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A modified matrix sign function method for projected Lyapunov equations

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Abstract

In this paper we discuss the numerical solution of projected generalized Lyapunov equations using the matrix sign function method. Such equations arise in stability analysis and control problems for descriptor systems including model reduction based on balanced truncation. It is known that the matrix sign function method applied to a matrix pencil $\lambda E - A$ converges if and only if $\lambda E - A$ is of index at most two. The convergence is quadratic if E is nonsingular, and it is linear, otherwise. We will propose a modification of the matrix sign function method that converges quadratically for pencils of arbitrary index. Numerical examples will be presented to demonstrate the properties of the modified method.

Key words: matrix sign function, matrix pencils, projected Lyapunov equations

1 Introduction

Consider a projected generalized continuous-time algebraic Lyapunov equation (GCALE)

$$E^T X A + A^T X E = -P_r^T G P_r, \quad X = P_l^T X P_l, \quad (1)$$

where $E, A, G \in \mathbb{R}^{n,n}$ are given matrices, P_l and P_r are the spectral projectors onto the left and right deflating subspaces corresponding to the finite eigenvalues of a regular pencil $\lambda E - A$ and $X \in \mathbb{R}^{n,n}$ is unknown. If the pencil $\lambda E - A$ is *stable*, i.e., all its finite eigenvalues have negative real part, then the projected GCALE (1) has a unique solution X for every G . If, additionally,

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G is symmetric and positive (semi)definite, then X is symmetric and positive semidefinite [36]. Projected Lyapunov equations of the form (1) arise in stability analysis and control design problems for descriptor systems including the characterization of controllability and observability properties, computing H_2 and Hankel norms, determining the minimal and balanced realizations as well as balanced truncation model order reduction [5,31,36,38]. In the literature, also other types of generalized Lyapunov equations have been considered that are useful in stability and optimal regulator problems for descriptor systems [23,28,40]. However, the application of such equations is usually limited to index one problems (see the definition of the index below), whereas the existence and uniqueness results for the projected GCALE (1) can be stated independently of the index of the pencil $\lambda E - A$.

There are several numerical methods for projected Lyapunov equations. In [35], generalizations of the Bartels-Stewart method [3,32] and the Hammarling method [22,32] have been proposed for (1) that are based on the preliminary transformation of the pencil $\lambda E - A$ into a generalized Schur form, solution of the generalized Sylvester and Lyapunov equations in (quasi)upper triangular form and back transformations. Since these methods cost $\mathcal{O}(n^3)$ operations and require $\mathcal{O}(n^2)$ memory location, they are restricted to the problems of small or medium size. Projected Lyapunov equations can also be solved by the iterative methods based on the ADI and Smith techniques [29,33,37]. These methods are especially efficient for large sparse Lyapunov equations with low-rank right-hand side.

In this paper, we consider the numerical solution of the projected GCALE (1) with large dense matrix coefficients using the matrix sign function method. This method was first proposed in [34] for standard Lyapunov equations, see also [13,24–26], and then extended to generalized Lyapunov equations with nonsingular E in [6,10,18,27,30]. The case of singular E was studied in the context of deflating subspace computations in [39]. It was observed there that the generalized matrix sign function method applied to the pencil $\lambda E - A$ converges only if $\lambda E - A$ is of index at most two. Furthermore, the convergence is quadratic if E is nonsingular, and it is linear, otherwise. We will propose a modification of the matrix sign function method for solving the projected GCALE (1) that ensures the quadratic convergence rate for matrix pencils of arbitrarily large index.

A major difficulty in the numerical solution of the projected GCALE (1) by iterative methods is that we need to compute the spectral projectors P_l and P_r . For large-scale problems this may be very expensive. Fortunately, in many applications such as computational fluid dynamics, electrical circuit simulation and constrained structural mechanics, the matrices E and A have some special block structure. This structure can be used to obtain the projectors P_l and P_r in explicit form [31,37]. Therefore, in the following we will assume that these

projectors are known.

In Section 2 we review some results on the matrix sign function. In Section 3 we present a modification of the matrix sign function method and its low-rank version for the projected GCALE (1). Section 4 contains some results of numerical experiments. Concluding remarks are given in Section 5.

Throughout the paper we will denote by $\mathbb{R}^{n,m}$ the space of $n \times m$ real matrices. The matrix A^T stands for the transpose of $A \in \mathbb{R}^{n,m}$, A^{-1} is the inverse of nonsingular $A \in \mathbb{R}^{n,n}$, and $A^{-T} = (A^{-1})^T$. An identity matrix of order n is denoted by I_n or simply by I .

2 The matrix sign function method

The *matrix sign function method* is one of the most popular approaches to solve large-scale dense Lyapunov equations [6,10,13,18,24–27,34]. In this section, we briefly summarize some results from there and show why the matrix sign function method cannot directly be applied to generalized Lyapunov equations with singular E .

Assume that a matrix $A \in \mathbb{R}^{n,n}$ has no eigenvalues on the imaginary axis. Let

$$A = T^{-1} \begin{bmatrix} J_- & 0 \\ 0 & J_+ \end{bmatrix} T$$

be the Jordan decomposition of A , where T is nonsingular, the eigenvalues of J_- lie in the open left half-plane and the eigenvalues of J_+ lie in the open right half-plane. Then a *matrix sign function* of A is defined via

$$\text{sign}(A) = T^{-1} \begin{bmatrix} -I & 0 \\ 0 & I \end{bmatrix} T.$$

If A has an eigenvalue on the imaginary axis, then $\text{sign}(A)$ is not defined.

Since $(\text{sign}(A))^2 = I$, the matrix $\text{sign}(A)$ can be computed by the Newton method applied to the nonlinear matrix equation $X^2 - I = 0$. The Newton iteration for the matrix sign function is given by

$$A_0 = A, \quad A_k = \frac{1}{2}(A_{k-1} + A_{k-1}^{-1}).$$

If A has no eigenvalues on the imaginary axis, then this iteration is quadratically convergent and $\lim_{k \rightarrow \infty} A_k = \text{sign}(A)$, see [24,34] for details.

The matrix sign function method has been extended to matrix pencils in [1,18,39]. For a pencil $\lambda E - A$ with $E, A \in \mathbb{R}^{n,n}$, a *generalized matrix sign function iteration* is given by

$$A_0 = A, \quad A_k = \frac{1}{2}(A_{k-1} + EA_{k-1}^{-1}E). \quad (2)$$

The convergence of this iteration strongly depends on the properties of the pencil $\lambda E - A$. If $\lambda E - A$ has no finite eigenvalues on the imaginary axis, then it can be reduced to the Weierstrass canonical form

$$E = W \begin{bmatrix} I & 0 & 0 \\ 0 & I & 0 \\ 0 & 0 & N \end{bmatrix} T, \quad A = W \begin{bmatrix} J_- & 0 & 0 \\ 0 & J_+ & 0 \\ 0 & 0 & I \end{bmatrix} T, \quad (3)$$

where W and T are nonsingular, the matrices J_- and J_+ have eigenvalues in the open left and right half-planes, respectively, and the matrix N is nilpotent with index of nilpotence ν , see [17]. The number ν is called the *index* of $\lambda E - A$. The eigenvalues of J_- and J_+ are the finite eigenvalues of the pencil $\lambda E - A$, and N corresponds to the eigenvalue at infinity. Using the Weierstrass canonical form (3), one can show by induction that the iteration matrices A_k generated by (2) have the form

$$A_k = W \begin{bmatrix} J_k^- & 0 & 0 \\ 0 & J_k^+ & 0 \\ 0 & 0 & N_k \end{bmatrix} T,$$

where

$$\begin{aligned} J_k^- &= -(I + (I - J_-)^{-2k}(I + J_-)^{2k})(I - (I - J_-)^{-2k}(I + J_-)^{2k})^{-1}, \\ J_k^+ &= (I + (I + J_+)^{-2k}(I - J_+)^{2k})(I - (I + J_+)^{-2k}(I - J_+)^{2k})^{-1}, \\ N_k &= 2^{-k}I + \frac{2^k - 2^{-k}}{3}N^2 + \mathcal{O}(N^4), \quad k = 1, 2, 3, \dots \end{aligned} \quad (4)$$

Here $\mathcal{O}(N^4)$ denotes the terms containing the powers of N^4 . Thus, if E is nonsingular and $\lambda E - A$ has no eigenvalues on the imaginary axis, then the iteration (2) converges quadratically to $E \text{sign}(E^{-1}A) = \text{sign}(AE^{-1})E$. For

singular E , the iteration (2) is convergent only if the pencil $\lambda E - A$ is of index at most two and it has no eigenvalues on the imaginary axis. In this case, the convergence rate is only linear, but not quadratic as for nonsingular E . If the index of $\lambda E - A$ is greater than two, i.e., $N^2 \neq 0$, then the iteration (2) diverges.

Consider now a generalized Lyapunov equation

$$E^T X A + A^T X E = -G, \quad (5)$$

where $E, A, G \in \mathbb{R}^{n,n}$ are given matrices and $X \in \mathbb{R}^{n,n}$ is unknown. The solution X of this equation can be computed by applying the generalized matrix sign function iteration (2) to the pencil

$$\lambda \begin{bmatrix} E & 0 \\ 0 & E^T \end{bmatrix} - \begin{bmatrix} A & 0 \\ G & -A^T \end{bmatrix}, \quad (6)$$

see [10,18,34] for details. Using a special block structure of the matrices in (6), this iteration can be written as

$$\begin{aligned} A_0 &= A, & A_k &= \frac{1}{2c_k} (A_{k-1} + c_k^2 E A_{k-1}^{-1} E), \\ G_0 &= G, & G_k &= \frac{1}{2c_k} (G_{k-1} + c_k^2 E^T A_{k-1}^{-T} G_{k-1} A_{k-1}^{-1} E), \end{aligned} \quad (7)$$

where c_k is a scalar parameter used to accelerate the convergence of the iteration. It can be chosen as $c_k = (|\det(A_{k-1})/\det(E)|)^{1/n}$ in the case of nonsingular E or $c_k = \sqrt{\|A_{k-1}\|/\|A_{k-1}^{-1}\|}$. Other scaling strategies can be found in [2,13,18,34]. If the matrix E is nonsingular and if the pencil $\lambda E - A$ is stable, then

$$\lim_{k \rightarrow \infty} A_k = -E, \quad \lim_{k \rightarrow \infty} G_k = 2E^T X E,$$

where X is the solution of (5). Therefore, as a stopping criterion in (7) the condition $\|A_k + E\| \leq tol$ can be taken with some matrix norm $\|\cdot\|$ and a tolerance tol .

For nonsingular E , comparison of the matrix sign function method to the generalized Bartels-Stewart and Hammarling methods with respect to the accuracy and computational cost can be found in [10]. It has been observed there that the matrix sign function method is about as expensive as the Bartels-Stewart method and that both methods require approximately the

same amount of work space. However, the matrix sign function method is more appropriate for parallelization [8] than the generalized Bartels-Stewart method and it is currently the only practicable approach to solve generalized Lyapunov equations with large dense matrix coefficients. An implementation of the matrix sign function method on parallel distributed computers can be found in the PARALLEL LIBRARY IN CONTROL¹ [11].

The computation of the solution (generalized) Lyapunov equations via the (generalized) matrix sign function method requires only basic linear algebra operations such as matrix-matrix multiplication and matrix inversion (or solution of linear systems). In this case, the data-sparse matrix representation like hierarchical matrix format [20,21] and the corresponding approximate arithmetic can be used for efficient implementation of the matrix sign function method [4,19].

The matrix sign function method has a disadvantage that the computation of an explicit inverse of A_k is required at every iteration. This may lead to significant roundoff errors for ill-conditioned A_k . Such difficulties may arise when eigenvalues of the pencil $\lambda E - A$ lie close to the imaginary axis or $\lambda E - A$ is nearly singular. It should also be noted that for the stable pencil $\lambda E - A$ of index one or two, even if the finite eigenvalues of $\lambda E - A$ are sufficiently far from the imaginary, the sequence of matrices A_k in (7) converges to a singular matrix. In [7], an inverse-free version of the matrix sign function method was proposed that is based on arithmetic-like operations for matrix pencils and does not involve matrix inverses. However, this method just like the iteration (2) is divergent if the index of the pencil $\lambda E - A$ exceeds two. Thus, the matrix sign function method cannot be directly utilized for generalized Lyapunov equations with singular E . In the next section, we present a possible extension of the matrix sign function method to the projected GCALE (1).

3 Sign function method for projected Lyapunov equations

Assume that the pencil $\lambda E - A$ is stable. Then $\lambda E - A$ can be reduced to the Weierstrass canonical form (3), where the block J_+ does not appear. In this case, the spectral projectors P_l and P_r onto the left and right deflating subspaces corresponding to the finite eigenvalues of $\lambda E - A$ have the form

$$P_l = W \begin{bmatrix} I & 0 \\ 0 & 0 \end{bmatrix} W^{-1}, \quad P_r = T^{-1} \begin{bmatrix} I & 0 \\ 0 & 0 \end{bmatrix} T. \quad (8)$$

¹ Available from <http://www.pscom.uji.es/plic/>

As mentioned above, the presence of the nilpotent block N in (3) makes the matrix sign iteration (2) divergent if $N^2 \neq 0$. In order to guarantee the convergence, we have to remove this block from E . This can be achieved, for example, if we multiply E by P_l from the left and/or by P_r from the right. Then the matrix sign function iteration takes the form

$$\hat{A}_k = \frac{1}{2}(\hat{A}_{k-1} + P_l E \hat{A}_{k-1}^{-1} E P_r) = W \begin{bmatrix} J_k^- & 0 \\ 0 & 2^{-k} I \end{bmatrix} T \quad (9)$$

with J_k^- as in (4). This iteration has the linear convergence rate and \hat{A}_k converges to a singular matrix. To get rid of the ill-conditioning of \hat{A}_k and to ensure the quadratic convergence as in the case of nonsingular E , we modify (9) as

$$A_k = \frac{1}{2}(A_{k-1} + P_l E A_{k-1}^{-1} E P_r + (I - P_l)A(I - P_r)) = W \begin{bmatrix} J_k^- & 0 \\ 0 & I \end{bmatrix} T.$$

Observe that

$$\begin{aligned} P_l E A_{k-1}^{-1} E P_r &= P_l E A_{k-1}^{-1} E = E A_{k-1}^{-1} E P_r, \\ (I - P_l)A(I - P_r) &= (I - P_l)A = A(I - P_r). \end{aligned}$$

Therefore, to reduce computations, the multiplication by P_l and $I - P_l$ can be left out. The iterations for G_k in (7) do not change. Note that if we start with $G_0 = P_r^T G P_r$, then all the iterates G_k satisfy $G_k = P_r^T G_k P_r$ and $\lim_{k \rightarrow \infty} A_k^{-T} G_k A_k^{-1} = 2X$ with $X = P_l^T X P_l$. The modified generalized matrix sign function method for the projected GCALE (1) is summarized in the following algorithm.

Algorithm 1 A modified matrix sign function method for projected GCALES

INPUT: $E, A, G, P_r \in \mathbb{R}^{n,n}$, $\lambda E - A$ is stable.

OUTPUT: An approximate solution X of the projected GCALE (1).

1. $A_0 = A, G_0 = P_r^T G P_r$.
2. FOR $k = 1, 2, \dots$

$$\begin{aligned} c_k &= \sqrt{\|A_{k-1}\| / \|A_{k-1}^{-1}\|}, \\ A_k &= \frac{1}{2c_k} \left(A_{k-1} + c_k^2 E A_{k-1}^{-1} E P_r + (2c_k - 1)A(I - P_r) \right), \\ G_k &= \frac{1}{2c_k} \left(G_{k-1} + c_k^2 E^T A_{k-1}^{-T} G_{k-1} A_{k-1}^{-1} E \right). \end{aligned} \quad (10)$$

END FOR

3. $X = \frac{1}{2} A_k^{-T} G_k A_k^{-1}$.
-

Since $\lim_{k \rightarrow \infty} A_k = -EP_r + A(I - P_r)$, the stopping criterion in Algorithm 1 can be chosen as $\|A_k + E_0\| \leq \text{tol}$ with $E_0 = EP_r - A(I - P_r)$ and some tolerance tol . Compared to the generalized sign function iteration (7), Algorithm 1 requires only two additional products EP_r and $A(I - P_r)$ at the beginning and one matrix addition at every iteration step.

Many practical applications lead to the projected GCALE (1) with a symmetric and positive semidefinite matrix G in factored form $G = C^T C$ with $C \in \mathbb{R}^{p,n}$. If $\lambda E - A$ is stable, then such an equation has a unique symmetric, positive semidefinite solution X that can also be factored as $X = L^T L$. Furthermore, if the number of rows in C is much smaller than the number of columns, or, equivalently, if the rank of G is much smaller compared to its size, then the eigenvalues of the solution X often decay very rapidly. Such a solution has a small numerical rank. The full numerical rank factor of X can be determined without forming the product $C^T C$ and computing X explicitly using the same approach as in the case of nonsingular E , see [12,27]. Exploiting the factored form of $G = C^T C$, we obtain the iteration

$$A_0 = A, \quad C_0 = CP_r, \quad (11)$$

$$A_k = \frac{1}{2c_k} \left(A_{k-1} + c_k^2 EA_{k-1}^{-1} EP_r + (2c_k - 1)A(I - P_r) \right), \quad (12)$$

$$\begin{bmatrix} C_{k-1} \\ c_k C_{k-1} A_{k-1}^{-1} E \end{bmatrix} = Q_k \begin{bmatrix} R_k \\ 0 \end{bmatrix} \Pi_k, \quad (13)$$

$$C_k = \frac{1}{\sqrt{2c_k}} R_k \Pi_k, \quad (14)$$

where (13) is the rank-revealing QR decomposition [14]. Here Q_k is orthogonal, Π_k is a permutation matrix and R_k has full row rank. The approximate full rank factor of the solution X can be computed as $L_k = (1/\sqrt{2})C_k A_k^{-1}$ and we have $X = L^T L \approx L_k^T L_k$.

4 Numerical examples

In this section we present some results of numerical experiments to demonstrate the properties of the modified matrix sign function method. Computations were done on IBM RS 6000 44P Modell 270 using MATLAB 7.0.4 with machine precision $\varepsilon \approx 2.22 \times 10^{-16}$.

Example 1 Consider the 2D instationary Stokes equation that describes the flow of an incompressible fluid in a domain. The spatial discretization of this

equation by the finite difference method on a uniform staggered grid leads to the descriptor system

$$\begin{aligned} E\dot{x}(t) &= Ax(t) + Bu(t), \\ y(t) &= Cx(t), \end{aligned} \tag{15}$$

with the matrices

$$E = \begin{bmatrix} I & 0 \\ 0 & 0 \end{bmatrix}, \quad A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & 0 \end{bmatrix},$$

where the matrices A_{12} and A_{21} have full rank. In this case, the pencil $\lambda E - A$ is of index two. The spectral projectors P_l and P_r for such a pencil can be found in [31,37]. The matrix G in the projected GCALE (1) is $G = C^T C$.

We compare the generalized sign function iteration (7) and the modified generalized sign function iteration (10), hereafter GSIGN and MGSIGN, respectively. We stop the iterations as soon as the condition $\phi(A_k) \leq n\sqrt{\varepsilon}$ is satisfied, where $\phi(A_k) = \|A_k + EP_r\|_F$ in the GSIGN method and

$$\phi(A_k) = \|A_k + EP_r - A(I - P_r)\|_F$$

in the MGSIGN method, and two additional iterations are performed. Here $\|\cdot\|_F$ denotes the Frobenius matrix norm. In both methods, we use the scaling

$$c_k = \begin{cases} \sqrt{\|A_k\|_F / \|A_k^{-1}\|_F} & \text{if } \phi(A_k) > 0.1 \text{ and } k > 3, \\ 1 & \text{otherwise.} \end{cases}$$

Figure 1 shows the convergence history $\phi(A_k)$ for the GSIGN and MGSIGN methods. One can see that the GSIGN method converges linearly, while the MGSIGN method has the quadratic convergence rate. In Figure 2, we present the condition numbers of A_k at every iteration step for both methods. As expected, the condition number of A_k in the GSIGN iteration (7) increases continuously, whereas the condition number of A_k in the MGSIGN iteration (10) remains bounded. Clearly, the solution provided by the GSIGN method may be inaccurate because of ill-conditioning of A_k . The normalized residuals

$$\frac{\|E^T X A + A^T X E + P_r^T C^T C P_r\|_F}{\|P_r^T C^T C P_r\|_F} \tag{16}$$

for the solutions X computed via the GSIGN and MGSIGN methods are $2.73 \cdot 10^{-12}$ and $1.03 \cdot 10^{-8}$, respectively. Note that for ill-conditioned problems, the small residual norm does not imply that the error in the computed solution is also small, see [35].

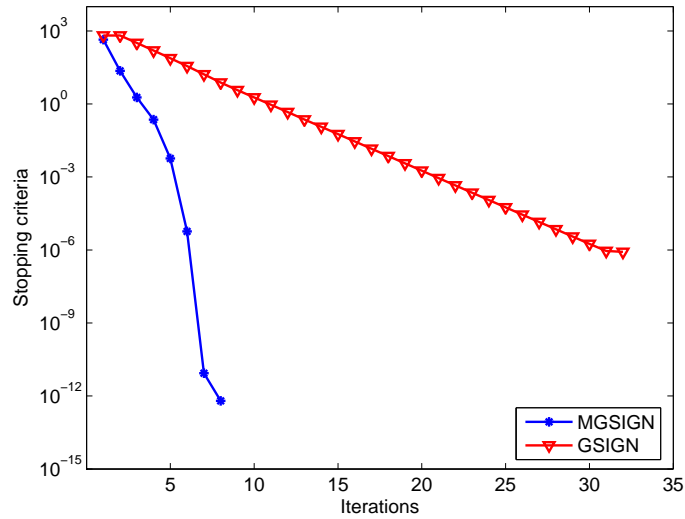


Fig. 1. Example 1: the convergence history for the generalized sign function method and the modified generalized sign function method.

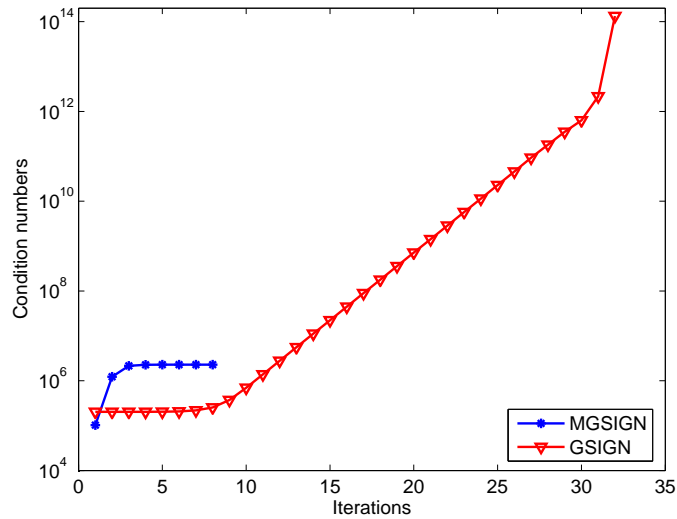


Fig. 2. Example 1: the condition numbers of A_k for the generalized sign function method and the modified generalized sign function method.

Example 2 Consider a damped mass-spring system with g masses as in [31]. The i th mass is connected to the $(i + 1)$ st mass by a spring and a damper and also to the ground by another spring and damper. Moreover, the first mass is connected to the last one by a rigid bar and it can be influenced by a control. The vibration of this system is described by the descriptor system (15) with

the matrices

$$E = \begin{bmatrix} I_g & 0 & 0 \\ 0 & M & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad A = \begin{bmatrix} 0 & I_g & 0 \\ K & D & -F^T \\ F & 0 & 0 \end{bmatrix}.$$

Here M is the symmetric, positive definite mass matrix, K is the stiffness matrix, D is the damping matrix and F is the full rank matrix of constraints. The pencil $\lambda E - A$ is of index three. The spectral projectors P_l and P_r for such a pencil can be found in [31,37]. The matrix C has the form $C = [e_1, e_2, e_{g-1}]^T \in \mathbb{R}^{3,n}$, where e_j denotes the j -th column of the identity matrix I_{2g+1} .

In this set of experiments, we compare computing the factorized solution of the projected GCALE (1) with $G = C^T C$ using the modified generalized sign function iteration (11)–(14) and the generalized Hammarling method [35]. The later was implemented using the GUPTRI routines² [15,16] for computing the generalized Schur form and the SLICOT library routines³ [9] for solving the upper (quasi)triangular Sylvester and Lyapunov equations called via the mex files in MATLAB. Figure 3 reports the execution time for the generalized Hammarling method (GHamm) and the 10 iterations of the modified generalized sign function iteration (MGSIGN) for different problem sizes increasing from $n = 101$ to $n = 1001$. The generalized Hammarling method provides the Cholesky factor $L \in \mathbb{R}^{n,n}$ of the solution $X = L^T L$, while the approximate factor L_k of $X \approx L_k^T L_k$ computed by the sign function iteration (11)–(14) has 75 rows in all experiments.

Figure 4 shows the normalized residuals (16) for the solutions computed via the MGSIGN iteration and the generalized Hammarling method. One can see that the residuals provided by the the MGSIGN iteration are smaller than those in the Hammarling method.

5 Conclusions

We have presented a modified method based on the matrix sign function iteration that can be used for solving projected generalized Lyapunov equations. Unlike the classical matrix sign function iteration, this method converges quadratically independent of the index of the underlying matrix pencil. Numerical experiments show that the modified matrix sign function method is competitive with direct methods for large dense problems. This method is well suited for parallelization and use of hierarchical matrix format is also possible.

² Available from http://www.cs.umu.se/research/nla/singular_pairs/guptri

³ Available from <http://www.slicot.de>

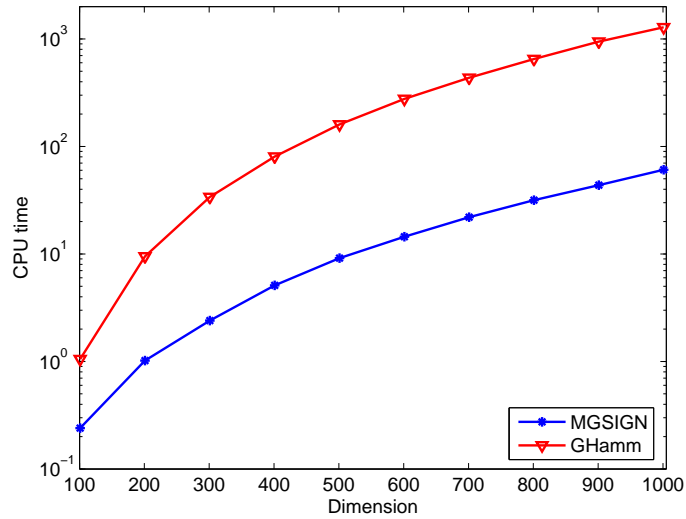


Fig. 3. Example 2: the execution time for the modified sign function method and the generalized Hammarling method.

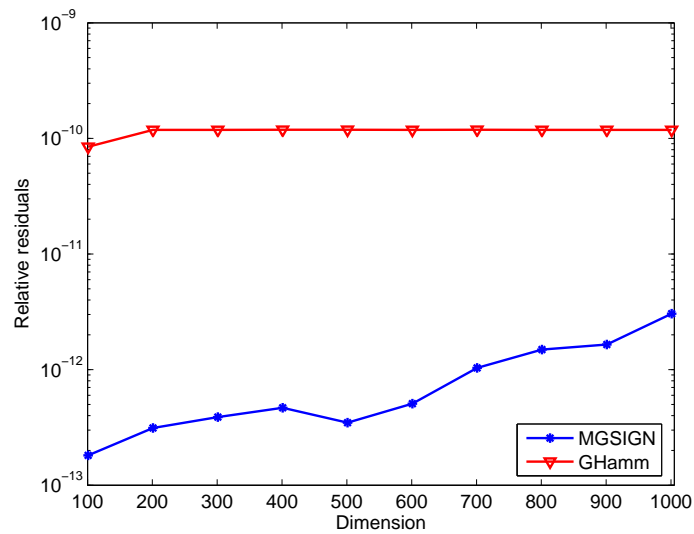


Fig. 4. Example 2: the normalized residuals for the modified sign function method and the generalized Hammarling method.

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