

Any positive residual curve is possible for the EKSM for Lyapunov equations

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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 that any positive residual curve is possible for the EKSM for Lyapunov matrix equations. In addition, we show how to systematically construct linear time invariant systems for which it is impractical to approximate the action of the product of the system Gramians using the EKSM. This is a property of the underlying Lyapunov matrix equations, rather than a defect of the EKSM.

Abstract Keywords Lyapunov matrix equations · extended Krylov subspaces · iterative methods

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1 Introduction and basic notation

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

$$AX + XA^T + BB^T = 0. \quad (1.1)$$

If A is stable, then there exists a unique solution X which is given by

$$X = \int_0^\infty e^{tA} BB^T e^{tA^T} dt.$$

The matrix X is symmetric positive semidefinite and the range of X is the smallest A invariant subspace which contains the range of B . If A is a dense matrix with

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$n = O(10^3)$, then we can solve equation (1.1) on a single processor using one of several dense methods [3, 7, 11, 33]. If A is a dense matrix with $n = O(10^5)$, then it is necessary to use a parallel machine, but efficient implementations have recently been completed [18, 19, 9, 8].

In many applications B is a tall matrix with $O(1)$ columns. Frequently, 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 [28, 2]. During the last 20 years a number of methods have been developed in order to compute good low rank approximations to X directly [29, 14, 17, 16, 27, 22, 30, 5, 4, 21]. Recently, the extended Krylov subspace method has been applied to this problem [6, 31, 20]. It is possible to treat the Lyapunov matrix equation as a standard linear system without using $O(n^2)$ resources [23]. 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.

Lyapunov equations are central to the analysis of dynamical systems. A linear time invariant system is a system of first order differential equations together with an algebraic equation

$$\begin{aligned}\dot{x}(t) &= Ax(t) + Bu(t), \\ y(t) &= Cx(t) + Du(t),\end{aligned}$$

where A , B , C , and D are real matrices of compatible size. Such systems can be found in every field of natural science. Frequently, the dimension n is so large that it is not possible to integrate the equation directly. In model reduction the primary objective is to compute a reduced order model, which can be used to simulate the original model [1]. Model reduction by balanced truncation [25, 26, 10] is a popular technique. The main problem is to compute the dominant eigenspace for the products PQ and QP , where the system Gramians P and Q are given as the solutions to a pair of Lyapunov matrix equations

$$AP + PA^T + BB^T = 0, \quad A^T Q + QA + C^T C = 0.$$

The two equations can either be solved separately or concurrently [15, 12] or the dominant subspaces can be estimated directly [35, 34].

In Section 2 we give a very brief description of the extended Krylov subspace method for Lyapunov equations. Our main result is derived and presented in Section 3. A secondary result with application to model reduction is presented in Section 4. Finally, Section 5 contains a short summary of our findings and an open question.

Our analysis centers around the sparsity patterns of the auxiliary matrices produced by the extended Krylov subspace method. We use the symbols “+”, “-”, and “*” to indicate respectively a positive, a negative and a nonzero number. The symbol “×” indicates a number which is not necessarily zero. Some zeros will be written explicitly to emphasize their presence. We illustrate our notation with the familiar example of inverting a nonsingular lower triangular matrix

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

2 The extended Krylov subspace method

This section contains a brief description of the extended Krylov subspace method for Lyapunov matrix equations. Let $A \in \mathbb{R}^{n \times n}$ and let $B \in \mathbb{R}^{n \times p}$. The standard Krylov subspace $K_j(A, B)$ is given by

$$K_j(A, B) = \text{span}\{B, AB, A^2B, \dots, A^{j-1}B\}.$$

It is clear that

$$K_j(A, B) \subseteq K_{j+1}(A, B)$$

and that

$$K(A, B) = \cup_{j=1}^{\infty} K_j(A, B) \subseteq \mathbb{R}^n$$

is the smallest A invariant subspace which contains the range of B . Now, if A is non-singular, then the extended Krylov subspace is given by

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

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 [6] who sought to approximate $f(A)$ for a specific class of analytical functions.

Simoncini [31] 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. In this paper we consider only the special case of

$$p = 1 \quad \text{and} \quad n = 2m. \quad (2.1)$$

For the sake of simplicity, we assume that

$$K(A, B) = \cup_{j=1}^{\infty} K_j(A, B) = \mathbb{R}^n. \quad (2.2)$$

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

$$V_j = [v_1 \ v_2 \ \dots \ v_{2j-1} \ v_{2j}].$$

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 $V_m^T V_m = I_n$. However, 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,

$$H_m = \begin{bmatrix} H_{11} & H_{12} & \dots & \dots & H_{1m} \\ H_{21} & H_{22} & \dots & \dots & \vdots \\ 0 & H_{32} & H_{33} & \dots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \dots & 0 & H_{m,m-1} & H_{mm} \end{bmatrix}$$

where $H_{ij} \in \mathbb{R}^{2 \times 2}$.

The extended Krylov subspace method seeks an approximation of the form

$$X_j = V_j Y_j V_j^T,$$

where $Y_j \in \mathbb{R}^{2j \times 2j}$ such that the corresponding residual given by

$$R(X_j) = AX_j + X_j A^T + BB^T$$

satisfies the Galerkin condition

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

It is easy to see that this condition is satisfied if and only if Y_j solves the reduced order equation

$$H_j Y_j + Y_j H_j^T + \beta^2 e_1^{(2j)} e_1^{(2j)T} = 0, \quad \beta = \|B\|_2 \quad (2.3)$$

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 (2.3) has a unique solution. It can be shown that the Frobenius norm of the residual satisfies

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

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

$$\text{Ran } V_m = \mathbf{EK}_m(A, B) = \mathbb{R}^n$$

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.

It is important to realize that X_j depends exclusively on $\mathbf{EK}_j(A, B)$. In particular, it is independent of the choice of orthonormal basis. Therefore, we are free to choose the basis which is most suitable to our analysis.

Simoncini [31] uses a clever variation of the Arnoldi algorithm to compute matrices

$$V_j = [v_1 \ v_2 \ \dots \ v_{2j-1} \ v_{2j}] \in \mathbb{R}^{n \times 2j}$$

such that

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

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 [3].

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 $H_{j+1, j}$. We will use this observation to prove that any positive residual curve is possible.

The extended Krylov subspace method differs from the original Arnoldi method introduced by Saad [29] and extended by Jaimoukha and Kasenally [14] 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 [32] and Knizhnerman and Simoncini [20]. 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 [24].

3 The main result

Our objective is to establish the following theorem.

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

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

The main problem is the nontrivial 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 $R(X_j)$. We must determine a class of matrices for which this relationship is particularly simple. Ideally, we would like $V_m = I_n$ and $H_m = A$.

Obviously, we require a detailed understanding of the structure of the matrices V_j and H_j . Let $A \in \mathbb{R}^{n \times n}$ be a nonsingular matrix and let $B \in \mathbb{R}^n$. Let $W_m \in \mathbb{R}^{n \times 2j}$ be the matrix given by

$$W_j = [w_1 \ w_2 \ w_3 \ w_4 \ \dots \ w_{2j-1} \ w_{2j}], \quad j = 1, 2, \dots, m$$

where

$$w_i = \begin{cases} A^{(i-1)/2}B, & i = \{1, 3, 5, \dots, 2m-1\}, \\ A^{-i/2}B, & i = \{2, 4, 6, \dots, 2m\}. \end{cases}$$

In particular,

$$W_m = [B \ A^{-1}B \ AB \ A^{-2}B \ A^2B \ A^{-3}B \ \dots \ A^{m-1}B \ A^{-m}B]. \quad (3.1)$$

By assumption (2.2), W_m is nonsingular. Let

$$V_m = [v_1 \ v_2 \ \dots \ v_{2m-1} \ v_{2m}] \in \mathbb{R}^{n \times n}$$

be any orthonormal matrix, such that

$$\text{span}\{w_1, w_2, \dots, w_i\} = \text{span}\{v_1, v_2, \dots, v_i\}, \quad i = 1, 2, 3, \dots, 2m-1, 2m.$$

Theoretically, V_m can be obtained by applying Gram-Schmidt orthogonalization to W_m . In any case, we have

$$\mathbf{EK}_j(A, B) = \text{Ran}W_j = \text{Ran}V_j, \quad V_j^T V_j = I_{2j}, \quad j = 1, 2, \dots, m.$$

Let H_m be the matrix given by

$$H_m = V_m^T A V_m$$

such that

$$A V_m = V_m H_m.$$

As explained in the previous section, H_m is upper block Hessenberg with block size 2. However, because of the structure of W_m , the last row of each of the subdiagonal blocks is zero, i.e.

$$H_{j+1,j} = \begin{bmatrix} \times & \times \\ 0 & 0 \end{bmatrix}, \quad j = 1, 2, \dots, m-1. \quad (3.2)$$

This phenomenon was first explained by Simoncini [31] in terms of the KPIK algorithm. Later, Jagels and Reichel [13] gave a different proof using orthogonal Laurent polynomials. The following paragraph contains a third proof. By definition, $v_1 = \alpha w_1$, $\alpha \in \mathbb{R}$, and $A v_1 = \alpha A B = \alpha w_3$. Therefore, $A v_1 \in \text{span}\{v_1, v_2, v_3\}$ and $h_{41} = 0$. Similarly, $v_2 = \beta w_1 + \gamma w_2$ for some β and γ . Hence, $A v_2 = \gamma B + 0 \cdot A^{-1}B + \beta A B \in \text{span}\{w_1, w_2, w_3\}$. Therefore, $A v_2 \in \text{span}\{v_1, v_2, v_3\}$ 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 will now collect information about H_m^{-1} . The matrix H_m is nonsingular, because A and V_m are both nonsingular. In general, if H is nonsingular, then H^{-1} is a dense matrix, regardless of the structure of H . However, in our case H_m^{-1} is upper block Hessenberg with block size 2! It is clear that

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

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

$$K_m = V_m^T A^{-1} V_m = (V_m^T A V_m)^{-1} = H_m^{-1}.$$

Now, 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,

$$K_m = \begin{bmatrix} K_{11} & K_{12} & \dots & \dots & K_{1m} \\ K_{21} & K_{22} & \dots & \dots & \vdots \\ 0 & K_{32} & K_{33} & \dots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \dots & 0 & K_{m,m-1} & K_{mm} \end{bmatrix}$$

where $K_{ij} \in \mathbb{R}^{2 \times 2}$. However, the first row of each of the subdiagonal blocks is zero, i.e.

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

This phenomenon is easy to explain. By definition, $v_1 = \alpha w_1 = \alpha B$ for some α . Hence, $A^{-1}v_1 = \alpha A^{-1}B = 0 \cdot w_1 + \alpha w_2 \in \text{span}\{w_1, w_2\} = \text{span}\{v_1, v_2\}$. Therefore, $k_{31} = k_{41} = 0$. In general, if $i \in \{3, 5, \dots\}$ we have $A^{-1}w_i = w_{i-2}$, but $A^{-1}w_{i-1} = w_{i+1}$. Therefore, $A^{-1}v_i \in \text{span}\{w_1, w_2, \dots, w_{i+1}\}$. 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.

In addition, it is possible to identify certain entries of H_m and K_m which are nonzero. To this end we consider the matrix

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

It easy to see that 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

$$H_m = \begin{bmatrix} \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \end{bmatrix} \wedge K_m = \begin{bmatrix} \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \end{bmatrix} \Rightarrow W_m = \begin{bmatrix} 1 & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \end{bmatrix}.$$

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

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

Therefore, $W_m(H_m, e_1)$ is nonsingular and its diagonal entries must be nonzero. It follows, that

$$H_m = \begin{bmatrix} \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ * & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \end{bmatrix} \wedge K_m = \begin{bmatrix} \times & \times & \times & \times & \times & \times \\ * & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ * & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ * & \times & \times & \times & \times & \times \end{bmatrix} \Leftrightarrow W_m = \begin{bmatrix} 1 & \times & \times & \times & \times & \times \\ * & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ * & \times & \times & \times & \times & \times \end{bmatrix}.$$

The key is to notice that every element on the diagonal of $W_m(H_m, e_1)$ is a product of certain key entries from either H_m or K_m . In short,

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

and the subdiagonal blocks satisfy

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

In addition, we claim that

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

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

$$H_m^{1-m} e_1, H_m^{2-m} e_1, H_m^{3-m} e_1, \dots, H_m^{m-1} e_1$$

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

We summarize these results in the following lemma.

Lemma 3.1 *Let $n = 2m$ be an even positive integer and let $A \in \mathbb{R}^{n \times n}$ be nonsingular. Let $B \in \mathbb{R}^n$ and assume that $K(A, B) = \mathbb{R}^n$. Let $W_m \in \mathbb{R}^{n \times n}$ be the matrix given by*

$$W_m = [B \ A^{-1}B \ AB \ A^{-2}B \ A^2B \ A^{-3}B \ \dots \ A^{m-1}B \ A^{-m}B],$$

and let

$$V_m = [v_1 \ v_2 \ \dots \ v_{2m-1} \ v_{2m}]$$

be any orthonormal matrix, such that

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

Let $H_m = V_m^T A V_m$. Then H_m is a nonsingular upper block Hessenberg matrix with block size 2, and

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

In addition, $K_m = H_m^{-1}$ is upper block Hessenberg with block size 2 and

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

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

$$W_m(H_m, e_1) = [w_1 \ w_2 \ \dots \ w_n] \in \mathbb{R}^{n \times n}$$

nonsingular, but more importantly

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

In particular,

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

which implies that the reduced order equations are immediately available. It remains to be seen if we can control the size of the residuals.

We now impose the extra condition that A be symmetric positive definite. Then H_m is symmetric positive definite with a special sparsity pattern which we exhibit in the case of $m = 3$ where

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

Now, let $H_m = L_m L_m^T$ be the Cholesky factorization of H_m . We will now show that L_m inherits its sparsity pattern from H_m . It is clear that H_m is a banded matrix with upper

and lower bandwidth at most 2. Therefore, L_m has a lower bandwidth of at most 2. We emphasize this by writing

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

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

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

As an illustration we exhibit the case of $m = 3$ where

$$L_m = \begin{bmatrix} + & & & \\ \times & + & & \\ * & \times & + & \\ \hline & & \times & + \\ & & * & \times & + \\ & & & \times & + \end{bmatrix}.$$

In addition, it is easy to see that $L_m L_m^T = H_m$ implies

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

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 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

$$T_m^T T_m = \begin{bmatrix} + & \times & \times & \times & \times & \times \\ & + & \times & \times & \times & \times \\ & & + & \times & \times & \times \\ \hline & & & + & \times & \times \\ & & & & + & \times \\ & & & & & + \end{bmatrix} \begin{bmatrix} + & & & & \\ \times & + & & & \\ \times & \times & + & & \\ \times & \times & \times & + & \\ \times & \times & \times & \times & + \\ \times & \times & \times & \times & \times & + \end{bmatrix} = \begin{bmatrix} \times & * & & & \\ * & \times & \times & * & \\ \times & \times & \times & & \\ * & \times & \times & \times & * \\ \hline & & \times & \times & \times \\ & & & * & \times & \times \end{bmatrix} = K_m.$$

Now, the key is to exploit the fact that the diagonal entries of T_m are nonzero. Starting with the last row of H_m^{-1} and working upwards, we deduce that the sparsity patterns of T_m and the lower triangular part of H_m^{-1} are identical. Specifically, in the case of $m = 3$, we have

$$T_m = \begin{bmatrix} + & & & \\ * & + & & \\ \times & + & & \\ * & \times & + & \\ \hline & & \times & + \\ & & * & \times & + \end{bmatrix}.$$

We summarize these results in the following lemma.

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*

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

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

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

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

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

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*

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

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

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

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

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

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

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

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

$$T_{jj} = \begin{bmatrix} + & 0 \\ * & + \end{bmatrix}, \quad j = 1, 2, \dots, m,$$

while

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

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

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

In the general case 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 seen if \hat{T}_{21} has the correct structure. We have

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

simply because the first row of L_{21} is orthogonal to the first column of L_{11} . It follows, that

$$\hat{T}_{21} = \begin{bmatrix} \begin{bmatrix} 0 & * \\ 0 & * \end{bmatrix} \\ O_2 \\ \vdots \\ O_2 \end{bmatrix}.$$

This completes the proof.

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*

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

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

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

and

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

The following examples emphasize that there is considerable freedom in the construction of H_m and K_m .

Example 1: If we choose

$$L_{jj} = \begin{bmatrix} + & 0 \\ - & + \end{bmatrix}, \quad j = 1, 2, \dots, m$$

as well as $\gamma_j > 0$ for $j < m$, then

$$T_{jj} = \begin{bmatrix} + & 0 \\ + & + \end{bmatrix}, \quad j = 1, 2, \dots, m$$

and

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

Naturally, this has implications for the sparsity patterns of H_m and K_m . As an illustration we display the case of $m = 3$ where

$$H_m = \begin{bmatrix} + & - & + & & & \\ - & + & - & & & \\ + & - & + & - & + & \\ - & + & - & & & \\ + & - & + & - & & \\ - & + & - & & & \end{bmatrix}, \quad \text{and} \quad K_m = \begin{bmatrix} + & + & & & & \\ + & + & + & + & & \\ + & + & + & & & \\ + & + & + & + & + & \\ + & + & + & & & \\ + & + & + & & & \end{bmatrix}.$$

Therefore, $W_m(H_m, e_1)$ is upper triangular with positive, rather than nonzero, diagonal entries.

Example 2: Let $0 < \varepsilon < 1$ and let

$$L_{jj} = \begin{bmatrix} 1 & 0 \\ -\varepsilon & 1 \end{bmatrix}.$$

Then,

$$L_{jj}^{-1} = \begin{bmatrix} 1 & 0 \\ \varepsilon & 1 \end{bmatrix} = T_{jj}, \quad L_{j+1,j} = \gamma_j \begin{bmatrix} \varepsilon & -1 \\ 0 & 0 \end{bmatrix}, \quad T_{j+1,j} = \gamma_j \begin{bmatrix} 0 & 1 \\ 0 & \varepsilon \end{bmatrix}, \quad \gamma_j > 0.$$

Now, if γ_j is small enough, then L is diagonally dominant by rows and if

$$\gamma_j(1 + \varepsilon) = \varepsilon \quad \Leftrightarrow \quad \gamma_j = \frac{\varepsilon}{1 + \varepsilon},$$

then the dominance factor is ε . It follows that

$$\kappa_\infty(L_m) \leq \frac{1 + \varepsilon}{1 - \varepsilon}.$$

In short, we can construct test matrices L_m and H_m which are well conditioned.

We are now ready to prove Theorem 3.1.

Proof We begin by considering Algorithm 1. 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 $\gamma_1, \gamma_2, \dots, \gamma_{j-1} > 0$. The matrices X_j are well defined and have full rank, simply because A_j is positive definite and

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

However, since we are free to choose $V_m = I_m$, we see that X_j is in fact the solution of the j th reduced order equation corresponding to

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

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

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

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

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

For the standard Arnoldi method it is much simpler to construct larger examples for which the residual curve is constant or nondecreasing for $j < n$, while the exact solution admits a good low rank approximation [24] and both symmetric and nonsymmetric equations can be constructed. At this point, we can not rule out the existence of such examples for the extended Krylov subspace method.

4 A secondary result

We now return to the situation of Lemma 3.1. Let $n = 2m$ be an even positive integer and let $A \in \mathbb{R}^{n \times n}$ be nonsingular. Let $B \in \mathbb{R}^n$ and assume $K(A, B) = \mathbb{R}^n$. Then the extended Krylov subspaces can be used to construct a matrix $V_m \in \mathbb{R}^{n \times n}$ with orthonormal columns such that if $H_m = V_m^T A V_m$, then H_m and H_m^{-1} are both upper block Hessenberg with block size 2. Now, suppose that A is negative definite. Then

$$H_m X + X H_m^T + e_1 e_1^T = 0$$

has a unique solution X which is symmetric positive definite. From the sparsity patterns of H_m and K_m we see that $W_m(H_m^T, H_m^T e_n)$ is nonsingular. It follows that the unique solution Y of

$$H_m^T Y + Y H_m + (H_m^T e_n)(H_m^T e_n)^T = 0$$

is symmetric positive definite. Now, the extended Krylov subspace method returns approximations X_i for X , such that

$$\text{Ran } X_i = \text{span}\{\underbrace{e_1, e_2, \dots, e_{2i-1}, e_{2i}}_{\text{the first } 2i \text{ columns of } I_n}\}$$

and approximations Y_j for Y , such that

$$\text{Ran } Y_j = \text{span}\{\underbrace{e_{n-2j+1}, e_{n-2j+2}, \dots, e_{n-1}, e_n}_{\text{the last } 2j \text{ columns of } I_n}\}.$$

It follows that

$$X_i Y_j = Y_j X_i = 0, \quad i + j \leq m$$

In short, it is impractical to use the extended Krylov subspace method to calculate the dominant eigenspaces for XY and YX . Naturally, this carries to the original problem. We state this as a theorem.

Theorem 4.1 *Let $m = 2n$ be an even positive integer and let $A \in \mathbb{R}^{n \times n}$ be a negative definite matrix. Let $B \in \mathbb{R}^n$ and assume that $K(A, B) = \mathbb{R}^n$. Then there exists a vector $C^T \in \mathbb{R}^n$, such that $K(A^T, C^T) = \mathbb{R}^n$, and if the extended Krylov subspace method is applied to the Lyapunov matrix equations*

$$AP + PA^T + BB^T = 0, \quad A^T Q + QA + C^T C = 0,$$

then the computed approximations P_i and Q_j satisfy

$$P_i Q_j = 0, \quad i + j \leq m.$$

Fig. 3.1 A MATLAB implementation of Algorithm 3.1

```

function [L A c f]=ieksm(l,r)

% IESKM = Invert EKSM.
%
% The function attempts to constructs a SPD matrix A, such
% that if the EKSM is applied to the Lyapunov equation
%  $A X + X A' = e1e1'$ , then the residual curve r is returned.
%
% Input:
% l : a parameter which determines the first block of L
% r : an array, containing the target residuals
%
% Output:
% L : the Cholesky factorization of A
% A : the desired matrix.
% c : the 2-norm condition number for certain principal
%     submatrices of A
% f : the residuals which EKSM would return,  $f(n)=0$ 
%

% Initialize L0 and determine the length of r.
L0=[1 0; sqrt(1/2) sqrt(1/2)]; n=length(r);

% Initialize the matrices
L=zeros(2*n,2*n); L(1:2,1:2)=L0; Q=zeros(2*n,2*n); Q(1,1)=1;

for i=1:n-1;
    % Assemble the matrix A
    A=L*L';

    % Solve the ith reduced order equation
    X=lyap(A(1:2*i,1:2*i),-Q(1:2*i,1:2*i));

    % Determine the next subdiagonal block of L up to a scaling
    aux=L(1+2*(i-1):2*i,1+2*(i-1):2*i)\[1; 0];

    % Determine the next subdiagonal block of A up to a scaling
    H=[aux(2) -aux(1); 0 0]*L(1+2*(i-1):2*i,1+2*(i-1):2*i)';

    % Determine the appropriate scaling factor
    gamma=r(i)/(sqrt(2)*norm(H*X(1+2*(i-1):2*i,:), 'fro'));

    % Apply the scaling to the next subdiagonal block of L
    L(1+2*i:2+2*i,1+2*(i-1):2*i)=-gamma*[aux(2) -aux(1); 0 0];

    % Select the next diagonal block of L
    l=abs(gamma*aux(1));
    L(1+2*i:2+2*i,1+2*i:2+2*i)=[1 0; sqrt(1/2) sqrt(1/2)];
end;

% Assemble the matrix A
A=L*L';

% Compute the indicated condition numbers
for i=1:n
    c(i)=cond(A(1:2*i,1:2*i));
end

% Compute the EKSM residuals. This is a shortcut, which relies on very
% special structure of L and A.

for i=1:n
    Xi=zeros(2*n,2*n); aux=lyap(A(1:2*i,1:2*i),-Q(1:2*i,1:2*i));
    Xi(1:2*i,1:2*i)=aux;
    Ri=A*Xi; Ri=Ri+Ri'-Q; f(i)=norm(Ri, 'fro');
end

```

We emphasize that this is a problem fundamental to the equations, rather than a defect of the algorithm. Specifically, there are linear time invariant systems (A, B, C) such that the system Gramians P and Q are orthogonal to machine precision. The simplest case known to us is that of a single n by n Jordan block

$$A = - \begin{bmatrix} d & & & \\ -1 & \ddots & & \\ & \ddots & \ddots & \\ & & -1 & d \end{bmatrix}.$$

If $d > 1$, then $A + A^T$ is symmetric negative definite by Gershgorin's circle theorem. Let J denote the antidiagonal matrix of size n . If we define

$$B = (\sqrt{2d}, 0, \dots, 0)^T, \quad \text{and} \quad C = JB = (0, \dots, 0, \sqrt{2d})^T,$$

then $Q = JPJ$ and a straight forward calculation shows that

$$p_{ij} = \binom{i+j-2}{j-1} v^{i-j-2}, \quad v = (2d)^{-1}.$$

We observe that P is a (graded) Pascal matrix. In particular, $p_{11} = 1$, so that $\|P\|_2 = \|Q\|_2 \geq 1$. Now, by Stirling's formula $p_{ij} \rightarrow 0$, for $i+j \rightarrow \infty$. Now, let $\text{fl}(x)$ denote the IEEE floating point representation of $x \in \mathbb{R}$. We see that, if n and d are sufficiently large, then not only is $\text{fl}(P)\text{fl}(Q) = 0$, but $\text{fl}(P\text{fl}(Qx)) = 0$ for all $\|x\|_2 \leq 1$. Why? Any number less than a certain threshold is rounded to zero. In short, it is effectively impossible to extract any information about the products of P and Q .

5 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 $A \in \mathbb{R}^n$ is symmetric negative definite and $B \in \mathbb{R}^n$ satisfies $K(A, B) = \mathbb{R}^n$. However, if A is symmetric negative definite, then a nondecreasing residual curve appears to be unlikely in the extreme and should only occur when A is very ill-conditioned.

If (A, B) is controllable, then we can find a vector $C^T \in \mathbb{R}^n$ such that (A^T, C^T) is observable and if the EKSM is applied to the Lyapunov equations

$$AP + PA^T + BB^T = 0, \quad A^T Q + QA + C^T C = 0,$$

then the approximations P_i and Q_j satisfy

$$P_i Q_j = 0$$

in exact arithmetic for all $i + j \leq m$, despite the fact that P and Q are nonsingular. This is a problem fundamental to the equations, rather than a defect of the algorithm.

Specifically, we presented an elementary example for which $\|P\|_2 = \|Q\|_2 \geq 1$, but $\text{fl}(P\text{fl}(Qx)) = 0$, where $x \in \mathbb{R}^n$ with $\|x\|_2 \leq 1$ and $\text{fl}(\cdot)$ denotes the floating point representation of the argument. Now, there are many real applications where this phenomenon is not an issue, but it would be interesting to chart the extent of the problem. Certainly, it is an issue in the analysis of general algorithms for Gramian based model reduction.

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