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Retracing the residual curve of a Lyapunov equation solver

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Abstract Let $A \in \mathbb{R}^{n\times n}$ and let $B \in \mathbb{R}^{n\times p}$ and consider the Lyapunov matrix equation $AX + XA^T + BB^T = 0$. If $A + A^T < 0$, then the extended Krylov subspace method (EKSM) can be used to compute a sequence of low rank approximations of X. In this paper we show how to construct a symmetric negative definite matrix A and a column vector B, for which the EKSM generates a predetermined residual curve.

Keywords Lyapunov matrix equations · the extended Krylov subspace method

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1 Introduction, basic notation, and general assumptions

Let $A \in \mathbb{R}^n$ and let $B \in \mathbb{R}^{n\times p}$ and consider the Lyapunov matrix equation

$$AX + XA^T + BB^T = 0. \tag{1.1}$$

This equation is uniquely solvable if and only if

$$\lambda + \mu \neq 0 \tag{1.2}$$

for all eigenvalues λ and μ of A, and the solution X is symmetric. If A is stable, then the central condition (1.2) is satisfied. Moreover, the solution X is symmetric positive semidefinite, and the range of X is the smallest A-invariant subspace containing the range of B, i.e.

$$\operatorname{Ran} X = K(A,B) = \cup_{j=1}^{\infty} K_j(A,B),$$

where $K_j(A,B)$ is the standard Krylov subspace given by

$$K_j(A,B) = \operatorname{span}\{A^i B : i = 0,1,2,\ldots,j-1\}, \quad 1 \leq j.$$

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If A is a dense matrix then we can solve equation (1.1) using one of several dense methods [2,6,10,28]. They all require $O(n^3)$ arithmetic operations and $O(n^2)$ words of storage, but efficient parallel algorithms have been implemented [15,16,8,7].

In many applications A is stable, even negative definite, and B is a tall matrix with $p \ll n$ columns. Frequently, but not universally, the eigenvalues for X decay rapidly and X can be approximated accurately with a low rank matrix. This is the low rank phenomenon for Lyapunov matrix equations [23,1]. During the last 20 years a number of iterative methods have been developed in order to compute good low rank approximations to X directly [24,12,14,13,22,19,25,4,3,18]. Recently the extended Krylov subspace method (EKSM) has been applied to this problem [5,26,17]. It is possible to treat the Lyapunov matrix equation as a standard linear system using $O(n)$ rather than $O(n^2)$ resources [20]. However, it is necessary to use a very compact representation of vectors in $\mathbb{R}^{n^2}$ which does not permit preconditioning in the usual sense.

In Section 2 we give a very brief description of the extended Krylov subspace method for Lyapunov equations. In Section 3 we show how to construct a symmetric negative definite matrix A and column vector B, for which the EKSM generates a predetermined residual curve.

Our analysis centers around the sparsity patterns of the auxiliary matrices produced by the EKSM. We use the symbols "+", "-", and "*" to indicate respectively a positive, a negative and a nonzero number. As usual, the symbol "$\times$" indicates a number which is not necessarily zero. A few zeros will be written explicitly to emphasize their presence, while the majority are left blank. We illustrate our notation with the familiar example of inverting a nonsingular lower triangular matrix

$$L = \begin{bmatrix} + & 0 \\ - & + \end{bmatrix} \in \mathbb{R}^{2\times 2} \quad \Rightarrow \quad L \in \mathrm{GL}_2(\mathbb{R}) \wedge L^{-1} = \begin{bmatrix} + & 0 \\ + & + \end{bmatrix}.$$

We will use the notation $e_j^{(k)}$ to denote the jth column vector of the k by k identity matrix I_k. The notation e_j refers exclusively to the case of $k = n$, i.e. $e_j = e_j^{(n)}$.

Our analysis is restricted to the case where n is even and B consists of a single column, i.e. $n = 2m$ for some positive integer m and $p = 1$. In addition, we assume that

$$K(A,B) = \mathbb{R}^n. \tag{1.3}$$

These assumptions simplify the analysis by eliminating the possibility of rank degradation and early breakdowns in the underlying Krylov process.

2 The extended Krylov subspace method

This section contains a brief description of the extended Krylov subspace method (EKSM) for Lyapunov matrix equations. Let $A \in \mathbb{R}^{n\times n}$ be a nonsingular matrix and let $B \in \mathbb{R}^n$. The extended Krylov subspace $\mathbf{EK}_j(A,B)$ is defined by

$$\mathbf{EK}_j(A,B) = \mathrm{span}\{A^{-j}B, A^{-j+1}B, \ldots, A^{-1}B, B, AB, \ldots, A^{j-1}B\}.$$

It is clear that
$$\mathbf{EK}_j(A,B) = K_{2j}(A,A^{-j}B)$$
and
$$\mathbf{EK}_j(A,B) \subseteq \mathbf{EK}_{j+1}(A,B).$$
The extended Krylov subspaces were introduced by Druskin and Knizhnerman [5] who sought to approximate $f(A)B$ for a class of analytic functions f.

Simoncini [26] was the first to apply the extended Krylov subspace method to the Lyapunov matrix equation
$$AX + XA^T + BB^T = 0,$$
where A is negative definite.

Now, let $\{v_i\}_{i=1}^n$ be any sequence of orthonormal vectors such that
$$\mathbf{EK}_j(A,B) = \text{span}\{v_1, v_2, \dots v_{2j}\},$$
and let $V_j \in \mathbb{R}^{n\times 2j}$ be the matrix given by
$$V_j = \begin{bmatrix} v_1 & v_2 & \dots & v_{2j-1} & v_{2j} \end{bmatrix}.$$
It is clear that
$$AV_m = V_m H_m$$
for some matrix $H_m \in \mathbb{R}^{n\times n}$, simply because the columns of V_m span $\mathbb{R}^n$. In fact, there is only one choice for H_m, namely
$$H_m = V_m^T A V_m$$
because $V_m^T V_m = I_n$. Moreover, since
$$A\mathbf{EK}_j(A,B) \subset \mathbf{EK}_{j+1}(A,B), \quad j = 1,2,\dots,m-1$$
and
$$\dim \mathbf{EK}_j(A,B) = 2j, \quad j = 1,2,\dots,m,$$
the matrix H_m must necessarily be upper block Hessenberg with block size 2. In short,
$$H_m = \begin{bmatrix} H_{11} & H_{12} & \dots & \dots & H_{1m} \\ H_{21} & H_{22} & \dots & \dots & \vdots \\ 0 & H_{32} & H_{33} & \dots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \dots & 0 & H_{m,m-1} & H_{mm} \end{bmatrix}, \quad H_{ij} \in \mathbb{R}^{2\times 2}.$$
The extended Krylov subspace method seeks an approximation of the form
$$X_j = V_j Y_j V_j^T, \quad Y_j \in \mathbb{R}^{2j\times 2j}$$
such that the corresponding residual given by
$$R(X_j) = AX_j + X_j A^T + BB^T$$

satisfies the Galerkin condition

$$V_j^T R(X_j) V_j = 0.$$

This condition is satisfied if and only if Y_j solves the reduced order equation

$$H_j Y_j + Y_j H_j^T + \beta^2 e_1^{(2j)} {e_1^{(2j)}}^T = 0, \quad \beta = \|B\|_2, \tag{2.1}$$

where

$$H_j = V_j^T A V_j \in \mathbb{R}^{2j \times 2j}.$$

If A is negative definite then H_j is negative definite and equation (2.1) has a unique solution. It can be shown that the Frobenius norm of the residual satisfies

$$\|R(X_j)\|_F = \sqrt{2} \|H_{j+1,j} E_j^T Y_j\|_F, \quad j < m, \tag{2.2}$$

where E_j consists of the last two columns of I_{2j} and $\|\cdot\|_F$ denotes the Frobenius norm. By assumption

$$\operatorname{Ran} V_m = EK_m(A,B) = \mathbb{R}^n$$

and it is easy to see that

$$R(X_m) = 0.$$

This is the finite termination property for the extended Krylov subspace method. It is primarily of theoretical interest as we can rarely afford to execute m iterations.

Simoncini [26] uses a clever variation of the Arnoldi algorithm to compute matrices

$$V_j = \begin{bmatrix} v_1 & v_2 & \dots & v_{2j-1} & v_{2j} \end{bmatrix} \in \mathbb{R}^{n \times 2j}$$

such that

$$\mathbf{EK}_j(A,B) = \operatorname{Ran} V_j, \quad V_j^T V_j = I_{2j}.$$

Simultaneously, the matrices

$$H_j = V_j^T A V_j \in \mathbb{R}^{2j \times 2j}$$

are extracted without explicitly forming the products, and the reduced order equations are solved using a dense method, say, the Bartel-Stewart method [2].

At this point we would like to emphasize that Y_j depends exclusively on H_j and β, i.e

$$Y_j = Y_j(H_j, \beta).$$

In particular, Y_j is independent of $H_{j+1,j}$ which determines the Frobenius norm of the residual via equation (2.2). We will use this observation to prove that any positive residual curve is possible. Moreover, since X_j depends exclusively on $\mathbf{EK}_j(A,B)$, rather than on any particular basis, we are free to choose whichever basis that will simplify our analysis.

The extended Krylov subspace method differs from the original Arnoldi method introduced by Saad [24] and extended by Jaimoukha and Kasenally [12] in the choice of the applied subspaces. Contributions to the analysis of the convergence rate for these two methods have been made by Simoncini and Druskin [27] and Knizhnerman and Simoncini [17]. Recently we have shown that any positive residual curve is possible for the standard Arnoldi method for Lyapunov equations. In fact, there is considerable freedom of choice, and both symmetric and nonsymmetric equations can be constructed [21].

3 The main result

Our primary objective is to establish the following theorem for the residual curve for the EKSM for Lyapunov matrix equations.

Theorem 3.1 *Let $n = 2m$ be an even positive integer and let $\{r_j\}_{j=1}^{m-1}$ be a sequence of positive real numbers. Then there exists a symmetric positive definite matrix $A \in \mathbb{R}^{n\times n}$ such that the residual curve for the extended Krylov subspace method applied to*

$$AX + XA^T = e_1 e_1^T$$

satisfies

$$\|R_j\|_F = r_j, \quad j = 1,2,\ldots,m-1, \quad \|R_m\|_F = 0.$$

The key to proving Theorem 3.1 is to understand the relationship between the matrices A and B which define the Lyapunov matrix equation, and the matrices V_m and H_m which determine the residuals. We now begin the process of constructing a class of matrices for which this relationship is particularly simple, i.e. $V_m = I_n$ and $H_m = A$, while retaining enough flexibility to control the norm of the residuals.

Let $W_m(A,B)$ be the matrix defined by

$$\begin{aligned} W_m(A,B) &= \left[B,\, A^{-1}B,\, AB,\, A^{-2}B,\, \ldots,\, A^{m-1}B,\, A^{-m}B\right] \\ &= \left[w_1,\, w_2,\, w_3,\, w_4,\, \ldots,\, w_{2m-1},\, w_{2m}\right]. \end{aligned}$$

The definition of $\mathbf{EK}_j(A,B)$ implies

$$\mathbf{EK}_j(A,B) = \text{span}\{w_1, w_2, \ldots, w_{2j-1}, w_{2j}\}, \quad j = 1,2,\ldots,m.$$

Now, let $V_m \in \mathbb{R}^{n\times n}$ be any orthonormal matrix such that

$$\text{span}\{v_1, v_2, \ldots v_i\} = \text{span}\{w_1, w_2, \ldots, w_i\}, \quad i = 1,2,\ldots,n. \tag{3.1}$$

Then, in particular

$$\mathbf{EK}_j(A,B) = \text{span}\{v_1, v_2, \ldots, v_{2j-1}, v_{2j}\}, \quad j = 1,2,\ldots,m.$$

The following Lemma 3.1 describes the sparsity patterns of the matrices H_m and K_m defined by

$$H_m = V_m^T A V_m \tag{3.2}$$

and

$$K_m = H_m^{-1} = V_m^T A^{-1} V_m. \tag{3.3}$$

Lemma 3.1 *Let $n = 2m$ be a positive integer, let $A \in \mathbb{R}^{n\times n}$ be a nonsingular matrix and let $B \in \mathbb{R}^n$ satisfy $K(A,B) = \mathbb{R}^n$. Let $V_m \in \mathbb{R}^{n\times n}$ be any orthonormal matrix such that equation (3.1) is satisfied and let H_m be defined by equation (3.2). Then H_m is upper block Hessenberg with block size 2 and the subdiagonal blocks satisfy*

$$H_{j+1,j} = \begin{bmatrix} \times & \times \\ 0 & 0 \end{bmatrix}, \quad j = 1,2,\ldots,m-1,$$

while

$$H_{mm} = \begin{bmatrix} \times & \times \\ * & \times \end{bmatrix}.$$

In addition, the matrix $K_m = H_m^{-1}$ *is upper block Hessenberg with block size* 2*, the first diagonal block of* K_m *satisfies*

$$K_{11} = \begin{bmatrix} \times & \times \\ * & \times \end{bmatrix},$$

while the subdiagonal blocks of K_m *satisfy*

$$K_{j+1,j} = \begin{bmatrix} 0 & \times \\ 0 & * \end{bmatrix}, \quad j = 1,2,\dots,m-1.$$

Proof We begin by illustrating the statement of the lemma in the case of $m = 3$ where the sparsity patterns of H_m and K_m are given by

$$H_m = \left[\begin{array}{cc|cc|cc} \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ \hline * & \times & \times & \times & \times & \times \\ & & \times & \times & \times & \times \\ \hline & & * & \times & \times & \times \\ & & & & * & \times \end{array}\right], \quad \text{and} \quad K_m = \left[\begin{array}{cc|cc|cc} \times & \times & \times & \times & \times & \times \\ * & \times & \times & \times & \times & \times \\ \hline & \times & \times & \times & \times & \times \\ & * & \times & \times & \times & \times \\ \hline & & & \times & \times & \times \\ & & & * & \times & \times \end{array}\right].$$

The fact that H_m is upper block Hessenberg can be extracted from the discussion in Section 2. We will now show why the subdiagonal blocks satisfy

$$H_{j+1,j} = \begin{bmatrix} \times & \times \\ 0 & 0 \end{bmatrix}.$$

This phenomenon was first explained by Simoncini [26] in terms of the KPIK algorithm[1]. Here we provide a proof in terms of the matrices W_m and V_m. We begin by examining the subdiagonal block H_{21}. By definition, $v_1 = \alpha w_1$, $\alpha \in \mathbb{R}$, and $Av_1 = \alpha AB = \alpha w_3$. Therefore, $Av_1 \in \text{span}\{v_1, v_2, v_3\}$ and $h_{41} = 0$. Similarly, $v_2 = \beta w_1 + \gamma w_2$ for some β and γ. Hence, $Av_2 = \gamma B + 0 \cdot A^{-1}B + \beta AB \in \text{span}\{w_1, w_2, w_3\}$. Therefore, $Av_2 \in \text{span}\{v_1, v_2, v_3\}$ and $h_{42} = 0$. This explains why

$$H_{21} = \begin{bmatrix} \times & \times \\ 0 & 0 \end{bmatrix}.$$

In general, we have $v_i \in \text{span}\{w_1, w_2, \dots, w_i\}$ for all i. If $i \in \{1,3,5,\dots,\}$, then $Aw_i = w_{i+2}$, and $Av_i \in \text{span}\{v_1, v_2, \dots, v_{i+2}\}$. If $i \in \{2,4,6,\dots\}$, then $Aw_i = w_{i-1}$, but since $Aw_{i-1} = w_{i+1}$ we have $Av_i \in \text{span}\{v_1, v_2, \dots, v_{i+1}\}$. This explains the general structure of the subdiagonal blocks $H_{j+1,j}$.

We still have to prove that certain entries of H_m are nonzero. To this end, we first examine the matrix K_m. It is clear that

$$A^{-1}V_m = V_m K_m$$

[1] Jagels and Reichel [11] have proved a similar result for the symmetric positive definite case using orthogonal Laurent polynomials.

for some matrix $K_m \in \mathbb{R}^{n\times n}$ simply because the columns of V_m span $\mathbb{R}^n$. In fact, there is only one choice namely

$$K_m = V_m^T A^{-1} V_m,$$

because the columns of V_m are orthonormal, and it is straightforward to verify that

$$K_m = H_m^{-1}.$$

From the definition of $\mathbf{EK}_j(A,B)$ it follows that

$$A^{-1}\mathbf{EK}_j(A,B) \subset \mathbf{EK}_{j+1}(A,B), \quad j = 1,2,\dots,m-1,$$

which immediately implies that K_m must be upper block Hessenberg. Again, the block size is 2 because $\dim \mathbf{EK}_j(A,B) = 2j$ for $j = 1,2,\dots,2m$. In short,

$$K_m = \begin{bmatrix} K_{11} & K_{12} & \dots & \dots & K_{1m} \\ K_{21} & K_{22} & \dots & \dots & \vdots \\ 0 & K_{32} & K_{33} & \dots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \dots & 0 & K_{m,m-1} & K_{mm} \end{bmatrix}, \quad K_{ij} \in \mathbb{R}^{2\times 2}.$$

We will now show that the first column of each of the subdiagonal blocks is zero, i.e.

$$K_{j+1,j} = \begin{bmatrix} 0 & \times \\ 0 & \times \end{bmatrix}, \quad j = 1,2,\dots,m-1.$$

We begin by examining the subdiagonal block K_{21}. By definition, $v_1 = \alpha w_1 = \alpha B$ for some α. Hence, $A^{-1}v_1 = \alpha A^{-1}B = 0\cdot w_1 + \alpha w_2 \in \operatorname{span}\{w_1,w_2\} = \operatorname{span}\{v_1,v_2\}$. Therefore, $k_{31} = k_{41} = 0$. This explains why

$$K_{21} = \begin{bmatrix} 0 & \times \\ 0 & \times \end{bmatrix}.$$

In general, if $i \in \{3,5,7,\dots\}$ then $A^{-1}w_i = w_{i-2}$, but $A^{-1}w_{i-1} = w_{i+1}$. Therefore, $A^{-1}v_i \in \operatorname{span}\{w_1,w_2,\dots,w_{i+1}\}$. If $i \in \{2,4,6,\dots\}$ then there is nothing to show, because we already know that K_m is upper block Hessenberg with block size 2.

We can now show the indicated entries of H_m and K_m are nonzero. To this end, we first consider the matrix

$$\begin{aligned} W_m(H_m,e_1) &= \left[e_1,\, H_m^{-1}e_1,\, H_m e_1,\, H_m^{-2}e_1,\, \dots,\, H_m^{m-1}e_1,\, H_m^{-m}e_1\right] \\ &= \left[e_1,\, K_m e_1,\, H_m e_1,\, K_m^2 e_1,\, \dots,\, H_m^{m-1}e_1,\, K_m^m e_1\right]. \end{aligned}$$

The structure of H_m and K_m implies that $W_m = W_m(H_m,e_1)$ is upper triangular. We exhibit the case of $m=3$ where

$$H_m = \left[\begin{array}{cc|cc|cc} \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ \hline \times & \times & \times & \times & \times & \times \\ & & \times & \times & \times & \times \\ \hline & & \times & \times & \times & \times \\ & & & & \times & \times \end{array}\right] \wedge K_m = \left[\begin{array}{cc|cc|cc} \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ \hline & \times & \times & \times & \times & \times \\ & \times & \times & \times & \times & \times \\ \hline & & & \times & \times & \times \\ & & & \times & \times & \times \end{array}\right] \Rightarrow W_m = \left[\begin{array}{cc|cc|cc} 1 & \times & \times & \times & \times & \times \\ & \times & \times & \times & \times & \times \\ \hline & & \times & \times & \times & \times \\ & & & \times & \times & \times \\ \hline & & & & \times & \times \\ & & & & & \times \end{array}\right].$$

However, since A and H_m are similar it is clear that

$$K(A,B) = \mathbb{R}^n \quad \Leftrightarrow \quad K(H_m, e_1) = \mathbb{R}^n.$$

Therefore, $W_m(H_m, e_1)$ is nonsingular and its diagonal entries must be nonzero. Now, the key is to notice that every element on the diagonal of $W_m(H_m, e_1)$ is a product of certain entries from either H_m or K_m. We must have

$$K_{11} = \begin{bmatrix} \times & \times \\ * & \times \end{bmatrix},$$

or the second diagonal entry of W_m is not sure to be nonzero. Similarly, it follows that

$$H_{j+1,j} = \begin{bmatrix} * & \times \\ 0 & 0 \end{bmatrix}, \quad K_{j+1,j} = \begin{bmatrix} 0 & \times \\ 0 & * \end{bmatrix} \quad j = 1,2,\dots,m-1.$$

Finally, it remains to be shown that

$$H_{mm} = \begin{bmatrix} \times & \times \\ * & \times \end{bmatrix}.$$

By examining the sparsity pattern of H_m we discover that it suffices to show that the last component of $H_m^m e_1$ is nonzero. However, the last component of each of the $2m-1$ vectors in the set

$$\{H_m^j e_1 \, : \, -(m-1) \leq j \leq m-1\}$$

is zero, but together with the vector $H_m^m e_1$ they span $\mathbb{R}^n$. This is only possible if the last component of $H_m^m e_1$ is nonzero. □

Lemma 3.1 characterizes the sparsity pattern for the matrix H_m generated by the EKSM as well as the sparsity pattern for the inverse matrix K_m. On the other hand, if we can find matrices H_m and K_m such that $H_m K_m = I_n$ and H_m and K_m have these sparsity patterns, then not only is

$$W_m(H_m, e_1) = \begin{bmatrix} w_1 & w_2 & \dots & w_n \end{bmatrix} \in \mathbb{R}^{n \times n}$$

nonsingular, but more importantly

$$\operatorname{span}\{w_1, w_2, \dots, w_i\} = \operatorname{span}\{e_1, e_2, \dots, e_i\}, \quad i = 1,2,\dots,n,$$

because $W_m(H_m, e_1)$ is upper triangular. In particular, we find that

$$\mathbf{EK}_j(H_m, e_1) = \operatorname{span}\{e_1, e_2, \dots, e_{2j-1}, e_{2j}\}, \quad j = 1,2,\dots,m.$$

We now impose the extra condition that A is symmetric positive definite. Let $H_m = L_m L_m^T$ be the Cholesky factorization of $H_m = V_m^T A V_m$. Lemma 3.2 describes the sparsity pattern for L_m and the inverse matrix $T_m = L_m^{-1}$.

Lemma 3.2 *Let $n = 2m$ be an even positive integer and let $A \in \mathbb{R}^{n\times n}$ be symmetric positive definite. Let $B \in \mathbb{R}^n$ and assume $K(A,B) = \mathbb{R}^n$. Let W_m and V_m be as in Lemma 3.1. Let $H_m = L_m L_m^T$ denote the Cholesky factorization of $H_m = V_m^T A V_m$. Then L_m is a lower block bidiagonal matrix with block size 2 and*

$$L_{j+1,j} = \begin{bmatrix} * & \times \\ 0 & 0 \end{bmatrix}, \quad j = 1,2,\ldots,m-1, \quad L_{mm} = \begin{bmatrix} + & 0 \\ * & + \end{bmatrix}.$$

In addition, $T_m = L_m^{-1}$ is a lower block diagonal matrix with block size 2 and

$$T_{11} = \begin{bmatrix} + & 0 \\ * & + \end{bmatrix}, \quad T_{j+1,j} = \begin{bmatrix} 0 & \times \\ 0 & * \end{bmatrix}, \quad j = 1,2,\ldots,m-1.$$

Lemma 3.2 states that L_m and T_m inherit their sparsity patterns from the lower half of H_m and K_m. We illustrate this by displaying the case of $m = 3$, where

$$L_m = \left[\begin{array}{cc|cc|cc} + & & & & & \\ \times & + & & & & \\ \hline * & \times & + & & & \\ & & \times & + & & \\ \hline & & * & \times & + & \\ & & & & * & + \end{array}\right], \quad \text{and} \quad T_m = \left[\begin{array}{cc|cc|cc} + & & & & & \\ * & + & & & & \\ \hline & \times & + & & & \\ & * & \times & + & & \\ \hline & & & \times & + & \\ & & & * & \times & + \end{array}\right].$$

The diagonal entries of L_m are positive simply because L_m is the Cholesky factor for the symmetric positive definite matrix H_m.

Proof We begin by examining the matrix L_m. The matrix H_m is banded with a lower bandwidth of 2. Therefore, L_m has a lower bandwidth of 2. We emphasize this by writing

$$L_m = \begin{bmatrix} L_{11} & & & \\ L_{21} & \ddots & & \\ & \ddots & \ddots & \\ & & L_{m,m-1} & L_{mm} \end{bmatrix}, \quad L_{j+1,j} = \begin{bmatrix} \times & \times \\ 0 & \times \end{bmatrix}, \quad j = 1,2,\ldots,m-1.$$

Now, since $H_m = L_m L_m^T$ and L_m is lower block bidiagonal, we have $H_{j+1,j} = L_{j+1,j} L_{jj}$. It follows that

$$L_{j+1,j} = H_{j+1,j} L_{jj}^{-T} = \begin{bmatrix} * & \times \\ 0 & 0 \end{bmatrix} \begin{bmatrix} + & \times \\ 0 & + \end{bmatrix} = \begin{bmatrix} * & \times \\ 0 & 0 \end{bmatrix}, \quad j = 1,2,\ldots,m-1.$$

Finally, by examining the lower right corner of the identity $H_m = L_m L_m^T$ we discover that

$$L_{mm} = \begin{bmatrix} + & 0 \\ * & + \end{bmatrix}.$$

We now consider the structure of $T_m = L_m^{-1}$. In general, if L is a nonsingular lower triangular matrix then $T = L^{-1}$ is a dense lower triangular matrix. However, in our case T_m inherits its sparsity pattern from K_m. As an illustration we exhibit the case of $m = 3$, where

$$T_m^T T_m = \left[\begin{array}{cc|cc|cc} + & \times & \times & \times & \times & \times \\ & + & \times & \times & \times & \times \\ \hline & & + & \times & \times & \times \\ & & & + & \times & \times \\ \hline & & & & + & \times \\ & & & & & + \end{array}\right] \left[\begin{array}{cc|cc|cc} + & & & & & \\ \times & + & & & & \\ \hline \times & \times & + & & & \\ \times & \times & \times & + & & \\ \hline \times & \times & \times & \times & + & \\ \times & \times & \times & \times & \times & + \end{array}\right] = \left[\begin{array}{cc|cc|cc} \times & * & & & & \\ * & \times & \times & * & & \\ \hline & \times & \times & \times & & \\ & * & \times & \times & \times & * \\ \hline & & & \times & \times & \times \\ & & & * & \times & \times \end{array}\right] = K_m.$$

Now, the key is to exploit the fact that the diagonal entries of T_m are nonzero. Starting with the last row of this identity and working upwards we deduce that the sparsity patterns of T_m and the lower triangular part of K_m are identical. This completes the proof. $\square$

It is clear that these patterns impose severe conditions on the entries of L_m. Specifically, since $I_n = L_m T_m$ and L_m and T_m are both lower block diagonal, we must have

$$\begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix} = I_{j+1,j} = L_{j+1,j} T_{jj} + L_{j+1,j+1} T_{j+1,j}$$
$$= \begin{bmatrix} \times & \times \\ 0 & 0 \end{bmatrix} \begin{bmatrix} + & 0 \\ \times & + \end{bmatrix} + \begin{bmatrix} + & 0 \\ \times & + \end{bmatrix} \begin{bmatrix} 0 & \times \\ 0 & \times \end{bmatrix} = \begin{bmatrix} \times & \times \\ 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & \times \\ 0 & \times \end{bmatrix}.$$

By considering entry $(1,1)$ of this equality we see that the first row of $L_{j+1,j}$ must necessarily be orthogonal to the first column of $T_{jj} = L_{jj}^{-1}$. On the other hand, we have the following lemma.

Lemma 3.3 *Let $n = 2m$ be an even positive integer and let*

$$L_{jj} = \begin{bmatrix} + & 0 \\ * & + \end{bmatrix} \in \mathbb{R}^{2\times 2} \quad j = 1,2,\ldots,m.$$

Let $(x_j, y_j)^T$ be the solution of

$$L_{jj} \begin{bmatrix} x_j \\ y_j \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad j = 1,2,\ldots,m-1,$$

and let $L_{j+1,j} \in \mathbb{R}^{2\times 2}$ be given by

$$L_{j+1,j} = \gamma_j \begin{bmatrix} y_j & -x_j \\ 0 & 0 \end{bmatrix}, \quad \gamma_j \neq 0, \quad j = 1,2,\ldots,m-1.$$

Then the matrix $L \in \mathbb{R}^{n\times n}$ given by

$$L = \begin{bmatrix} L_{11} & & & \\ L_{21} & \ddots & & \\ & \ddots & \ddots & \\ & & L_{m,m-1} & L_{mm} \end{bmatrix}$$

is nonsingular and $T = L^{-1}$ satisfies

$$T = \begin{bmatrix} T_{11} & & & \\ T_{21} & \ddots & & \\ & \ddots & \ddots & \\ & & T_{m,m-1} & T_{mm} \end{bmatrix},$$

where

$$T_{jj} = \begin{bmatrix} + & 0 \\ * & + \end{bmatrix}, \quad 1 \le j \le m, \qquad \textit{and} \qquad T_{j+1,j} = \begin{bmatrix} 0 & * \\ 0 & * \end{bmatrix}, \quad 1 \le j < m.$$

Proof The proof is by induction on the number m of diagonal blocks. For $m = 1$ there is little to show, as

$$L = \begin{bmatrix} + & 0 \\ * & + \end{bmatrix} \in \mathbb{R}^{2\times 2} \quad \Rightarrow \quad L \in \mathrm{GL}_2(\mathbb{R}) \wedge T = L^{-1} = \begin{bmatrix} + & 0 \\ * & + \end{bmatrix}.$$

In general, we partition L_m as follows

$$L_m = \begin{bmatrix} \hat{L}_{11} & \\ \hat{L}_{21} & \hat{L}_{22} \end{bmatrix},$$

where

$$\hat{L}_{11} = L_{11} \quad \text{and} \quad \hat{L}_{22} = \begin{bmatrix} L_{22} & & & \\ L_{32} & L_{33} & & \\ & \ddots & \ddots & \\ & & L_{m,m-1} & L_{mm} \end{bmatrix}.$$

Then

$$\hat{T}_m = \begin{bmatrix} \hat{T}_{11} & \\ \hat{T}_{21} & \hat{T}_{22} \end{bmatrix},$$

where

$$\hat{T}_{ii} = \hat{L}_{ii}^{-1}, \quad i = 1,2 \quad \text{and} \quad \hat{T}_{21} = -\hat{L}_{22}^{-1}\hat{L}_{21}\hat{L}_{11}^{-1}.$$

By assumption, the conclusion applies to $\hat{L}_{22}$, and $\hat{T}_{22}$ has the correct structure. It remains to be shown that $\hat{T}_{21}$ has the correct structure. We have

$$\hat{L}_{21}\hat{L}_{11}^{-1} = -\gamma_1 \begin{bmatrix} \begin{bmatrix} y_1 & -x_1 \\ 0 & 0 \end{bmatrix} \\ O_2 \\ \vdots \\ O_2 \end{bmatrix} L_{11}^{-1} = \begin{bmatrix} \begin{bmatrix} 0 & * \\ 0 & 0 \end{bmatrix} \\ O_2 \\ \vdots \\ O_2 \end{bmatrix}, \quad \text{where} \quad O_2 = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix},$$

because, by construction, the first row of L_{21} is orthogonal to the first column of L_{11}^{-1}. The proof is completed by exploiting the structure of the first column of $\hat{L}_{22}^{-1}$. □

The following corollary is an immediate consequence of the sparsity patterns of L_m and T_m.

Corollary 3.1 *Let $n = 2m$ be an even positive integer and let L_m and T_m be as in Lemma 3.3. If we define*

$$H_m = L_m L_m^T > 0, \quad \textit{and} \quad K_m = H_m^{-1} = T_m^T T_m > 0,$$

then H_m and K_m are block tridiagonal with block size 2, and

$$H_{j+1,j} = \begin{bmatrix} * & \times \\ 0 & 0 \end{bmatrix}, \quad j = 1, 2 \dots, m-1, \quad H_{mm} = \begin{bmatrix} + & * \\ * & + \end{bmatrix},$$

and

$$K_{11} = \begin{bmatrix} + & * \\ * & + \end{bmatrix}, \quad K_{j+1,j} = \begin{bmatrix} 0 & \times \\ 0 & * \end{bmatrix}, \quad j = 1, 2 \dots, m-1.$$

We illustrate the statement of Corollary 3.1 in the case of $m = 3$ where

$$H_m = \left[\begin{array}{cc|cc|cc} + & \times & * & & & \\ \times & + & \times & & & \\ \hline * & \times & + & \times & * & \\ & & \times & + & \times & \\ \hline & & * & \times & + & * \\ & & & & * & + \end{array}\right] \quad \text{and} \quad K_m = \left[\begin{array}{cc|cc|cc} + & * & & & & \\ * & + & \times & * & & \\ \hline & \times & + & \times & & \\ & * & \times & + & \times & * \\ \hline & & & \times & + & \times \\ & & & * & \times & + \end{array}\right].$$

The diagonal entries are positive simply because H_m and K_m are symmetric positive definite, a property inherited from the original matrix A.

It is clear that the matrix $W_m(H_m, e_1)$ satisfies

$$W_m(H_m, e_1) = \left[\begin{array}{cc|cc|cc} 1 & \times & \times & \times & \times & \times \\ & * & \times & \times & \times & \times \\ \hline & & * & \times & \times & \times \\ & & & * & \times & \times \\ \hline & & & & * & \times \\ & & & & & * \end{array}\right],$$

which implies that

$$\mathbf{EK}_j(H_m, e_1) = \operatorname{span}\{e_1, e_2, \dots, e_{2j-1}, e_{2j}\}, \quad j = 1, 2, \dots, m.$$

We are finally ready to prove Theorem 3.1 in the general case.

Proof Consider Algorithm 1 which produces a sequence of matrices $\{A_j\}_{j=1}^m$. We claim that $A = A_m$ realizes the given residual curve. Each of the matrices L_j satisfies Lemma 3.3. It follows, that $A_j \in \mathbb{R}^{2j \times 2j}$ is symmetric positive definite and the matrix $W_j(A_j, e_1^{(2j)}) \in \mathbb{R}^{2j \times 2j}$ given by

$$W_j(A_j, e_1^{(2j)}) = \begin{bmatrix} e_1^{(2j)} & A_j^{-1} e_1^{(2j)} & A_j e_1^{(2j)} & A_j^{-2} e_1^{(2j)} & \dots & A_j^{j-1} e_1^{(2j)} & A_j^{-j} e_1^{(2j)} \end{bmatrix}$$

is upper triangular with nonzero diagonal entries, regardless of the choices made for $\gamma_i > 0$, $i = 1, 2, \dots, j-1$. The matrices X_j are well defined and have full rank, simply because A_j is positive definite and

$$\operatorname{Ran} X_j = K(A_j, e_1^{(2j)}) = \mathbb{R}^{2j}.$$

In addition, we see that X_j is in fact the jth approximation returned by the EKSM when applied to the Lyapunov matrix equation

$$AX + XA^T = e_1 e_1^T,$$

where $A = A_m$. If $r < m$, then the corresponding residual $R(X_j)$ satisfies

$$\|R(X_j)\|_F = \sqrt{2}\|A_{j+1,j}E_j^T X_j\|_F,$$

where E_j consists of the last two columns of the $2j$ by $2j$ identity matrix I_{2j}. Now, since

$$A_{j+1,j} = L_{j+1,j}L_{jj}^T = \gamma_j \begin{bmatrix} y_j & -x_j \\ 0 & 0 \end{bmatrix} \begin{bmatrix} + & * \\ 0 & + \end{bmatrix} = \gamma_j \begin{bmatrix} * & \times \\ 0 & 0 \end{bmatrix}$$

it follows that the first row of $A_{j+1,j}E_j^T X_j$ is a nontrivial linear combination of the last two rows of the nonsingular matrix X_j. Therefore, there exists a unique $\gamma_j > 0$, such that

$$\|R(X_j)\|_F = r_j.$$

□

Algorithm 1 Construction of A_m

1: **for** $j = 1, 2, \ldots, m$ **do**
2: Choose $L_{jj} \in \mathbb{R}^{2\times 2}$ such that
$$L_{jj} = \begin{bmatrix} + & 0 \\ * & + \end{bmatrix}.$$
3: Define
$$L_j = \begin{bmatrix} L_{11} & & & \\ L_{21} & \ddots & & \\ & \ddots & \ddots & \\ & & L_{j,j-1} & L_{jj} \end{bmatrix}, \quad A_j = L_j L_j^T.$$
4: **if** $j < m$ **then**
5: Let X_j be the solution of
$$A_j X_j + X_j A_j^T = e_1^{(2j)} e_1^{(2j)^T}.$$
6: Let $\begin{bmatrix} x_j & y_j \end{bmatrix}^T$ be the solution of
$$L_{jj} \begin{bmatrix} x_j \\ y_j \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$
and define
$$L_{j+1,j} = \gamma_j \begin{bmatrix} y_j & -x_j \\ 0 & 0 \end{bmatrix},$$
where $\gamma_j > 0$ is the unique positive real number, such that
$$\|R(X_j)\|_F = r_j.$$
7: **end if**
8: **end for**

The proof of Theorem 3.1 is constructive and a MATLAB implementation is available from the author by request. However, numerically Algorithm 1 is highly sensitive to the choices made when selecting the diagonal blocks of L_m. In particular, given a residual curve and a positive number ν we can always find a symmetric positive definite matrix A which reproduces the residual curve and satisfies

$$\kappa_2(A) \geq \nu.$$

This follows immediately from the fact that we are free to choose L_{11} and Cauchy's interlacing theorem which ensures that

$$\kappa_2(A) = \kappa_2(A_m) \geq \kappa_2(A_{11}) = \kappa_2(L_{11}L_{11}^T).$$

It follows, that even an ill-conditioned matrix A can generate a rapidly decreasing, but positive residual curve. Refining Algorithm 1 to the point where $\kappa_2(A_m)$ is minimal is an open question.

4 Conclusion

We have shown that any positive residual curve is possible for the extended Krylov subspace method (EKSM) for the Lyapunov equation $AX + XA^T + BB^T = 0$, where $A \in \mathbb{R}^{n\times n}$ is symmetric negative definite and $B \in \mathbb{R}^n$ satisfies $K(A,B) = \mathbb{R}^n$. The algorithm is well defined whenever A is negative definite, but this condition does not ensure that the residual curve decreases rapidly or monotonically to zero. Theorems guaranteeing such behavior must necessarily impose additional assumptions on A and B.

Acknowledgments

This work is reminiscent of the analysis of GMRES for standard linear systems by Greenbaum, Pták and Strakoš [9] and an early copy of the manuscript was entitled "Any positive residual curve is possible for the extended Krylov subspace method for Lyapunov matrix equations" in recognition of their work. Size considerations ultimately lead to the selection of the current title. The author would like to thank the two anonymous referees as well as Bo Kågström whose comments allowed him to improve the presentation. The work is supported by eSSENCE, a collaborative e-Science programme funded by the Swedish Research Council within the framework of the strategic research areas designated by the Swedish Government. In addition, support has been provided by the Swedish Foundation for Strategic Research under the frame program A3 02:128 and the EU Mål 2 Project UMIT.

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