+BB' = 0$. The interest in this problem stems from *model reduction* where the task is to approximate high-dimensional models by ones of lower order. The two recently developed Krylov subspace methods exploited in this paper are the *Arnoldi method* [Saad, *Math. Comput.*, 37 (1981), pp. 105–126] and the *Generalised Minimum Residual method* (GMRES) [Saad and Schultz, *SIAM J. Sci. Statist. Comput.*, 7 (1986), pp. 856–869]. Exact expressions for the approximation errors incurred are derived in both cases. The numerical solution of the *low-dimensional* linear matrix equation arising from the GMRES method is discussed and an algorithm for its solution is proposed. Low rank solutions of discrete time Lyapunov equations and continuous time algebraic Riccati equations are also considered. Throughout this paper, the authors tackle problems in which B has more than one column with the use of block Krylov schemes.

Key words. Arnoldi, GMRES, iterative methods, model reduction, Krylov subspace methods, Lyapunov matrix equation, large-scale systems

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1. Introduction.

In this paper, we focus on low-rank approximate solutions of large Lyapunov matrix equations

$$AP + PA' + BB' = 0, \quad A, P \in \mathcal{R}^{N\times N}, \quad \text{and} \quad B \in \mathcal{R}^{N\times p}, \tag{1}$$

in which N is large (typically greater than 200) and $p \ll N$. Lyapunov equations play an important role in control and communications theory. They arise naturally in $\mathcal{H}^\infty$ optimal control theory [11], system balancing [20], [22], stability analysis of dynamical systems [21], and model reduction of linear time invariant systems [22], [29].

The need for model reduction arises in many areas of engineering, where high-order mathematical models are used to describe complex dynamical behaviour. These occur whenever models are described by partial differential equations that culminate in large, linear finite element models. For practical reasons, it is desirable to replace these high-order models by low-order approximations; for example, in control system applications, high-order models may result in high-order controllers and the subsequent implementation of these controllers is cumbersome and expensive. Consider a stable linear state-space model of the form

$$\dot{x}(t) = Ax(t) + Bu(t), \tag{2}$$

$$y(t) = Cx(t) + Du(t), \tag{3}$$

in which $x(t)$ is the state vector of dimension N, $u(t)$ is a control vector of length p, and $y(t)$ is the output vector of length q. The matrices A, B, C, and D are real with their dimensions fixed by those of x, u, and y. The associated transfer function is given by $G(s) = C(sI - A)^{-1}B + D$. The task of any model reduction algorithm is

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to find an approximate stable model

$$\dot{x}_k(t) = A_k x_k(t) + B_k u(t), \tag{4}$$

$$y_k(t) = C_k x_k(t) + D_k u(t), \tag{5}$$

in which $x_k(t) \in \mathcal{R}^k$, with $k \ll N$ and the low-order transfer function is given by $G_k(s) = C_k(sI - A_k)^{-1}B_k + D_k$. Well-established model reduction methods such as optimal Hankel norm [10] and balanced truncation [22], [29] begin by solving the linear matrix equations

$$AP + PA' + BB' = 0 \tag{6}$$

and

$$A'Q + QA + C'C = 0, \tag{7}$$

which have unique solutions if and only if $\lambda_i(A) + \bar{\lambda}_j(A) \neq 0$ for all i, j. The requisite for P and Q stems from the easily computable $\mathcal{L}^\infty$ error bound [10]

$$\|G(s) - G_k(s)\|_\infty \leq 2\sum_{k+1}^{N} \sigma_i(PQ), \tag{8}$$

where the σ_i's are the Hankel singular values of $G(s)$ defined as $\sigma_i = \lambda_i^{1/2}(PQ)$ and arranged in decreasing order of magnitude.

The low-rank approximate solution to large Lyapunov equations has received only modest attention; the references [1], [15], [16], and [25] are to the authors' knowledge the only available literature on the topic. In the case of low-dimensional problems (for $N \leq 50$) there are numerous solution techniques based on iterative approximation methods, numerical integration, Kronecker matrix products, Jordan decompositions, and eigenvalue decompositions. Of these various procedures, the Bartels–Stewart algorithm [3] is probably the most efficient and widely used. The Bartels–Stewart algorithm transforms A into a real Schur form $H = U'AU$ in which U is orthogonal and H is quasi upper-triangular. This gives

$$H\tilde{P} + \tilde{P}H' + U'BB'U = 0, \tag{9}$$

in which $\tilde{P} = U'PU$, and this equation is easily solved by back substitution. Unfortunately, none of these methods are suitable for solving large Lyapunov equations, since the computation time and storage requirements are prohibitive. The Schur decompositions of sparse matrices are dense in general as are their orthogonal transformation matrices. Furthermore, their respective solutions P and $\tilde{P}$ in (1) and (9) will generally be dense even when A is diagonal. To remedy this situation, this paper presents algorithms that compute approximate solutions to (1) for large A and low rank B. Our approach is based on the work of Saad [25], which uses classical Krylov subspace techniques.

Krylov subspace techniques are a class of iterative methods that are playing an increasing role in the solution of numerous scientific problems. Originally proposed for the solution of large eigenvalue problems, they have successfully found their way into a variety of applications in the areas of control theory, computational chemistry, and physics. Much of the theoretical research on the applications of Krylov subspace techniques relates to the solution of linear systems of equations $Ax = b$ [8], [23],

[28] with recent extensions to nonlinear systems [7] employing hybrid schemes and ordinary differential equations [6], [9]; a good survey of recent research activity in this area with an emphasis on supercomputers may be found in [26]. In [25] Saad considers the low-rank approximate solutions to (1) in which $p = 1$; this paper extends his work to the general case via the use of block schemes and gives an expression for the corresponding residual error. We subsequently address the problem of computing a low rank approximate solution to (1) which meets an optimality condition. The GMRES method we consider minimises the Frobenius norm of the error for which we also give an exact expression.

Recently, several researchers have proposed alternative iterative methods for the approximate solution to large Sylvester equations of the form $AX + XB = -C$. In [31], the *Alternating-Direction-Implicit* (ADI) iteration is applied to refine an initial approximate solution. The block *Successive Overrelaxation* iterative method may also be used to iteratively refine an initial approximate solution; this idea was first proposed by Starke and Niethammer [30]. Both the ADI and SOR methods do not necessarily yield low-rank approximate solutions; consequently, storing and manipulating the solution may be expensive.

In [18], Hu and Reichel consider low-rank approximate solutions to Sylvester equations. Their technique is similar to ours and was developed independently. Their Galerkin method produces a low-dimensional Sylvester equation whose solution is used to build a low-rank approximation, while the GMRES method yields a large system of linear equations via the use of Kronecker tensors. The main difference between [18] and the results presented in this paper is that our computations are performed in the low dimension and expressions for the residual errors are provided.

Section 2 describes the type of approximations employed and studies the *Arnoldi* and *GMRES* methods, deriving exact expressions for the errors incurred in both schemes. Section 3 considers the practical problem of solving the linear matrix equation arising from the GMRES method. Section 4 employs the solution techniques presented in §2 to give low-rank solutions and residual error expressions for the discrete Lyapunov matrix equation and for the continuous time algebraic Riccati equation. Two illustrative examples in §5 show how the Lyapunov solvers behave in practice, and finally, some concluding remarks are given in §6.

2. Krylov subspace techniques. The purpose of this section is to establish the type of low-rank approximation used throughout this paper. Based on this choice, we describe the Arnoldi and GMRES methods and give a full error analysis for each case.

In practice, solutions to large Lyapunov equations (1) frequently admit good low-rank approximations, in addition to which one is generally interested in computing only the dominant eigenspace of the solution P^*, rather than P^* itself, since the dominant eigenspace of P^* is known to be associated with the dominant modes of the system described by (2) and (3) [20]. Ideally, we would therefore like to compute a rank m approximation P_m, where $m \ll N$ such that $\|P^* - P_m\|_F$ is minimised. Throughout this paper we shall make use of the Frobenius norm defined as $\|Z\|_F = \sqrt{\mathrm{tr}(ZZ')}$ in which Z' denotes the transpose of Z.

Consider the Schur decomposition of P^* given by $P^* = U\Sigma U'$ in which $U \in \mathcal{R}^{N\times N}$ is an orthogonal matrix and $\Sigma = \mathrm{diag}\{\sigma_1, \sigma_2, \ldots, \sigma_N\}$ is a matrix of eigenvalues ordered such that $|\sigma_1| \geq |\sigma_2| \geq \cdots |\sigma_N| \geq 0$. Then the optimal rank m Frobenius norm

approximation of P^* is given by

$$P_m := U \begin{bmatrix} \Sigma_m & 0 \\ 0 & 0 \end{bmatrix} U' = U_m \Sigma_m U_m', \tag{10}$$

where $\Sigma_m = \text{diag}\{\sigma_1, \sigma_2, \ldots, \sigma_m\}$ (i.e., the first m diagonal elements of Σ) and $U_m \in \mathcal{R}^{N \times m}$ is the first m columns of U. In [25] a low-rank approximation is computed by choosing an orthogonal matrix $V_m \in \mathcal{R}^{N \times m}$ and calculating the exact solution X_m to the reduced-order Lyapunov equation

$$(V_m' A V_m) X_m + X_m (V_m' A' V_m) + V_m' B B' V_m = 0. \tag{11}$$

The estimate of P^* is then given by $P_m = V_m X_m V_m'$. Compared with the optimal approximation given in (10), it is apparent that to compute a good estimate of P^*, V_m must be an accurate approximation of U_m, or in other words, the m most dominant eigenvectors of P^*. Unfortunately, minimising $\|P^* - P_m\|_F$ is intractable when P^* is unknown.

We will therefore turn our attention to the problem of selecting V_m and X_m. Let K_m be the mp-dimensional Krylov space defined as

$$K_m = \text{span}\left\{[B \; AB \; A^2B \; \cdots \; A^{m-1}B]\right\}, \tag{12}$$

then following [25], we will select V_m to be an orthogonal basis of K_m. Throughout the remainder of this paper, we will exploit approximations to the solution P^* which have the form

$$P_m = V_m X_m V_m', \tag{13}$$

where $X_m \in \mathcal{R}^{mp \times mp}$ is an arbitrary symmetric matrix. The key point here is that even though $P_m \in \mathcal{R}^{N \times N}$, it may be efficiently stored as the product of smaller matrices $V_m \in \mathcal{R}^{N \times mp}$ and $X_m \in \mathcal{R}^{mp \times mp}$. We observe that P_m is symmetric for symmetric X_m and $\text{rank}(P_m) = \text{rank}(X_m) \leq mp$.

The remainder of this section is devoted to the appropriate selection of a symmetric X_m. We begin by defining the residual error function associated with a particular choice of X_m as

$$R_m(X_m) := A(V_m X_m V_m') + (V_m X_m V_m') A' + BB'. \tag{14}$$

The solution techniques presented in this paper are based on seeking a symmetric X_m so as to give $R_m(X_m)$ desirable properties. Section 2.1 addresses the problem of constructing X_m such that $R_m(X_m)$ has an orthogonality property with respect to K_m and gives a computable expression for $\|R_m(X_m)\|_F$. Section 2.2 deals with finding a symmetric X_m which minimises $\|R_m(X_m)\|_F$ for which a simple expression is also derived.

2.1. The Arnoldi method. Next we use the well established Arnoldi algorithm [32] to calculate an orthonormal basis V_m for the Krylov subspace K_m. The basic outline of a block Arnoldi process is given next.

Arnoldi process.

- Compute $B = Q_1 R_1$ and set $p_1 :=$ number of columns of Q_1 (QR factorisation).

- Do $j = 1, \ldots, m$.
  (a) Set $V_j = [Q_1\ Q_2 \cdots Q_j]$.
  (b) Compute $\begin{bmatrix} A_{1j} \\ A_{2j} \\ \vdots \\ A_{jj} \end{bmatrix} = V_j' A Q_j$.
  (c) $Q_{j+1} A_{j+1,j} = AQ_j - \sum_{k=1}^{j} Q_k A_{kj}$ (QR factorisation) and $p_{j+1} :=$ number of columns of Q_{j+1}.

End Do.

In practice, it is advisable to compute the QR factorisations of the Arnoldi process via the Gram–Schmidt (GS) or modified Gram–Schmidt (MGS) orthogonalisation processes. A brief description of such a factorisation process is given next; column partition B as $B = [b_1, b_2, \ldots, b_p]$; then

$$\begin{array}{lll} \text{Step 1:} & n_{q_1} = b_1, & q_1 = n_{q_1}/\|n_{q_1}\|_2, \\ \text{Step 2:} & n_{q_2} = b_2 - (q_1' b_2) q_1, & q_2 = n_{q_2}/\|n_{q_2}\|_2, \\ \vdots & \vdots & \vdots \\ \text{Step k:} & n_{q_k} = b_k - \sum_{j=1}^{k-1} (q_j' b_k) q_j, & q_k = n_{q_k}/\|n_{q_k}\|_2; \end{array}$$

construct the orthogonal matrix $Q_1 := [q_1\ q_2\ \cdots\ q_p]$, and finally, define the upper triangular matrix R_1, where

$$R_1 = \begin{bmatrix} \|n_{q_1}\|_2 & q_1' b_2 & q_1' b_3 & \cdots & q_1' b_p \\ 0 & \|n_{q_2}\|_2 & q_2' b_3 & \cdots & \vdots \\ 0 & 0 & \|n_{q_3}\|_2 & \cdots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & 0 & \|n_{q_p}\|_2 \end{bmatrix}. \tag{15}$$

Poor numerical properties of the GS method make it necessary to occasionally employ the MGS approach, which is a rearrangement of the calculations outlined above [12]. The main point we wish to highlight is that to effect the QR factorisation of B in this setting, one only needs to construct an orthogonal basis Q_1 of B such that $Q_1 \in \mathcal{R}^{N \times p}$ and an upper-triangular matrix $R \in \mathcal{R}^{p \times p}$.

In the case that B does not have full column rank, GS and MGS do not generally yield an orthogonal basis for B. The QR factorisation is then given by

$$B\Pi = [\hat{Q}_1\ \hat{Q}_2] \begin{bmatrix} \hat{R}_{11} & \hat{R}_{12} \\ 0 & 0 \end{bmatrix}$$

in which $\hat{R}_{11}$ is upper-triangular and Π is a permutation matrix. In such a situation, we set $Q_1 := \hat{Q}_1$ and $R_1 := [\hat{R}_{11}\ \hat{R}_{12}]\Pi'$. Finally, $p_1 := \operatorname{rank}(Q_1) = \operatorname{rank}(B)$, and hence V_1 has only p_1 columns. Similarly, the QR factorisation of $AQ_j - \sum_{k=1}^{j} Q_k A_{kj}$ in the main loop of the Arnoldi process is given by

$$[\hat{Q}_{j1}\ \hat{Q}_{j2}] \begin{bmatrix} \hat{R}_{j1} & \hat{R}_{j2} \\ 0 & 0 \end{bmatrix} = \left(AQ_j - \sum_{k=1}^{j} Q_k A_{kj} \right) \Pi, \tag{16}$$

in which we set

$$Q_{j+1} := \hat{Q}_{j1} \quad \text{and} \quad A_{j+1,j} := [\hat{R}_{j1}\ \hat{R}_{j2}]\Pi'. \tag{17}$$

We observe that the upper-triangular structure of $\hat{R}_{j1}$ is lost since Π' permutes the columns of $[\hat{R}_{j1}\ \hat{R}_{j2}]$. The matrices R_1 and A_{j+1}, j are nonsquare and will have row rank of p_1 and p_{j+1} respectively. We refer to any rank drop in B or $AQ_j - \sum_{k=1}^{j} Q_k A_{kj}$ as a *curable* (or partial) breakdown since it does not adversely affect the Arnoldi process if tackled in the manner just described. For the most part, we will assume that this type of breakdown does not occur; consequently, m steps of the Arnoldi process generate $V_m \in \mathcal{R}^{N \times mp}$.

By construction, the algorithm above produces an orthonormal basis $V_m = [Q_1\ Q_2\ \cdots\ Q_m]$ for the Krylov subspace K_m. Defining the $mp \times mp$ block upper-Hessenberg matrix A_m as

$$A_m = \begin{bmatrix} A_{11} & A_{12} & \cdots & \cdots & A_{1m} \\ A_{21} & A_{22} & \cdots & \cdots & \vdots \\ 0 & A_{32} & A_{33} & \cdots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & A_{m,m-1} & A_{mm} \end{bmatrix}, \tag{18}$$

it is easy to verify that

$$AV_m = V_m A_m + Q_{m+1} A_{m+1,m} E_m' \tag{19}$$

and

$$A_m = V_m' A V_m, \tag{20}$$

where E_m is a matrix of the last p columns of the mp identity matrix.

Remark 2.1. Boley and Golub [4] give a similar treatment of the block Arnoldi process; however, their algorithm computes an orthogonal basis of the entire controllable subspace (i.e., the Krylov space $K(A, B)$), the construction of A_m is carried out using (20) rather than by the Arnoldi process and finally, they do not consider (19). In our algorithm, we use their implementation of (16) for the updates given in (17). This ensures that (19) is satisfied.

If we set $B_m := [R_1'\ 0_{p \times l}]'$ where $l = p(m-1)$, then $B = V_m B_m$, the residual error (14) is then given by

$$R_m(X_m) := A(V_m X_m V_m') + (V_m X_m V_m')A' + V_m B_m B_m' V_m'. \tag{21}$$

Substituting (19) into (21) gives

$$R_m(X_m) = V_{m+1} \begin{bmatrix} A_m X_m + X_m A_m' + B_m B_m' & X_m E_m A_{m+1,m}' \\ A_{m+1,m} E_m' X_m & 0 \end{bmatrix} V_{m+1}', \tag{22}$$

where $V_{m+1} = [V_m\ Q_{m+1}]$. The Arnoldi–Lyapunov solver considered in this subsection seeks a symmetric X_m by imposing the condition that the residual error $R_m(X_m)$ has an orthogonality property with respect to K_m; we can state the problem we wish to address as follows.

PROBLEM 2.1. Find an approximate solution $P_m := V_m X_m V_m'$ that satisfies the Galerkin type condition $V_m' R_m(X_m) V_m = 0$.

The following theorem is the main result of this subsection and gives the solution to Problem 2.1.

THEOREM 2.1. *Suppose that m steps of the Arnoldi process have been taken and that the residual error is defined by* (21); *then if* $\lambda_i(A_m) + \bar{\lambda}_j(A_m) \neq 0$, *for all* i, j,

(a) $V_m' R_m(X_m) V_m = 0$ *if and only if* $X_m = X_m^A$, *where* X_m^A *satisfies*

$$A_m X_m^A + X_m^A A_m' + B_m B_m' = 0; \tag{23}$$

(b) *If the conditions of* (a) *are met, then the residual error norm is given by*

$$\|R_m^A\|_F := \|R_m(X_m^A)\|_F = \sqrt{2}\|A_{m+1,m} E_m' X_m^A\|_F. \tag{24}$$

Proof. Pre- and post-multiplying (22) by V_m' and V_m, respectively, gives

$$\begin{aligned} V_m' R_m(X_m) V_m &= V_m' V_{m+1} \begin{bmatrix} A_m X_m + X_m A_m' + B_m B_m' & X_m E_m A_{m+1,m}' \\ A_{m+1,m} E_m' X_m & 0 \end{bmatrix} V_{m+1}' V_m \\ &= \begin{bmatrix} I & 0 \end{bmatrix} \begin{bmatrix} A_m X_m + X_m A_m' + B_m B_m' & X_m E_m A_{m+1,m}' \\ A_{m+1,m} E_m' X_m & 0 \end{bmatrix} \begin{bmatrix} I \\ 0 \end{bmatrix} \\ &= A_m X_m + X_m A_m' + B_m B_m', \end{aligned}$$

since $V_{m+1} = [V_m \; Q_{m+1}]$ is part of an orthogonal matrix. The result follows immediately, establishing the proof of part (a). Substituting (23) into the (1,1) block of (22) gives

$$R_m^A := R_m(X_m^A) = V_{m+1} \begin{bmatrix} 0 & X_m^A E_m A_{m+1,m}' \\ A_{m+1,m} E_m' X_m^A & 0 \end{bmatrix} V_{m+1}', \tag{25}$$

$$\begin{aligned} \|R_m^A\|_F &= \sqrt{\mathrm{tr}(X_m^A E_m A_{m+1,m}' A_{m+1,m} E_m' X_m^A) + tr(A_{m+1,m} E_m' X_m^A X_m^A E_m A_{m+1,m}')} \\ &= \sqrt{2}\sqrt{\mathrm{tr}(X_m^A E_m A_{m+1,m}' A_{m+1,m} E_m' X_m^A)} \\ &= \sqrt{2}\|A_{m+1,m} E_m' X_m^A\|_F, \end{aligned} \tag{26}$$

since V_{m+1} is part of an orthogonal matrix that completes the proof. □

An implication of the above result is that as m is increased, the residue is confined to a progressively smaller and smaller subspace of $\mathcal{R}^{N \times N}$. This, however, does not imply that the Arnoldi will produce a sequence of nonincreasing residual error norms. The residual error norm in (24) provides a useful stopping criterion in a practical implementation of the algorithm; it allows one to economically evaluate the error norm and gauge the quality of the low rank approximation. The key points here are the following. Firstly, (23) is a Lyapunov equation of dimension mp, which can be solved accurately using the Bartels–Stewart algorithm [3]; secondly, P_m may be efficiently stored as the product of low-order matrices; and thirdly, the residual error norm does not require the computation of the approximate solution P_m at each step, instead (24) is computed via low-dimensional matrix products. Finally, we mention that $\mathrm{Re}(\lambda_i(A_m)) < 0$ is guaranteed whenever $A + A' < 0$. The complete algorithm may now be summarised in the following procedure.

Arnoldi–Lyapunov solver.

- Start: Specify a tolerance $\epsilon > 0$, set an integer parameter m_1, and, set $k = 0$ and $m := m_1$.
- The Arnoldi process:
  1. Compute $B = Q_1 R_1$ (QR factorisation).

2. Do $j = k+1, k+2, \ldots, k+m_1$
   (a) Set $V_j = [Q_1\ Q_2 \cdots Q_j]$.
   (b) Compute $\begin{bmatrix} A_{1j} \\ A_{2j} \\ \vdots \\ A_{jj} \end{bmatrix} = V_j' A Q_j$.
   (c) $Q_{j+1} A_{j+1,j} = AQ_j - \sum_{k=1}^{j} Q_k A_{kj}$ (QR factorisation).
   End Do.

- Find the symmetric X_m^A which uniquely satisfies the low-order Lyapunov equation $A_m X_m^A + X_m^A A_m' + B_m B_m' = 0$.
- Compute $\|R_m^A\|_F := \sqrt{2}\|A_{m+1,m} E_m' X_m^A\|_F$.
- Stopping test: If $\|R_m^A\|_F > \epsilon$, set $k := k + m_1$, $m := k + m_1$ and go to step 2 of the Arnoldi process.
- Form the approximate solution: $P_m := V_m X_m^A V_m'$.

Remark 2.2. Computing the residual error norm $\|R_m^A\|_F$ at the end of each Arnoldi process iteration requires $\frac{25}{2}(mp)^3$ floating point operations and $2.5(mp)^2$ words of storage [12]. As mp increases, the cost of calculating X_m^A becomes excessive, to counter this, the procedure above introduces the variable m_1 (typically 3 or 4) which translates into the residual error norm being evaluated every m_1 iterations of the Arnoldi process. Note that in the stopping test, m is the total number of iterations.

It is important to note that the algorithm converges in at most $\mathrm{mod}(N/p) + 1$ steps using exact arithmetic (provided no curable breakdown occurs), at which point it yields the exact solution P^*. The point we wish to make here is that in practice, accurate solutions may be computed for mp significantly smaller than N. The problem therefore rests with establishing theoretical error bounds for $\|P^* - P_m\|_F$, which would be useful in selecting an integer value for m to give a good approximate solution.

A drawback of the algorithm above is that as m increases, manipulations with V_m become expensive and storage requirements become excessive. One way to avoid this type of buildup is to truncate the orthogonalisation process by forcing the new Q_{m+1} to be orthogonal to only the last l columns of V_m, where l is a user specified integer parameter. The resulting block Hessenberg matrix A_m is block-banded with a superdiagonal bandwidth $l-1$. An advantage of implementing such an incomplete orthogonalisation process is that it requires only the storage of the last l columns of V_m; for further details we refer the reader to [6], [23], and [24]. Unfortunately, the simple formula of (24) no longer holds when incomplete orthogonalisation is in service, making it difficult to gauge how well the method is performing on a particular problem.

In [14], it is shown that numerical methods for solving (1) suffer from numerical instability; in particular, no numerical method will be backward stable. The following result gives one perturbation of the data in (1) for which the low-rank solution given in Theorem 2.1 is an exact solution.

COROLLARY 2.2. *Suppose that m steps of the Arnoldi process have been taken and let* $P_m := V_m X_m^A V_m'$ *be the low-rank approximate solution of* (1), *where* X_m^A *satisfies* (23). *Then*

$$(A - \Delta_m) P_m + P_m (A - \Delta_m)' + BB' = 0, \tag{27}$$

where $\Delta_m = Q_{m+1}A_{m+1,m}Q_m'$ *and* $\|\Delta_m\|_F = \|A_{m+1,m}\|_F$.

Proof. Substituting $X_m := X_m^A$ into (21) and using (25) gives

$$\begin{aligned} &A(V_m X_m^A V_m') + (V_m X_m^A V_m')A' + BB' \\ &\quad = V_{m+1}\begin{bmatrix} 0 & X_m^A E_m A_{m+1,m}' \\ A_{m+1,m}E_m' X_m^A & 0 \end{bmatrix} V_{m+1}' \\ &\quad = Q_{m+1}A_{m+1,m}E_m' X_m^A V_m' + V_m X_m^A E_m A_{m+1,m}' Q_{m+1}'. \end{aligned} \tag{28}$$

Equation (27) follows by rearranging (28) and noting that $E_m' = Q_m' V_m$. The expression for $\|\Delta_m\|_F$ follows from the fact that Q_m and Q_{m+1} are parts of an orthogonal matrix. Finally, observe that Δ_m is at most a rank p perturbation. □

2.2. The Generalised Minimum Residual method (GMRES). In this section we address the problem of computing an approximate solution to (1) that meets some optimality condition. The method we propose is based on finding a symmetric X_m that minimises the norm of the residual error $R(X_m)$. We have termed this a *Generalised Minimum Residual* method (GMRES), as it is based on a similar idea of Saad and Schultz [28], developed in the context of solving linear systems. The problem we would like to solve can be stated as follows.

PROBLEM 2.2. Find a symmetric $X_m \in \mathcal{R}^{mp\times mp}$ that minimises the residual error norm, namely,

$$\|R_m^{GM}\|_F := \min_{X_m = X_m'} \left\| V_{m+1}\begin{bmatrix} A_m X_m + X_m A_m' + B_m B_m' & X_m E_m A_{m+1,m}' \\ A_{m+1,m}E_m' X_m & 0 \end{bmatrix} V_{m+1}' \right\|_F.$$

DEFINITION 2.1. The solution of Problem 2.2 relies on the following definitions:

(a) Let v_j denote the jth column of the matrix $V \in \mathcal{R}^{n\times m}$ and $\mathrm{vec}(V)$ be defined as

$$\mathrm{vec}(V) = \begin{bmatrix} v_1' & v_2' & \cdots & v_n' \end{bmatrix}' \in \mathcal{R}^{nm}; \tag{29}$$

(b) $A \otimes B$ denotes the Kronecker product of matrices $A \in \mathcal{R}^{k\times l}$ and $B \in \mathcal{R}^{n\times m}$; and is the matrix whose (i,j) block is $a_{ij}B$.

$$A \otimes B = \begin{bmatrix} & a_{ij}B & \end{bmatrix} \in \mathcal{R}^{(kn)\times(lm)} \quad \text{for } i = 1 \text{ to } k \quad \text{and} \quad j = 1 \text{ to } l, \tag{30}$$

from which we deduce

$$\mathrm{vec}(ABC) = (C' \otimes A)\mathrm{vec}(B), \tag{31}$$

$$\mathrm{vec}(A)'\mathrm{vec}(B) = \mathrm{tr}(A'B), \tag{32}$$

$$(A \otimes B)(C \otimes D) = (AC \otimes BD), \tag{33}$$

$$(A \otimes B)' = A' \otimes B'. \tag{34}$$

The following theorem is the main result of this subsection and gives the solution to Problem 2.2.

THEOREM 2.3. *Suppose that* m *steps of the Arnoldi process have been taken and that the residual error is given by* (22)*, then if* $\lambda_i(A_m) + \bar{\lambda}_j(A_m) \neq 0$*, for all* i, j

$$\|R_m^{GM}\|_F = \sqrt{\mathrm{tr}(B_m'(A_m X_m^{GM} + X_m^{GM} A_m' + B_m B_m')B_m)}, \tag{35}$$

where X_m^{GM} satisfies the mp-dimensional linear matrix equation

$$
\begin{aligned}
&A'_m(A_m X_m^{GM} + X_m^{GM} A'_m + B_m B'_m) + (A_m X_m^{GM} + X_m^{GM} A'_m + B_m B'_m)A_m \\
&\quad + E_m A'_{m+1,m} A_{m+1,m} E'_m X_m^{GM} + X_m^{GM} E_m A'_{m+1,m} A_{m+1,m} E'_m = 0.
\end{aligned} \tag{36}
$$

Proof. The first part of the proof will establish that X_m^{GM} satisfies the linear matrix equation (36), while the residual error norm given in (35) is derived in the second part.

Starting with (22), we have

$$
\begin{aligned}
\|R_m(X_m)\|_F^2 &= \operatorname{tr}\left([A_m X_m + X_m A'_m + B_m B'_m]^2\right) \\
&\quad + \operatorname{tr}\left(X_m E_m A'_{m+1,m} A_{m+1,m} E'_m X_m\right) \\
&\quad + \operatorname{tr}\left(A_{m+1,m} E'_m X_m X_m E_m A'_{m+1,m}\right)
\end{aligned} \tag{37}
$$

since V_{m+1} is part of an orthogonal matrix. Using (31) and (32) of Definition 2.1,

$$
\begin{aligned}
\|R_m(X_m)\|_F^2 &= \|(I \otimes A_m + A_m \otimes I)\operatorname{vec}(X_m) + \operatorname{vec}(B_m B'_m)\|_2^2 \\
&\quad + \|(I \otimes A_{m+1,m} E'_m)\operatorname{vec}(X_m)\|_2^2 + \|(A_{m+1,m} E'_m \otimes I)\operatorname{vec}(X_m)\|_2^2
\end{aligned} \tag{38}
$$

$$
= \left\| \begin{bmatrix} I \otimes A_m + A_m \otimes I \\ I \otimes A_{m+1,m} E'_m \\ A_{m+1,m} E'_m \otimes I \end{bmatrix} \operatorname{vec}(X_m) + \begin{bmatrix} \operatorname{vec}(B_m B'_m) \\ 0_{mp \times 1} \\ 0_{mp \times 1} \end{bmatrix} \right\|_2^2 \tag{39}
$$

$$
\equiv \left\| \bar{A}_m \bar{x}_m + \bar{b}_m \right\|_2^2 \tag{40}
$$

with a one-to-one correspondence between (39) and (40).

Since (40) is a least squares problem, it follows that its minimum is achieved when

$$
\bar{A}'_m \left(\bar{A}_m \bar{x}_m + \bar{b}_m\right) = 0 \tag{41}
$$

[12]. Substituting the terms of (39) into (41) and using (33) and (34) yields

(42)

$$
\begin{aligned}
&(I \otimes A_m + A_m \otimes I)' \{(I \otimes A_m + A_m \otimes I)\operatorname{vec}(X_m) + \operatorname{vec}(B_m B'_m)\} \\
&+ (I \otimes E_m A'_{m+1,m} A_{m+1,m} E'_m)\operatorname{vec}(X_m) + (E_m A'_{m+1,m} A_{m+1,m} E'_m \otimes I)\operatorname{vec}(X_m) = 0.
\end{aligned}
$$

Using (31) and (34),

$$
\begin{aligned}
0 &= (I \otimes A_m + A_m \otimes I)' \operatorname{vec}(A_m X_m + X_m A'_m + B_m B'_m) \\
&\quad + \operatorname{vec}(E_m A'_{m+1,m} A_{m+1,m} E'_m X_m) + \operatorname{vec}(X_m E_m A'_{m+1,m} A_{m+1,m} E'_m)
\end{aligned} \tag{43}
$$

$$
\begin{aligned}
0 &= A'_m(A_m X_m + X_m A'_m + B_m B'_m) + (A_m X_m + X_m A'_m + B_m B'_m)A_m \\
&\quad + E_m A'_{m+1,m} A_{m+1,m} E'_m X_m + X_m E_m A'_{m+1,m} A_{m+1,m} E'_m,
\end{aligned} \tag{44}
$$

which is the linear matrix equation given in (36). This completes the proof of the first part.

Suppose X_m^{GM} satisfies (36); then substituting $\operatorname{tr}\left(X_m^{GM} \times (36)\right)$ into (37), and using the property $\operatorname{tr}(AB) = \operatorname{tr}(BA)$ followed by some algebra, we get that

$$
\left\|R_m^{GM}\right\|_F^2 = \operatorname{tr}\left(B'_m(A_m X_m^{GM} + X_m^{GM} A'_m + B_m B'_m)B_m\right) \tag{45}
$$

from which (35) follows, thereby completing the proof. □

Remark 2.3. In the proof above, we have elected to use the Kronecker tensor approach because of the close parallel it shows with GMRES à la Saad and Schultz [28]. Since the Frobenius norm of the residue $R_m(X_m)$ is expressed as

$$\|R_m(X_m)\|_F^2 = \mathrm{tr}(R_m(X_m)R_m(X_m)');$$

an alternative way to establish (36) is to use trace differentiation as defined in [2].

COROLLARY 2.4. *X_m^{GM} satisfies the mp-dimensional linear equation* (36) *if and only if the solution residue R_m^{GM} satisfies the Galerkin type condition*

$$V_m' \left(A' R_m^{GM} + R_m^{GM} A\right) V_m = 0. \tag{46}$$

Proof. Substituting (22) into the left-hand side of (46) gives

$$\begin{aligned} &V_m' \left(A' R_m^{GM} + R_m^{GM} A\right) V_m \\ &\quad = V_m' A' [V_m \; Q_{m+1}] \\ &\qquad \cdot \begin{bmatrix} A_m X_m^{GM} + X_m^{GM} A_m' + B_m B_m' & X_m^{GM} E_m A_{m+1,m}' \\ A_{m+1,m} E_m' X_m^{GM} & 0 \end{bmatrix} \begin{bmatrix} V_m' \\ Q_{m+1}' \end{bmatrix} V_m \\ &\qquad + V_m' [V_m \; Q_{m+1}] \\ &\qquad \cdot \begin{bmatrix} A_m X_m^{GM} + X_m^{GM} A_m' + B_m B_m' & X_m^{GM} E_m A_{m+1,m}' \\ A_{m+1,m} E_m' X_m^{GM} & 0 \end{bmatrix} \begin{bmatrix} V_m' \\ Q_{m+1}' \end{bmatrix} A V_m. \end{aligned} \tag{47}$$

Substituting (19) into (47) followed by some simple algebra yields

$$\begin{aligned} &V_m' \left(A' R_m^{GM} + R_m^{GM} A\right) V_m \\ &\quad = \begin{bmatrix} A_m' & E_m A_{m+1,m}' \end{bmatrix} \begin{bmatrix} A_m X_m^{GM} + X_m^{GM} A_m' + B_m B_m' \\ A_{m+1,m} E_m' X_m^{GM} \end{bmatrix} \\ &\qquad + \begin{bmatrix} A_m X_m^{GM} + X_m^{GM} A_m' + B_m B_m' & X_m^{GM} E_m A_{m+1,m}' \end{bmatrix} \begin{bmatrix} A_m \\ A_{m+1,m} E_m' \end{bmatrix}. \end{aligned} \tag{48}$$

The right-hand side of (48) is the *mp*-dimensional linear matrix equation given in (36). The result follows immediately. □

This corollary shows that an equivalent way of posing the GMRES problem is to determine an approximate solution $P_m := V_m X_m V_m'$ that meets the Galerkin type condition $V_m'(A' R_m(X_m) + R_m(X_m) A) V_m = 0$. The complete GMRES–Lyapunov algorithm is summarised in the following procedure.

GMRES–Lyapunov solver.

- Start: Specify a tolerance $\epsilon > 0$, set an integer parameter m_1, and, set $k = 0$ and $m := m_1$.
- The Arnoldi process:
  1. Compute $B = Q_1 R_1$ (QR factorisation).
  2. Do $j = k+1, k+2, \ldots, k+m_1$.
     (a) Set $V_j = [Q_1 \; Q_2 \cdots Q_j]$.
     (b) Compute $\begin{bmatrix} A_{1j} \\ A_{2j} \\ \vdots \\ A_{jj} \end{bmatrix} = V_j' A Q_j$.

(c) $Q_{j+1}A_{j+1,j} = AQ_j - \sum_{k=1}^{j} Q_k A_{kj}$ (QR factorisation).

End Do.

- Find the symmetric X_m^{GM} which uniquely satisfies $A'_m(A_m X_m^{GM} + X_m^{GM} A'_m + B_m B'_m) + (A_m X_m^{GM} + X_m^{GM} A'_m + B_m B'_m)A_m + E_m \times A'_{m+1,m} A_{m+1,m} E'_m X_m^{GM} + Xm^{GM} E_m A'_{m+1,m} A_{m+1,m} E'_m = 0$.
- Compute $\left\|R_m^{GM}\right\|_F := \sqrt{\mathrm{tr}(B'_m(A_m X_m^{GM} + X_m^{GM} A'_m + B_m B'_m)B_m)}$.
- Stopping test: If $\left\|R_m^{GM}\right\|_F > \epsilon$, set $k := k + m_1$, $m := k + m_1$ and go to step 2 of the Arnoldi process.
- Form the approximate solution: $P_m := V_m X_m^{GM} V'_m$.

Suppose that m steps of the Arnoldi process are taken, then under certain conditions, the right-hand side of step (c) may be zero. In such a situation, Q_{m+1} cannot be calculated and consequently, the algorithm terminates prematurely, yielding

$$AV_m = V_m A_m. \tag{49}$$

This type of breakdown is referred to as *happy breakdown* [27] and takes place when the span of V_m is invariant with respect to A. The exact solution may thus be computed.

COROLLARY 2.5. *In the event of* happy breakdown *after m steps of the Arnoldi process, Arnoldi and* GMRES *yield the same solution, namely, the exact solution* P^*.

Proof. Substituting (49) into (21) gives $R_m(X_m) = V_m(A_m X_m + X_m A'_m + B_m B'_m)V'_m$. In the case of Arnoldi, $V'_m R_m(X_m) V_m = 0 \Leftrightarrow A_m X_m^A + X_m^A A'_m + B_m B'_m = 0$, while in the case of GMRES, it is clear that $\min \|R_m(X_m)\|_F = 0$ from which it follows that $A_m X_m^{GM} + X_m^{GM} A'_m + B_m B'_m = 0$. Arnoldi and GMRES have a solution residue $R_m^A = R_m^{GM} = 0$, and exact solutions $P^* = P_m = V_m X_m^A V'_m = V_m X_m^{GM} V'_m$. □

If, on the other hand, the right-hand side of step (c) is "small," it becomes difficult to construct Q_{m+1}, which is orthogonal to V_m. Wilkinson [32] recommends reorthogonalising the newly computed Q_{m+1} which, although expensive, yields a $[V_m\ Q_{m+1}]$ orthogonal to within working precision.

The following corollary gives theoretical bounds on the quality of the approximate solution for Arnoldi and GMRES, which are specialisations of those in [13].

COROLLARY 2.6. *Suppose that m steps of the Arnoldi process are taken and that* $\lambda_{\max}(A + A') < 0$; *then*

$$\frac{\sqrt{2}|\eta|}{\sqrt{N}\|A\|_F\|B\|_F^2}\left\|A_{m+1,m}E'_m X_m^A\right\|_F \le \frac{\|P^* - P_m\|_F}{\|P^*\|_F} \le \frac{\sqrt{2N}\|A\|_F}{|\eta|\|B\|_F^2}\left\|A_{m+1,m}E'_m X_m^A\right\|_F$$

for the Arnoldi, and

$$\frac{|\eta|}{\sqrt{N}\|A\|_F\|B\|_F^2}\sqrt{\mathrm{tr}(B'_m(A_m X_m^{GM} + X_m^{GM} A'_m + B_m B'_m)B_m)} \le \frac{\|P^* - P_m\|_F}{\|P^*\|_F}, \tag{50}$$

$$\frac{\|P^* - P_m\|_F}{\|P^*\|_F} \le \frac{\sqrt{N}\|A\|_F}{|\eta|\|B\|_F^2}\sqrt{\mathrm{tr}(B'_m(A_m X_m^{GM} + X_m^{GM} A'_m + B_m B'_m)B_m)} \tag{51}$$

for GMRES, *where* $|\eta| = -\lambda_{\max}(A + A')/2$ *is the logarithmic norm of* A [12].

In this section, we have presented two methods for computing low-rank approximate solutions to large-scale Lyapunov equations. The first method computes an approximate solution $P_m := V_m X_m V'_m$ such that $V'_m R(X_m) V_m = 0$, while the second minimises $\|R_m(X_m)\|_F$. Finally, simple expressions for the residual error norm are

derived in each case. In the above discussion we have not alluded to any practical way of solving (36). This is the object of the next section, where we will consider a solution technique for the mp-dimensional linear matrix equation arising from the GMRES method.

3. The GMRES linear matrix equation. In this section we present an algorithm for the solution of the linear matrix equation given in (36). Since A_m is block upper-Hessenberg and $B_m B_m'$ is banded and symmetric, we will show how to exploit this rich structure to facilitate the calculation of X_m.

In an early paper, Howland and Senez [17] gave a simplified solution to the Lyapunov matrix equation

$$AX + XA' + D = 0, \tag{52}$$

in which A is lower-Hessenberg and D is diagonal. In this development, we extend and adapt their method to solve the linear matrix equation of (36) arising from the GMRES problem. Throughout this section, we will set $A := A_m$, $D := B_m B_m'$. E is the matrix of the last p columns of the mp-identity matrix and $A_{m+1,m}$ remains as defined in §3. Finally, we will assume for the purposes of brevity that curable breakdown has not taken place during the first m iterations. In this simplified notation, (36) may be rewritten as

$$\begin{aligned} &A'(AX + XA' + D) + (AX + XA' + D)A + EA_{m+1,m}'A_{m+1,m}E'X \\ &\quad + XEA_{m+1,m}'A_{m+1,m}E' = 0. \end{aligned} \tag{53}$$

In this section, the solution to (53) is derived as a linear combination $X := \sum_{i=1}^{n} \rho_i X_i$ for $n := \sum_{i=1}^{p}(mp + 1 - i)$ linearly independent, symmetric matrices X_i where each X_i is constructed to satisfy $AX_i + X_iA' + D_i = M_i$ for some banded symmetric D_i, and symmetric M_i. Finally, the ρ_i's are obtained by solving the nonsingular linear system $\sum_{i=1}^{n} \rho_i D_i = D$. We start with the following definitions and preliminary results needed to establish the main result of this subsection.

DEFINITION 3.1. A matrix X_i and a banded, symmetric matrix D_i of bandwidth $p-1$ [12] are called a GMRES pair with respect to A if they satisfy the linear matrix equation

$$\begin{aligned} &A'(AX_i + X_iA' + D_i) + (AX_i + X_iA' + D_i)A + EA_{m+1,m}'A_{m+1,m}E'X_i \\ &\quad X_iEA_{m+1,m}'A_{m+1,m}E' = 0. \end{aligned} \tag{54}$$

LEMMA 3.1. *If $\lambda_i(A)+\bar{\lambda}_j(A) \neq 0$ for all i, j then* (53) *admits a unique symmetric solution, $X = 0$ if and only if $D = 0$.*

Proof. If $D = 0$, then (53) becomes

$$A'(AX+XA') + (AX+XA')A + EA_{m+1,m}'A_{m+1,m}E'X + XEA_{m+1,m}'A_{m+1,m}E' = 0. \tag{55}$$

The vec form of (55) is given by

$$\begin{aligned} 0 &= \{(I \otimes A'A) + (A \otimes A') + (A' \otimes A) + (A'A \otimes I)\}\,\mathrm{vec}(X) \\ &\quad + \{(I \otimes EA_{m+1,m}'A_{m+1,m}E') + (EA_{m+1,m}'A_{m+1,m}E' \otimes I)\}\,\mathrm{vec}(X) \\ &= [(I\otimes A+A\otimes I)'\ (A_{m+1,m}E'\otimes I)'\ (I\otimes A_{m+1,m}E')'] \begin{bmatrix} I\otimes A+A\otimes I \\ A_{m+1,m}E'\otimes I \\ I\otimes A_{m+1,m}E' \end{bmatrix} \mathrm{vec}(X), \end{aligned} \tag{56}$$

using the identities given in (33) and (34). It is well known that if $\lambda_i(A) + \bar{\lambda}_j(A) \neq 0$ for all i, j, then $(I \otimes A + A \otimes I)$ is nonsingular [10]; consequently, the solution to (56) is $\mathrm{vec}(X) = 0$ and therefore, the only solution to (55) is $X = 0$. Conversely, if $X = 0$, then (53) becomes $A'D + DA = 0$, which can only be true if $D = 0$ since $\lambda_i(A) + \bar{\lambda}_j(A) \neq 0$ for all i, j. □

Consider n GMRES pairs $(X_1, D_1), (X_2, D_2), \ldots, (X_n, D_n)$ with respect to A, then for any constants $\rho_1, \rho_2, \ldots, \rho_n$, $(\sum_{i=1}^n \rho_i X_i, \sum_{i=1}^n \rho_i D_i)$ is also a GMRES pair with respect to A; therefore,

$$
\begin{aligned}
&A'\left(A\left(\sum_{i=1}^n \rho_i X_i\right) + \left(\sum_{i=1}^n \rho_i X_i\right) A' + \left(\sum_{i=1}^n \rho_i D_i\right)\right) \\
&\quad + EA'_{m+1,m} A_{m+1,m} E' \left(\sum_{i=1}^n \rho_i X_i\right) \\
&\quad + \left(A\left(\sum_{i=1}^n \rho_i X_i\right) + \left(\sum_{i=1}^n \rho_i X_i\right) A' + \left(\sum_{i=1}^n \rho_i D_i\right)\right) A \\
&\quad + \left(\sum_{i=1}^n \rho_i X_i\right) EA'_{m+1,m} A_{m+1,m} E' = 0.
\end{aligned} \tag{57}
$$

Subtracting (57) from (53) gives

$$
\begin{aligned}
&A'\left(A\left(X - \sum_{i=1}^n \rho_i X_i\right) + \left(X - \sum_{i=1}^n \rho_i X_i\right) A' + \left(D - \sum_{i=1}^n \rho_i D_i\right)\right) \\
&\quad + \left(A\left(X - \sum_{i=1}^n \rho_i X_i\right) + \left(X - \sum_{i=1}^n \rho_i X_i\right) A' + \left(D - \sum_{i=1}^n \rho_i D_i\right)\right) A \\
&\quad + EA'_{m+1,m} A_{m+1,m} E' \left(X - \sum_{i=1}^n \rho_i X_i\right) \\
&\quad + \left(X - \sum_{i=1}^n \rho_i X_i\right) EA'_{m+1,m} A_{m+1,m} E' = 0.
\end{aligned} \tag{58}
$$

Lemma 3.1 states that $X = \sum_{i=1}^n \rho_i X_i$ if and only if $D = \sum_{i=1}^n \rho_i D_i$. The solution to (53) will be taken to have the form $X = \sum_{i=1}^n \rho_i X_i$, for which we will give constructions for D_i, X_i, and ρ_i such that

$$
D = \sum_{i=1}^n \rho_i D_i. \tag{59}
$$

Matrices D and D_i each have a bandwidth of $p - 1$, therefore, (59) has a unique solution if and only if (a) $n := \sum_{i=1}^p (mp + 1 - i)$ and (b) $D_1, D_2, \ldots, D_n$ are linearly independent.

The construction of X relies on selecting the last p columns (rows) of n X_i's in such a way that they are linearly independent. The following lemma shows that if the n X_i's are linearly independent, then so too are the D_i's.

LEMMA 3.2. *If $\lambda_i(A) + \bar{\lambda}_j(A) \neq 0$ for all i, j, then,if $X_1, X_2, \ldots, X_n$ and $D_1, D_2, \ldots, D_n$ are GMRES pairs, with respect to A, then when $X_1, X_2, \ldots, X_n$ are linearly independent so are $D_1, D_2, \ldots, D_n$.*

Proof. Suppose that $D_1, D_2, \ldots, D_n$ are linearly dependent, so that, for some constants $\alpha_1, \alpha_2, \ldots, \alpha_n$, not all zero, $\sum_{i=1}^{n} \alpha_i D_i = 0$, then substituting into (53) gives

$$
\begin{aligned}
&A'\left(A\left(\sum_{i=1}^{n}\alpha_i X_i\right) + \left(\sum_{i=1}^{n}\alpha_i X_i\right)A' + \left(\sum_{i=1}^{n}\alpha_i D_i\right)\right) \\
&+ EA'_{m+1,m}A_{m+1,m}E'\left(\sum_{i=1}^{n}\alpha_i X_i\right) \\
&+ \left(A\left(\sum_{i=1}^{n}\alpha_i X_i\right) + \left(\sum_{i=1}^{n}\alpha_i X_i\right)A' + \left(\sum_{i=1}^{n}\alpha_i D_i\right)\right)A \\
&+ \left(\sum_{i=1}^{n}\alpha_i X_i\right)EA'_{m+1,m}A_{m+1,m}E' = 0,
\end{aligned} \tag{60}
$$

which is uniquely satisfied by $\sum_{i=1}^{n} \alpha_i X_i = 0$ following Lemma 3.1, hence $X_1, X_2, \ldots, X_n$ are linearly dependent. Since these are assumed linearly independent, the result follows by contradiction. □

Lemma 3.2 shows that since the X_i's are linearly independent by construction, so too are the D_i's; consequently, (59) is a nonsingular system and the ρ_i's may be uniquely determined. All that remains is to construct the unknown elements of X_i and D_i, which are given in the following result.

THEOREM 3.3. *Assume that* $\lambda_i(A) + \bar{\lambda}_j(A) \neq 0$ *for all* i, j; *then there exists at least* n *linearly independent* GMRES *pairs* $(X_1, D_1), \ldots, (X_n, D_n)$ *with respect to* A *where* $n := \sum_{i=1}^{p}(mp + 1 - i)$.

Proof. Consider $X_1, X_2, \ldots, X_n$ symmetric matrices whose last p columns (rows) have been selected as follows. Firstly, the n X_j's have their last p columns (rows) set to zero; then the first mp X_j's each have their last column (row) set, respectively, to the columns (rows) of the mp identity matrix; the next $(mp-1)$ X_j's have their $(mp-1)$th column (row) set, respectively, to the columns (rows) of the $(mp-1)$ identity matrix, etc. It is clear that this selection of the last p columns (rows) of X_j leads to n linearly independent X_j's since each of their last $mp \times p$, $(p \times mp)$ blocks are linearly independent. The key observation is that fixing the last p columns (rows) of X_j fully determines the last two terms of (54) since $E'X_j$, (X_jE) is the last p rows (columns) of X_j. Defining $Q_j := EA'_{m+1,m}A_{m+1,m}E'X_j + X_jEA'_{m+1,m}A_{m+1,m}E'$ and substituting into (54) yields

$$A'M_j + M_jA + Q_j = 0, \tag{61}$$

in which $M_j := AX_j + X_jA' + D_j$; furthermore, (61) admits a unique solution M_j. Substituting M_j into its definition gives

$$AX_j + X_jA' + D_j = M_j, \tag{62}$$

from which it follows that X_j satisfies (54) if it satisfies (62). We determine the remaining elements of X_j by considering the skew symmetric T_j and banded symmetric D_j matrices defined by

$$AX_j - \tfrac{1}{2}M_j = T_j - \tfrac{1}{2}D_j, \tag{63}$$

it is clear that if the GMRES pair (X_j, D_j) satisfies (63), then it satisfies (62). It will be shown by induction that the remaining unknown elements of X_j and the elements of D_j and T_j may be derived uniquely by (63). When this is the case, the X_j's are clearly independent. So by Lemma 3.2, the D_j are also independent. Block partitioning (63) gives

$$
\begin{array}{c} \\ \text{(m-k-1)p} \\ \text{p} \\ \text{p} \\ \text{(k-1)p} \end{array}
\begin{array}{c}
\begin{array}{cccc} \text{(m-k-1)p} & \text{p} & \text{p} & \text{(k-1)p} \end{array} \\
\begin{bmatrix} A_{11} & A_{12} & A_{13} & A_{14} \\ A_{21} & A_{22} & A_{23} & A_{24} \\ 0 & A_{32} & A_{33} & A_{34} \\ 0 & 0 & A_{43} & A_{44} \end{bmatrix}
\end{array}
\begin{bmatrix} X_{11} & X_{12} & X_{13} & X_{14} \\ X'_{12} & X_{22} & X_{23} & X_{24} \\ X'_{13} & X'_{23} & X_{33} & X_{34} \\ X'_{14} & X'_{24} & X'_{34} & X_{44} \end{bmatrix}
$$

$$
-\frac{1}{2}\begin{bmatrix} M_{11} & M_{12} & M_{13} & M_{14} \\ M'_{12} & M_{22} & M_{23} & M_{24} \\ M'_{13} & M'_{23} & M_{33} & M_{34} \\ M'_{14} & M'_{24} & M'_{34} & M_{44} \end{bmatrix} = \begin{bmatrix} T_{11} & T_{12} & T_{13} & T_{14} \\ -T'_{12} & T_{22} & T_{23} & T_{24} \\ -T'_{13} & -T'_{23} & T_{33} & T_{34} \\ -T'_{14} & -T'_{24} & -T'_{34} & T_{44} \end{bmatrix}
$$

$$
-\frac{1}{2}\begin{bmatrix} D_{11} & D_{12} & 0 & 0 \\ D'_{12} & D_{22} & D_{23} & 0 \\ 0 & D'_{23} & D_{33} & D_{34} \\ 0 & 0 & D'_{34} & D_{44} \end{bmatrix}. \tag{64}
$$

Suppose that the last kp columns (rows) of X_j and the last $(k-1)p$ columns (rows) of T_j and D_j are given. The following development shows that this is sufficient to determine the remaining elements of X_j, T_j, and D_j. The blocks X_{12} and X_{22} may be derived from the following blocks of (64):

$$(65)\quad (1,3),\qquad T_{13} = A_{11}X_{13} + A_{12}X_{23} + A_{13}X_{33} + A_{14}X'_{34} - \tfrac{1}{2}M_{13},$$

$$(66)\quad (3,1),\qquad X_{12} = -(X_{13}A'_{33} + X_{14}A'_{34} + T_{13} - \tfrac{1}{2}M_{13})(A'_{32})^{-1},$$

$$(67)\quad (2,3),\qquad T_{23} - \tfrac{1}{2}D_{23} = A_{21}X_{13} + A_{22}X_{23} + A_{23}X_{33} + A_{24}X'_{34} - \tfrac{1}{2}M_{23},$$

$$(68)\quad (3,2),\qquad -T'_{23} - \tfrac{1}{2}D'_{23} = A_{32}X_{22} + A_{33}X'_{23} + A_{34}X'_{24} - \tfrac{1}{2}M'_{23}.$$

Adding (67) to the transpose of (68) gives

$$
\begin{aligned} X_{22} = {} & (M_{23} - X_{23}A'_{33} - X_{24}A'_{34} - A_{21}X_{13} - A_{22}X_{23} - A_{23}X_{33} - A_{24}X'_{34})(A'_{32})^{-1} \\ & - D_{23}(A'_{32})^{-1}. \end{aligned} \tag{69}
$$

Since curable breakdown has not occurred during the first m iterations, $Q_{j+1}A_{j+1,j} = AQ_j - \sum_{k=1}^{j} Q_k A_{kj}$ (step (c) of the Arnoldi process) has full column rank. Hence each subdiagonal block of (18) is nonsingular by the construction in the Arnoldi process; consequently, A_{32} is nonsingular. The only unknown in the right-hand side of (69) is D_{23}. Observe that D_j is banded; therefore, D_{23} is strictly lower-triangular, and since A'_{32} is lower-triangular, $D_{23}(A'_{32})^{-1}$ is strictly lower-triangular. The upper-triangular part of $-(X_{23}A'_{33} + X_{24}A'_{34} + A_{21}X_{13} + A_{22}X_{23} + A_{23}X_{33} + A_{24}X'_{34} - M_{23})(A'_{32})^{-1}$ therefore determines the upper-triangular part of X_{22} and by the required symmetry of X_j the lower-triangular part of X_{22}. Substituting X_{22} into (69) yields D_{23}; T_{23} is then evaluated from (67). T_{33} and D_{33} are derived from

$$(70)\qquad (3,3)\quad T_{33} - \tfrac{1}{2}D_{33} = A_{32}X_{23} + A_{33}X_{33} + A_{34}X'_{34} - \tfrac{1}{2}M_{33},$$

adding (70) to its transpose. Using the facts that T_j is skew symmetric and D_j and M_j are symmetric gives

$$(71)\quad D_{33} = -\left(A_{32}X_{23} + A_{33}X_{33} + A_{34}X'_{34} + X'_{23}A'_{32} + X_{33}A'_{33} + X_{34}A'_{34} - M_{33}\right).$$

Back-substituting into (70) finally yields T_{33}. It follows by induction that fixing the last p columns (rows) of X_j uniquely determines the remaining elements of X_j and the elements of D_j and T_j. An important observation is that none of the calculations changes the last p columns (rows) of X_j so that n repetitions with n linearly independent X_j will generate n independent GMRES pairs (X_j, D_j) by Lemma 3.2, thereby completing the proof. □

The solution to the linear matrix equation given in (53) may now be written as a linear combination of n linearly independent GMRES pairs (X_j, D_j) obtained by the construction of Theorem 3.3. The constants $\rho_1, \rho_2, \ldots, \rho_n$ are obtained by solving the nonsingular system (59) and hence $X = \sum_{i=1}^{n} \rho_i X_i$ is the required solution.

Remark 3.1. Suppose that d_i^j and d_j are vectors of the jth super-diagonal elements of D_i and D, respectively, for $i = 1, \ldots, n$, and $j = 0, \ldots, p-1$. Then (59) may be written as $Lx = b$, in which

(72)
$$L = \begin{bmatrix} d_1^0 & d_2^0 & \cdots & d_n^0 \\ d_1^1 & d_2^1 & \cdots & d_n^2 \\ \vdots & \vdots & \vdots & \vdots \\ d_1^{p-1} & d_2^{p-1} & \cdots & d_n^{p-1} \end{bmatrix} \in \mathcal{R}^{n\times n},\ x = \begin{bmatrix} \rho_1 \\ \rho_2 \\ \vdots \\ \rho_n \end{bmatrix} \in \mathcal{R}^n,\ \text{and } b = \begin{bmatrix} d_1 \\ d_2 \\ \vdots \\ d_n \end{bmatrix} \in \mathcal{R}^n.$$

This linear system has a unique solution since the D_i's are linearly independent (by Lemma 3.2).

The following procedure summarises the block solution of the GMRES linear matrix equation (53).

Block GMRES linear equation solver.

- Initialise by constructing n linearly independent matrices which are obtained by forming the last p columns (rows) of X_j.
- Do $j = 1$ to n.
  1. Form $Q_j := E_m A'_{m+1,m} A_{m+1,m} E'_m X_j + X_j E_m A'_{m+1,m} A_{m+1,m} E'_m$ and solve the Lyapunov equation $A'M_j + M_j A + Q_j = 0$ for the unknown M_j.
  2. Do $k = 1$ to $m-1$
     - Partition X_j, A, and M_j as in (64) where the first $(m-k)p \times (m-k)p$ block of X and the first $(m-k+1)p \times (m-k+1)p$ blocks of T_j and D_j are unknown.
     - Compute X_{12} from (64).
     - Compute the upper triangular part of X_{22} and symmetrise.
     - Compute T_{13}, T_{23}, and T_{33}, and, D_{23} and D_{33}.
     - End Do (k).
  3. End Do (j).
- Using Remark 3.1, solve the linear system $\sum_{i=1}^{n} \rho_i D_i = D$ to determine ρ_i.
- Form the solution; $X := \sum_{i=1}^{n} \rho_i X_i$.

The residual error norm for the GMRES problem is given by

$$\|R(X_m^{GM})\|_F = \sqrt{\mathrm{tr}(B'_m(A_m X_m^{GM} + X_m^{GM} A'_m + B_m B'_m)B_m)}. \tag{73}$$

Evaluating equation (73) may be efficiently implemented without forming X_m^{GM} since $\sum_{i=1}^{n} \rho_i M_i = A_m X_m^{GM} + X_m^{GM} A'_m + B_m B'_m$. In such an implementation, the D_j's

may be stored as vectors while only the upper-triangular part of the M_j's need be stored. It must be pointed out that we require only that the starting matrices be linearly independent and consequently, other starting matrices for X_j may be used to compute the whole solution. In practice, the selection of these independent matrices appears to affect the quality of the computed X_m^{GM}. We have as yet not investigated the conditioning of the linear system in (59).

Remark 3.2. Although n low-dimensional Lyapunov equations are solved in step 1, the transformation of A to Schur form need only be carried out once.

In this section we have presented an algorithm for solving the linear matrix equation arising from the GMRES method. This solver exhibits features that may be exploited on parallel processors, this, together with update schemes, are topics of our ongoing research. The conditioning of the linear system of equations in (59) is not well understood and work continues on numerically enhancing this algorithm.

4. Extensions to other matrix equations. In this section we will show how the Krylov subspace techniques considered above can be applied to two other large matrix equation problems. The first is the approximate solution of large discrete-time Lyapunov equations which arise in the model reduction of large models described by first-order difference equations [10]. The second type of problem we address in this section is the approximate solution to large continuous time algebraic Riccati equations. Equations of this type arise in $\mathcal{H}^\infty$, classical linear optimal control and filtering theories, and spectral factorisation problems [11], [19]. As these extensions are relatively straightforward, we will state the results without giving any proofs.

4.1. The discrete-time Lyapunov equation. Consider the discrete-time Lyapunov equation

$$APA' - P + BB' = 0 \tag{74}$$

in which A, $P \in \mathcal{R}^{N\times N}$, $B \in \mathcal{R}^{N\times p}$, and, N is large and $p \ll N$. The Arnoldi process then generates an orthogonal basis V_m for the Krylov space given in (12), and the residual error for any approximate low-rank solution of the form $P_m = V_m X_m V_m'$ is given by

$$R_m(X_m) := A(V_m X_m V_m')A' - (V_m X_m V_m') + BB'. \tag{75}$$

Substituting (19) into (75) gives

(76)
$$R_m(X_m) = V_{m+1}\begin{bmatrix} A_m X_m A_m' - X_m + B_m B_m' & A_m X_m E_m A_{m+1,m}' \\ A_{m+1,m}E_m' X_m A_m' & A_{m+1,m}E_m' X_m E_m A_{m+1,m}' \end{bmatrix} V_{m+1}'$$

since $V_m B_m = B$. We then seek a solution $P_m := V_m X_m V_m'$ by imposing the condition that $R_m(X_m)$ has an orthogonality property with respect to K_m.

PROBLEM 4.1. Find an approximate solution $P_m := V_m X_m V_m'$ that satisfies the Galerkin type condition $V_m' R_m(X_m) V_m = 0$.

THEOREM 4.1. *Suppose that m steps of the Arnoldi process have been taken and that the residual error is given by* (76); *then if* $|\lambda_i(A_m)(\lambda_j(A_m))^{-1}| \neq 1$ *for all* i, j,

(a) $V_m' R_m(X_m) V_m = 0$ *if and only if* $X_m = X_m^A$, *where* X_m^A *satisfies*

$$A_m X_m^A A_m' - X_m^A + B_m B_m' = 0. \tag{77}$$

(b) *If the conditions of* (a) *are met, then the residual error norm is given by*

$$\|R_m^A\|_F := \|R_m(X_m^A)\|_F = \|A_{m+1,m}E'_m X_m^A \begin{bmatrix} \sqrt{2}A'_m & E_m A'_{m+1,m} \end{bmatrix}\|_F. \tag{78}$$

Proof. The proof is essentially the same as that of Theorem 2.1 except that it uses (76). □

Next, we address the problem of computing a symmetric, an approximate solution to (74) which minimises the residual error norm.

PROBLEM 4.2. Find a symmetric $X_m \in \mathcal{R}^{m\times m}$ that minimises the residual error norm, namely,

$$\|R_m^{GM}\|_F := \min \left\| V_{m+1} \begin{bmatrix} A_m X_m A'_m - X_m + B_m B'_m & A_m X_m E_m A'_{m+1,m} \\ A_{m+1,m}E'_m X_m A'_m & A_{m+1,m}E'_m X_m E_m A'_{m+1,m} \end{bmatrix} V'_{m+1} \right\|_F.$$

THEOREM 4.2. *Suppose that m steps of the Arnoldi process have been taken and that the residual error is given by* (76), *then if* $|\lambda_i(A_m)(\lambda_j(A_m))^{-1}| \neq 1$, *for all* i, j,

$$\|R_m^{GM}\|_F = \sqrt{\operatorname{tr}(B'_m(A_m X_m^{GM} A'_m - X_m^{GM} + B_m B'_m)B_m)}, \tag{79}$$

where X_m^{GM} *satisfies the mp-dimensional linear matrix equation*

$$\begin{aligned} &A'_m(A_m X_m^{GM} A'_m - X_m^{GM} + B_m B'_m)A_m - (A_m X_m^{GM} A'_m - X_m^{GM} + B_m B'_m) \\ &+ E_m A'_{m+1,m} A_{m+1,m} E'_m X_m^{GM} A'_m A_m + A'_m A_m X_m^{GM} E_m A'_{m+1,m} A_{m+1,m} E'_m \\ &+ E_m A'_{m+1,m} A_{m+1,m} E'_m X_m^{GM} E_m A'_{m+1,m} A_{m+1,m} E'_m = 0. \end{aligned} \tag{80}$$

Proof. The proof is essentially the same as that of Theorem 2.2 except that it uses (76). □

The following procedure summarises the solution of large discrete Lyapunov equations.

Arnoldi (GMRES)-Discrete Lyapunov solver.

- Calculate V_m, Q_{m+1}, A_m, $A_{m+1,m}$, and B_m via the Arnoldi process.
- **Arnoldi:** Find X_m^A which satisfies $A_m X_m^A A'_m - X_m^A + B_m B'_m = 0$. Compute the residual error norm $\|R_m^A\|_F := \|A_{m+1,m}E'_m X_m^A \begin{bmatrix} \sqrt{2}A'_m & E_m A'_{m+1,m} \end{bmatrix}\|_F$ and form the approximate solution: $P_m := V_m X_m^A V'_m$.
- **GMRES:** Find X_m^{GM}, which satisfies (80). Compute $\|R_m^{GM}\|_F := \sqrt{\operatorname{tr}(B'_m(A_m X_m^{GM} A'_m - X_m^{GM} + B_m B'_m)B_m)}$ and form the approximate solution: $P_m := V_m X_m^{GM} V'_m$.

The solution to the linear matrix equation in (80) may be computed using a variant of the construction presented in §3.

4.2. The algebraic Riccati equation. Consider the continuous-time algebraic Riccati equation

$$AP + PA' - PC'CP + BB' = 0 \tag{81}$$

in which A, $P \in \mathcal{R}^{N\times N}$, $B \in \mathcal{R}^{N\times p}$, $C \in \mathcal{R}^{q\times N}$. The method of solution we will consider makes use of the following $2N \times 2N$ Hamiltonian matrix that is associated

with (81),

$$\mathcal{H} = \begin{bmatrix} A' & -C'C \\ -BB' & -A \end{bmatrix}. \tag{82}$$

The matrix $\mathcal{H}$ in (82) has a number of important properties.

1. The Hamiltonian matrix $\mathcal{H}$ has no imaginary axis eigenvalues if and only if $[j\omega I - A' \; B_m]$ and $[(j\omega I - A')' \; C_m']'$ have full row and column rank, respectively, for all $\omega \in \mathcal{R}$.

2. Suppose that W transforms $\mathcal{H}$ into a Jordan form; $W^{-1}\mathcal{H}W = J$, where $W = [w_1, w_2, \ldots, w_{2N}]$ are the eigenvectors of $\mathcal{H}$. Then each solution to the Riccati equation in (81) may be expressed as $P := W_{21}W_{11}^{-1}$, where W_{11} is assumed nonsingular and $[W_{11}' \; W_{21}']' \in \mathcal{R}^{2N\times N}$ is a matrix of N eigenvectors of $\mathcal{H}$ partitioned such that $W_{11}, \; W_{21} \in \mathcal{R}^{N\times N}$.

For further details, we refer the reader to [19] and the references therein.

Consider the Riccati equation in (81) where N is large and $p, \; q \ll N$. The Arnoldi process then generates an orthogonal basis V_m for the Krylov space $K_m := \text{span}\{[B \; AB \; A^2B \cdots A^{m-1}B]\}$. The residual error for any approximate solution of the form $P_m = V_m X_m V_m'$ is then given by

$$R_m(X_m) := A(V_m X_m V_m') + (V_m X_m V_m')A' - (V_m X_m V_m')C'C(V_m X_m V_m') + BB' = 0. \tag{83}$$

Substituting (19) into (83) gives

$$R_m(X_m) = V_{m+1}\begin{bmatrix} A_m X_m + X_m A_m' - X_m C_m' C_m X_m + B_m B_m' & X_m E_m A_{m+1,m}' \\ A_{m+1,m}E_m' X_m & 0 \end{bmatrix} V_{m+1}', \tag{84}$$

where $C_m := CV_m$ and $V_m B_m = B$. We seek a solution $P_m = V_m X_m V_m'$ in which V_m is an orthogonal basis of the Krylov space by imposing an orthogonality condition on K_m We can state the approximation problem as the following.

PROBLEM 4.3. Find an approximate solution $P_m := V_m X_m V_m'$ that satisfies the Galerkin type condition $V_m' R_m(X_m) V_m = 0$.

THEOREM 4.3. *Suppose that m steps of the Arnoldi process have been taken and that the residual error is given by* (84). *Then provided that* $[j\omega I - A_m' \; B_m]$ *and* $[(j\omega I - A_m')' \; C_m']'$ *have full row and column rank, respectively, for all* $\omega \in \mathcal{R}$,

(a) $V_m' R_m(X_m) V_m = 0$ *if and only if* $X_m = X_m^A$, *where* X_m^A *satisfies*

$$A_m X_m^A + X_m^A A_m' - X_m^A C_m' C_m X_m^A + B_m B_m' = 0; \tag{85}$$

(b) *If the conditions of* (a) *are met, then the residual error norm is given by*

$$\|R_m^A\|_F := \|R_m(X_m^A)\|_F = \sqrt{2}\|A_{m+1,m}E_m' X_m^A\|_F. \tag{86}$$

Proof. The proof is essentially the same as that of Theorem 2.1 except that it uses (84). □

The following procedure summarises the solution of large algebraic Riccati equations.

Arnoldi-Continuous-Riccati solver.

- Calculate V_m, Q_{m+1}, A_m, $A_{m+1,m}$, and B_m via the Arnoldi process.
- Then find X_m^A which satisfies the low-dimensional algebraic Riccati equation $A_m X_m^A + X_m^A A_m' - X_m^A C_m' C_m X_m^A + B_m B_m' = 0$ (via the ordered Schur method [19]).
- Compute $\|R_m^A\|_F := \sqrt{2}\|A_{m+1,m} E_m' X_m^A\|_F$.
- Form the approximate solution: $P_m := V_m X_m^A V_m'$.

In control problems, typically, one is interested in computing a solution to the Riccati equation from either the stable or antistable basis for the eigenspace of the Hamiltonian matrix since it yields a symmetric and (semi) definite solution [19]. The discrete time Riccati equation may also be treated in a similar way to yield a residual error norm and a constraining linear matrix equation, the derivation of which we omit.

5. Numerical experiments. The purpose of this section is to illustrate with the help of two examples the behaviour of the residual error formulae presented in §3. The tests reported here were performed on a Sparc-10 Sun workstation using Pro-MATLAB running under Unix.

Example 1. In this example, we have chosen $A \in \mathcal{R}^{N\times N}$ and $B \in \mathcal{R}^{N\times p}$, where $N = 1000$ and $p = 4$. A is a diagonal matrix with its elements uniformly distributed in the interval [0 1] by taking $a_{jj} := (j+1)/(N+1)$. The B matrix has the form

$$B = \begin{bmatrix} J_1 & 0 & 0 & 0 \\ 0 & J_2 & 0 & 0 \\ 0 & 0 & J_3 & 0 \\ 0 & 0 & 0 & J_4 \end{bmatrix}, \tag{87}$$

which is defined as follows. Let J be a vector of ones in $\mathcal{R}^{\frac{N}{4}}$; then $J_1 = J/15$, $J_2 = J/150$, $J_3 = J/1500$, and $J_4 = J/15000$. Figure 1 shows the evolution of the residual error norm of the Arnoldi and GMRES methods for increasing rank of P_m. We make the following observations: the Arnoldi error is larger than that of GMRES as predicted and both exhibit nonincreasing profiles, although the theory predicts this behaviour only for GMRES.

Table 1 compares a few CPU run times for the Arnoldi and GMRES methods for increasing rank of P_m. The times reported in this table are in seconds. The larger CPU times needed for the GMRES method are attributed to the computationally intensive algorithm of §3. Step 1 of the block GMRES solver presented in §3 must be implemented as suggested in Remark 3.2. The following is a breakdown of the

TABLE 1
CPU *run times for the Arnoldi and* GMRES *methods.*

m	Arnoldi (secs)	GMRES (secs)
4	2.6923000e-02	3.7431300e-01
8	4.7045000e-02	1.6965540e+00
12	8.0165000e-02	4.9038100e+00
16	1.2784200e-01	1.1461245e+01
20	2.0119000e-01	2.2708456e+01
24	3.2316100e-01	3.6983727e+01
28	3.8514500e-01	6.1250413e+01
32	5.0988800e-01	9.3542215e+01

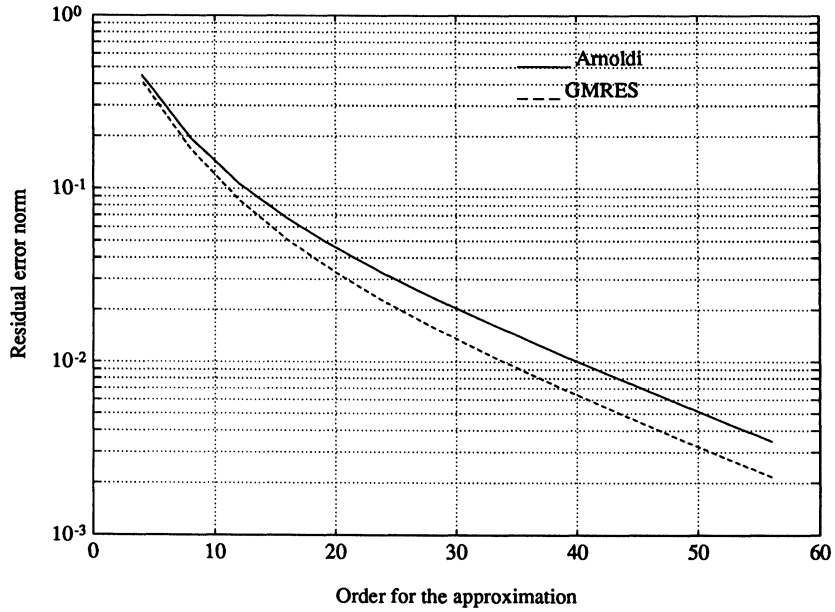

FIG. 1. *Evolution of* $\|R_m(X_m)\|_F$ *for Arnoldi and* GMRES *methods for increasing* mp.

work load in terms of floating point operations and memory requirements for each algorithm. The main difference in the two methods proposed is in the computation of a symmetric X_m; in the following, m is the iteration count; therefore, A_m, $X_m \in \mathcal{R}^{mp\times mp}$, and $n = mp^2 + \frac{p}{2} - \frac{p^2}{2}$ are defined in Theorem 3.3.

Bartels–Stewart [3] *Schur decomposition*: $10(mp)^3$. Solving linear systems: $0.5(mp)^3$. Obtaining the final solution: $2(mp)^3$. The total flop count is approximately $12.5(mp)^3$ with storage needs of approximately $2.5(mp)^2$, assuming that data are overwritten.

Block GMRES *Schur decomposition*: $10(mp)^3$. Solving linear systems: $0.5n(mp)^3$. Form the M_j's: $2n(mp)^3$. Evaluate X_{12}, X_{22}, T_{13}, D_{23}, and D_{33}: no less than $(m^4+\frac{m}{2}+1)(m-1)p^4n$. Solve the linear system (59): $2n^3$ and form the final solution: $2n(mp)^2$. The total flop count is approximately $2n^3+2n(mp)^2+n(2.5(mp)^3+(m^4+\frac{m}{2}+1)(m-1)p^4)+10(mp)^3$ with storage needs of $n(mp)^2+n^2$, assuming that the data are overwritten.

The flop count for GMRES is higher than for the Bartels–Stewart algorithm; however, the extra computations generally yield smaller residual errors. The two expensive steps in the GMRES algorithm are (i) the repeated solution of the Lyapunov equation in (61) for M_j; and (ii) the construction of the unknown elements in X_j and D_j. Finally, we observe that the GMRES algorithm consists of n independent constructions which are combined using (59) and $X = \sum_{i=1}^{n} \rho_i X_i$ to yield X_m^{GM}. This structure makes the algorithm suitable for parallel implementation. The large difference in CPU times between the Arnoldi based technique and the GMRES motivate the search for numerically efficient solvers for (36).

Example 2. In this example, we have chosen $A \in \mathcal{R}^{N\times N}$ and $B \in \mathcal{R}^{N\times p}$, where $N = 200$ and $p = 4$. A is a diagonal matrix with its first 100 elements uniformly

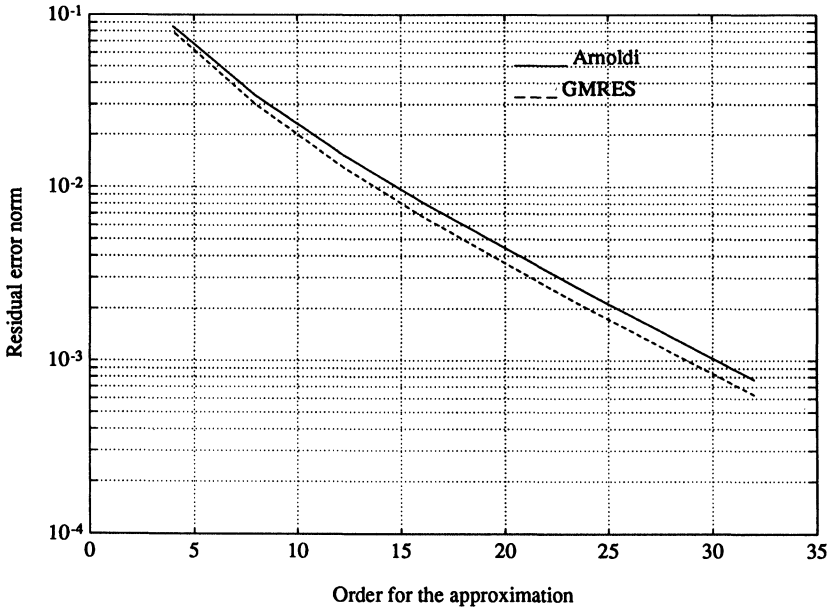

FIG. 2. *Evolution of* $\|R_m(X_m)\|_F$ *for Arnoldi and* GMRES *methods for increasing* mp.

distributed in the interval [0 1] by taking $a_{jj} := (j+1)/(0.5N+1)$, while the second 100 elements are distributed between [9 10] by taking $a_{jj} := 9 + (j+1)/(0.5N+1)$. The B matrix has the form given in (87) in which J is a vector of ones in $\mathcal{R}^{\frac{N}{4}}$ and J_1, J_2, J_3, and J_4 are as defined in Example 1. Figure 2 shows the evolution of the residual error norm of the Arnoldi and GMRES methods for increasing rank of P_m. We make the following observations: the Arnoldi error is larger than that of GMRES as predicted and both exhibit nonincreasing profiles although the theory predicts this behaviour only for GMRES. The main point of this example is to illustrate that there is no apparent degradation in the algorithms' performances when A is a nonnormal matrix.

6. Conclusions. In this paper we have presented and tested two numerical techniques for calculating low-rank approximate solutions to large Lyapunov matrix equations. We have given simple expressions for the residual error norms of the Arnoldi and GMRES that are useful as stopping criteria in any practical implementation. Of the two methods proposed, we regard GMRES as the superior in view of its minimum residue norm property; however, this is achieved at the expense of more calculation as reported in §5. We have proposed an algorithm for the solution of block GMRES linear matrix equations that exploit the block-Hessenberg structure of A_m. We have carried out some simple extensions that address the approximate solution of large discrete Lyapunov and algebraic Riccati equations. Throughout this paper, we have opted to use block schemes to retain generality. The results and algorithms presented here are in matrix form of which scalar (vector) instances are special cases.

Many questions remain unanswered and more effort is required in order to better understand the performance characteristics of these methods. Some open questions that we will continue to investigate are the following.

- Is X_m updatedable in a cheap way?
- Is there a simple connection between the Arnoldi and GMRES solutions as was found in [5]?
- What are the inertia properties of X_m^{GM}?
- What are good starting matrices for the GMRES linear equation solver?
- Is preconditioning possible?

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