

# Efficient methods for solving a nonsymmetric algebraic Riccati equation arising in stochastic fluid models<sup>1</sup>

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## Abstract

We consider the nonsymmetric algebraic Riccati equation  $XM_{12}X + XM_{11} + M_{22}X + M_{21} = 0$ , where  $M_{11}, M_{12}, M_{21}, M_{22}$  are real matrices of sizes  $n \times n, n \times m, m \times n, m \times m$ , respectively, and  $M = [M_{ij}]_{i,j=1}^2$  is an irreducible singular  $M$ -matrix with zero row sums. The equation plays an important role in the study of stochastic fluid models, where the matrix  $-M$  is the generator of a Markov chain. The solution of practical interest is the minimal nonnegative solution. This solution may be found by basic fixed-point iterations, Newton's method and the Schur method. However, these methods run into difficulties in certain situations. In this paper we provide two efficient methods that are able to find the solution with high accuracy even for these difficult situations.

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*Key words:* Nonsymmetric algebraic Riccati equation;  $M$ -matrix; Minimal nonnegative solution; Schur method; Latouche–Ramaswami algorithm

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## 1 Introduction

In [7] we studied the nonsymmetric algebraic Riccati equation (ARE)

$$XM_{12}X + XM_{11} + M_{22}X + M_{21} = 0, \quad (1)$$

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where  $M_{11}, M_{12}, M_{21}, M_{22}$  are real matrices of sizes  $n \times n, n \times m, m \times n, m \times m$ , respectively, and

$$M = \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix} \quad (2)$$

is a nonsingular  $M$ -matrix or an irreducible singular  $M$ -matrix. (A square matrix  $A$  is called an  $M$ -matrix if  $A = sI - B$  with  $B \geq 0$  (elementwise order) and  $s \geq \rho(B)$ , where  $\rho(\cdot)$  is the spectral radius. It is called a singular  $M$ -matrix if  $s = \rho(B)$ ; it is called a nonsingular  $M$ -matrix if  $s > \rho(B)$ .) Nonsymmetric AREs of this type appear in the study of fluid models through Wiener–Hopf factorization of Markov chains (see [23] and the references therein). The solution of practical interest is the minimal nonnegative solution. In this paper we limit our attention to the most important situation that  $M$  is an irreducible singular  $M$ -matrix with  $Me = 0$ , where  $e$  is a column vector with all components equal to one. The dimension of  $e$  is often clear from the context. Otherwise, we use  $e^{(k)}$  to indicate that the dimension is  $k$ .

The following result is a special case of the results established in [7]. (The main results of [7] have been summarized and updated in [11].)

**Theorem 1** *Let  $M$  be an irreducible singular  $M$ -matrix with  $Me = 0$ . Then (1) has a minimal nonnegative solution  $S$  and  $Se \leq e$ .*

It has been shown in [9] that the minimal nonnegative solution  $S$  is positive.

Let  $\hat{S}$  be the minimal nonnegative solution of

$$XM_{21}X + XM_{22} + M_{11}X + M_{12} = 0, \quad (3)$$

the dual equation of (1). Then we also have  $\hat{S}e \leq e$  and  $\hat{S} > 0$ . It has been shown in [7] that the matrices  $Z = M_{11} + M_{12}\hat{S}$  and  $\hat{Z} = M_{22} + M_{21}\hat{S}$  are irreducible  $M$ -matrices and that  $Ze \geq 0$  and  $\hat{Z}e \geq 0$ .

Three types of methods for finding the minimal nonnegative solution  $S$  have been studied in [7]. They are basic fixed-point iterations, Newton’s method and the Schur method. The most difficult situation for these methods occurs when  $u_1^T e = u_2^T e$ , where  $u_1 \in \mathbb{R}^n$  and  $u_2 \in \mathbb{R}^m$  are positive vectors such that  $(u_1^T \ u_2^T)M = 0$ . (The vectors  $u_1$  and  $u_2$  are uniquely determined if we assume  $u_1^T e + u_2^T e = 1$ , for example.) In this situation, the convergence of the fixed-point iterations is sublinear and the convergence of Newton’s method is typically linear with rate  $1/2$ . Difficulties also arise when  $u_1^T e \approx u_2^T e$ . The Schur method also runs into difficulties when  $u_1^T e \approx u_2^T e$ , as we will explain later.

On the other hand, the difficult situation is also an important situation. In the study of Markov chains,  $-M$  is the generator of the Markov chain. Since  $M$  has a zero eigenvalue, the chain will live forever. (If  $M$  were an irreducible nonsingular  $M$ -matrix with nonnegative row sums, the chain would die out.) In the Wiener–Hopf factorization of the Markov chain (see [23]), we get two new Markov chains with generators  $-Z$  and  $-\hat{Z}$ , respectively. The difficult situation ( $u_1^T e = u_2^T e$ ) is precisely the situation where both chains will live forever.

In this paper we present two efficient methods for finding the solution  $S$ . The first one is a modified Schur method presented in Section 3. To put this method in a proper setting, the original Schur method is discussed in Section 2. The modified Schur method is expected to have high accuracy even when  $u_1^T e \approx u_2^T e$ . However, there is not much we can do if the accuracy is not high enough when  $u_1^T e \approx u_2^T e$ , since Newton’s method (the standard tool for iterative refinement) runs into difficulties in this case. The second method is based on an important observation by Ramaswami [22] that the equation (1) is closely related to a quadratic matrix equation arising in quasi-birth-death processes (QBDs), for which the powerful Latouche–Ramaswami (LR) algorithm [18] can be applied. The LR algorithm is an iterative procedure and is much easier to use than the Schur method. However, a direct application of the LR algorithm would require about  $\frac{400}{3}n^3$  flops each iteration when  $m = n$ , while the Schur method (modified or not) only requires roughly  $200n^3$  flops for the whole computation. In Section 4, we present a simplified LR algorithm using the special structure of the QBD. The simplified algorithm requires about  $\frac{124}{3}n^3$  flops each iteration when  $m = n$ . The (simplified) LR algorithm has quadratic convergence when  $u_1^T e \neq u_2^T e$ . In many cases, the LR algorithm requires only a small number of iterations, so the computational work of the simplified LR algorithm is comparable to that for the (modified) Schur method. When  $u_1^T e = u_2^T e$ , however, the convergence of the LR algorithm is expected to be linear with rate  $1/2$ . In this case, the simplified LR algorithm is still much more expensive than the Schur method. In Section 5, for the case  $u_1^T e \geq u_2^T e$ , we use a modification of a shift technique proposed in [14] to speed up the convergence of the simplified LR algorithm without increasing the computational work per iteration. In particular, quadratic convergence is recovered for the (simplified) LR algorithm for the case  $u_1^T e = u_2^T e$ . In Section 6, we present some numerical results to show the efficiency and accuracy of the modified Schur method and the simplified LR algorithm with a shift.

## 2 The Schur method

It has been pointed out in [20] that the Schur method can be used to find solutions of general nonsymmetric AREs. In particular, the Schur method can

find the minimal solution  $S$  of (1) by using an appropriate invariant subspace of the matrix

$$R = \begin{bmatrix} M_{11} & M_{12} \\ -M_{21} & -M_{22} \end{bmatrix}. \quad (4)$$

So we first provide some information about the eigenvalues of the matrix  $R$ . We denote the open left half-plane and the open right half-plane by  $\mathbb{C}_<$  and  $\mathbb{C}_>$ , respectively. The next result is an update of some results in [7] and [11]. See also [23] for relevant results in the context of Markov chains, which are obtained using probabilistic arguments and interpretations.

**Theorem 2** *With previous notations, we have*

- (1) *If  $u_1^T e = u_2^T e$ , then  $R$  has  $n-1$  eigenvalues in  $\mathbb{C}_>$ ,  $m-1$  eigenvalues in  $\mathbb{C}_<$ , and two zero eigenvalues with only one linearly independent eigenvector. Moreover,  $Se = e$  and  $\hat{S}e = e$ .*
- (2) *If  $u_1^T e > u_2^T e$ , then  $R$  has  $n-1$  eigenvalues in  $\mathbb{C}_>$ ,  $m$  eigenvalues in  $\mathbb{C}_<$ , and one zero eigenvalue. Moreover,  $Se = e$ ,  $\hat{S}e \leq e$  and  $\hat{S}e \neq e$ .*
- (3) *If  $u_1^T e < u_2^T e$ , then  $R$  has  $n$  eigenvalues in  $\mathbb{C}_>$ ,  $m-1$  eigenvalues in  $\mathbb{C}_<$ , and one zero eigenvalue. Moreover,  $Se \leq e$ ,  $Se \neq e$  and  $\hat{S}e = e$ .*

**Remark 3** *In [7] and [11], the conclusion  $Se = e$  ( $\hat{S}e = e$ ) was made under the additional assumption that  $M_{12}$  ( $M_{21}$ ) has no zero columns. The additional assumption can be removed by using a continuity argument. We shall not give the argument here since the conclusion also follows from Theorem 6 and Propositions 7 and 8 in Section 4.*

We can easily verify the so-called Wiener–Hopf factorization for the matrix (2) (see [7,23]):

$$\begin{bmatrix} M_{11} & M_{12} \\ -M_{21} & -M_{22} \end{bmatrix} \begin{bmatrix} I & \hat{S} \\ S & I \end{bmatrix} = \begin{bmatrix} I & \hat{S} \\ S & I \end{bmatrix} \begin{bmatrix} Z & 0 \\ 0 & -\hat{Z} \end{bmatrix}. \quad (5)$$

It is shown in [7] that the eigenvalues of  $Z$  are the  $n$  eigenvalues of  $R$  with largest real parts and that the eigenvalues of  $\hat{Z}$  are the negative of the  $m$  eigenvalues of  $R$  with smallest real parts, even when the matrix

$$\begin{bmatrix} I & \hat{S} \\ S & I \end{bmatrix}$$

is singular. Recall that the matrices  $Z$  and  $\hat{Z}$  are irreducible  $M$ -matrices. Thus, by the Perron–Frobenius theory (see [4,24]), for case (2) in Theorem 2 the eigenvalue of  $R$  that is in  $\mathbb{C}_{<}$  and closest to the imaginary axis must be real and simple; for case (3) in Theorem 2 the eigenvalue of  $R$  that is in  $\mathbb{C}_{>}$  and closest to the imaginary axis must be real and simple. We can also see from (5) that the column space of  $(I - S^T)^T$  is the unique  $n$ -dimensional invariant subspace of  $R$  corresponding to the  $n$  eigenvalues of  $R$  with largest real parts. This means that the solution  $S$  may be obtained by the Schur method as described below (see [7] for a slight different presentation).

**Theorem 4** *Let  $U$  be an orthogonal matrix such that*

$$U^T R U = N$$

*is a real Schur form of  $R$ , where the  $1 \times 1$  or  $2 \times 2$  diagonal blocks of  $N$  corresponding to eigenvalues in  $\mathbb{C}_{>}$  come before the  $1 \times 1$  block(s) corresponding to the zero eigenvalue(s), which is (are) followed by the diagonal blocks corresponding to eigenvalues in  $\mathbb{C}_{<}$ . If  $U$  is partitioned as*

$$\begin{bmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{bmatrix}, \tag{6}$$

*where  $U_{11} \in \mathbb{R}^{n \times n}$ , then  $U_{11}$  is nonsingular and  $S = U_{21} U_{11}^{-1}$ .*

In the theorem, the solution  $S$  is found by solving  $S U_{11} = U_{21}$ . The accuracy of  $S$  is thus dependent on  $\kappa(U_{11})$ , the condition number of the matrix  $U_{11}$ . An upper bound for the 2-norm condition number can be obtained by applying the next result, noting that an upper bound for  $\|S\|_2$  can be obtained from  $S e \leq e$  (see Theorem 1).

**Proposition 5** *Let  $U$  be an orthogonal matrix partitioned as in (6). If  $U_{11}$  is nonsingular and  $W = U_{21} U_{11}^{-1}$ , then*

$$\kappa_2(U_{11}) \leq 1 + \|W\|_2^2.$$

The proof of this result is essentially the same as that of corresponding results in [15] and [16], where the results are stated for specific matrix equations.

We use subroutines DGEHRD, DORGHR, DHSEQR, and DTREXC from LAPACK [1] to compute in double precision an ordered real Schur form described in Theorem 4. The  $1 \times 1$  or  $2 \times 2$  diagonal blocks in the real Schur form obtained by DHSEQR do not generally have the required ordering. The subroutine DTREXC is used to reorder the diagonal blocks by using orthogonal

transformations to interchange consecutive diagonal blocks (see [2]). To keep the number of interchanges of consecutive blocks at a minimum, we use the original ordering within the group of diagonal blocks associated with eigenvalues in  $\mathbb{C}_>$  and within the group of diagonal blocks associated with eigenvalues in  $\mathbb{C}_<$ .

When  $u_1^T e = u_2^T e$ , zero is a double eigenvalue of  $R$  with index two (see Theorem 2). Thus, without any special treatment, we can only expect half of the machine precision for the two computed eigenvalues near zero when  $u_1^T e = u_2^T e$ . (For a discussion of perturbation of a multiple eigenvalue, see [17], for example.) When  $u_1^T e \approx u_2^T e$ , the exact Schur form of  $R$  should contain  $1 \times 1$  diagonal blocks  $(0)$  and  $(\mu)$ , where  $\mu \approx 0$  is a real number. In the computed Schur form, however, the accuracy of the two approximate eigenvalues is in general far lower than the level of the machine precision. We make the reasonable assumption that, in the computed real Schur form,  $n - 1$  of the remaining eigenvalues are in  $\mathbb{C}_>$  and  $m - 1$  of the remaining eigenvalues are in  $\mathbb{C}_<$  (as is the case for the exact Schur form). If the computed Schur form displays a  $2 \times 2$  diagonal block for the two approximate eigenvalues, we will not attempt to compute an approximate minimal solution from the Schur form. If the computed Schur form displays two  $1 \times 1$  diagonal blocks for the two approximate eigenvalues  $\lambda_1 \geq \lambda_2$ , an approximate solution will be computed in the following way: (a) If  $\lambda_1 > 0$  and  $\lambda_2 \leq 0$ , then we can compute the minimal solution as described in Theorem 4. (b) If  $\lambda_1 \leq 0$ , then we replace the  $n$ th column of  $U$  by  $(1, 1, \dots, 1)^T / \sqrt{n + m}$ , a normalized eigenvector corresponding to the exact zero eigenvalue, and then compute the minimal solution as in Theorem 4. (c) If  $\lambda_2 > 0$ , we use DTREXC to bring  $(\lambda_2)$  to the  $(n + 1, n + 1)$  position (If  $\lambda_1 = \lambda_2$ , we assume that  $\lambda_2$  is closer to the  $(n + 1, n + 1)$  position than  $\lambda_1$  is.) and then compute the minimal solution as in Theorem 4.

Therefore, when  $u_1^T e \approx u_2^T e$  the Schur method as described in Theorem 4 may still provide an approximate solution, but the accuracy of the approximate solution is very much in doubt. This kind of inaccuracy has already been reported for symmetric AREs when the Hamiltonian matrix has eigenvalues on the imaginary axis (see [3], for example).

In order to find an accurate solution, we will provide a new procedure based on the Schur decomposition. We will separate the known zero eigenvalue from the rest of eigenvalues of  $R$  in the beginning, and bring the tamed zero eigenvalue back into play only when necessary.

### 3 A modified Schur method

Our first step is to separate the known zero eigenvalue of the matrix  $R$  in (4) from the rest of its eigenvalues. Let  $P_k$  ( $k = m, n$ ) be Householder transformations such that  $P_k e^{(k)} = -\sqrt{k} e_1^{(k)}$  ( $k = m, n$ ), where  $e_1^{(k)} = (1, 0, \dots, 0)^T$  is  $k$ -dimensional. Thus,

$$P_k = I_k - 2w_k w_k^T$$

with

$$w_k = (e^{(k)} + \sqrt{k} e_1^{(k)}) / \|e^{(k)} + \sqrt{k} e_1^{(k)}\|_2.$$

Note that  $P_k^{-1} = P_k^T = P_k$ . Let

$$T = \begin{bmatrix} I_n & 0 \\ -\sqrt{\frac{m}{n}} I_{m \times n} & I_m \end{bmatrix} \begin{bmatrix} P_n & 0 \\ 0 & P_m \end{bmatrix}.$$

Then we have

$$T \begin{bmatrix} e^{(n)} \\ e^{(m)} \end{bmatrix} = \begin{bmatrix} -\sqrt{n} e_1^{(n)} \\ 0 \end{bmatrix}$$

and thus

$$TRT^{-1} \begin{bmatrix} -\sqrt{n} e_1^{(n)} \\ 0 \end{bmatrix} = TR \begin{bmatrix} e^{(n)} \\ e^{(m)} \end{bmatrix} = 0. \quad (7)$$

The matrix

$$V = TRT^{-1} = \begin{bmatrix} V_{11} & V_{12} \\ V_{21} & V_{22} \end{bmatrix}$$

can be formed by computing in  $O((n+m)^2)$  flops the matrices

$$V_{11} = \tilde{M}_{11} + \sqrt{\frac{m}{n}} \tilde{M}_{12} I_{m \times n}, \quad V_{12} = \tilde{M}_{12},$$

$$V_{21} = -\tilde{M}_{21} - \sqrt{\frac{m}{n}} (I_{m \times n} \tilde{M}_{11} + \tilde{M}_{22} I_{m \times n}) - \frac{m}{n} I_{m \times n} \tilde{M}_{12} I_{m \times n},$$

$$V_{22} = -\tilde{M}_{22} - \sqrt{\frac{m}{n}}I_{m \times n}\tilde{M}_{12},$$

where

$$\tilde{M}_{11} = P_n M_{11} P_n, \quad \tilde{M}_{12} = P_n M_{12} P_m, \quad \tilde{M}_{21} = P_m M_{21} P_n, \quad \tilde{M}_{22} = P_m M_{22} P_m.$$

By (7), the first column of  $V$  is zero. So we can write

$$V = \begin{bmatrix} 0 & z \\ 0 & \tilde{V} \end{bmatrix}, \quad (8)$$

where  $\tilde{V}$  is of size  $(n+m-1) \times (n+m-1)$ . Note that  $V$  and  $R$  have the same eigenvalues. So the zero eigenvalue of  $R$  has been separated from the rest of its eigenvalues.

Next we explain how the solution  $S$  of (1) can be obtained from a proper solution of the Riccati equation corresponding to the matrix  $V$ , i.e., the equation

$$XV_{12}X + XV_{11} - V_{22}X - V_{21} = 0. \quad (9)$$

Recall that the column space of  $(I \ S^T)^T$  is the unique  $n$ -dimensional invariant subspace of  $R$  corresponding to its  $n$  eigenvalues with largest real parts. Let the column space of  $(S_1^T \ S_2^T)^T$ , where  $S_1 \in \mathbb{R}^{n \times n}$ , be the invariant subspace of  $V$  corresponding to these same eigenvalues. Since the column space of  $(S_1^T \ S_2^T)^T$  is the same as the column space of  $T(I \ S^T)^T$ , there exists a nonsingular  $n \times n$  matrix  $W$  such that

$$\begin{bmatrix} S_1 \\ S_2 \end{bmatrix} = T \begin{bmatrix} I \\ S \end{bmatrix} W = \begin{bmatrix} P_n W \\ (P_m S - \sqrt{\frac{m}{n}}I_{m \times n}P_n)W \end{bmatrix}.$$

Therefore, (9) has a solution

$$\tilde{S} = S_2 S_1^{-1} = (P_m S - \sqrt{\frac{m}{n}}I_{m \times n}P_n)P_n^{-1} = P_m S P_n - \sqrt{\frac{m}{n}}I_{m \times n}.$$

Thus, the solution  $S$  of (1) can be obtained from  $\tilde{S}$  by using

$$S = P_m(\tilde{S} + \sqrt{\frac{m}{n}}I_{m \times n})P_n. \quad (10)$$

Our task is then to find  $\tilde{S}$  accurately.

Let  $\tilde{Q}^T \tilde{V} \tilde{Q} = \tilde{N}$  be a real Schur form of the matrix  $\tilde{V}$  in (8). Since one zero eigenvalue of  $V$  has been left out, the remaining eigenvalues of  $V$  can (normally) be found accurately by the real Schur form for  $\tilde{V}$ . Therefore, we know all eigenvalues of  $R$  and thus all eigenvalues of  $Z = M_{11} + M_{12}S$  and  $\hat{Z} = M_{22} + M_{21}\hat{S}$ . We arrange the  $1 \times 1$  or  $2 \times 2$  diagonal blocks of  $\tilde{N}$  in such a way that diagonal blocks associated with eigenvalues in  $\mathbb{C}_>$  appear in the top left corner. As before, the ordered real Schur form for  $\tilde{V}$  is computed by using the subroutines DGEHRD, DORGHR, DHSEQR, and DTREXC. A Schur form for  $V$  is obtained by using

$$Q^{(1)} = \begin{bmatrix} 1 & 0 \\ 0 & \tilde{Q} \end{bmatrix}.$$

By Theorem 2,  $\tilde{N}$  has either  $n-1$  or  $n$  eigenvalues in  $\mathbb{C}_>$ . If  $\tilde{N}$  has  $n-1$  eigenvalues in  $\mathbb{C}_>$ , then the separated zero eigenvalue is one of the  $n$  eigenvalues of  $V$  with largest real parts. Therefore, the solution  $\tilde{S}$  is determined by the first  $n$  columns of the orthogonal matrix  $Q^{(1)}$ . If  $n=1$  then  $\tilde{S}=0$ . For  $n>1$ , we let

$$\tilde{Q} = \begin{bmatrix} \tilde{Q}_{11} & \tilde{Q}_{12} \\ \tilde{Q}_{21} & \tilde{Q}_{22} \end{bmatrix}$$

with  $\tilde{Q}_{11} \in \mathbb{R}^{(n-1) \times (n-1)}$ , and let

$$L = \begin{bmatrix} 1 & 0 \\ 0 & \tilde{Q}_{11} \end{bmatrix}.$$

Then

$$\tilde{S} = \begin{bmatrix} 0 & \tilde{Q}_{21} \end{bmatrix} L^{-1} = \begin{bmatrix} 0 & \tilde{Q}_{21}(\tilde{Q}_{11})^{-1} \end{bmatrix}.$$

Note that the invertibility of  $L$  is guaranteed by the existence of the solution  $\tilde{S}$ . Moreover, by Proposition 5,

$$\kappa_2(\tilde{Q}_{11}) \leq \kappa_2(L) \leq 1 + \|\tilde{S}\|_2^2. \quad (11)$$

If  $\tilde{N}$  has  $n$  eigenvalues in  $\mathbb{C}_>$ , then the zero eigenvalue is not one of the  $n$  eigenvalues of  $V$  with largest real parts. So, for the Schur form of  $V$ , we

use DTREXC to move the zero eigenvalue from the  $(1, 1)$  position to the  $(n + 1, n + 1)$  position. If  $u_1^T e \approx u_2^T e$  then, at one stage in this process, we need to swap the zero eigenvalue with a very small positive eigenvalue. The swapping can be performed with high accuracy since we swap two  $1 \times 1$  blocks (see [2]). Let  $Q^{(2)}$  be the orthogonal matrix used to move the zero eigenvalue to the right position and let  $Q = Q^{(1)}Q^{(2)}$ . Then

$$Q^T V Q = N$$

is a new real Schur form with the  $n$  eigenvalues in  $\mathbb{C}_>$  appearing first in  $N$ . Let  $Q$  be partitioned as

$$Q = \begin{bmatrix} Q_{11} & Q_{12} \\ Q_{21} & Q_{22} \end{bmatrix}$$

with  $Q_{11} \in \mathbb{R}^{n \times n}$ . Then  $\tilde{S} = Q_{21}Q_{11}^{-1}$ . Again, the invertibility of  $Q_{11}$  is guaranteed by the existence of the solution  $\tilde{S}$ . Moreover,

$$\kappa_2(Q_{11}) \leq 1 + \|\tilde{S}\|_2^2. \quad (12)$$

After  $\tilde{S}$  has been computed, the solution  $S$  is found by (10) in  $O((n + m)^2)$  flops. The whole procedure described in this section will be called the modified Schur method.

The upper bound in (11) and (12) involves  $\|\tilde{S}\|_2$ . We note that the difference between  $\|\tilde{S}\|_2$  and  $\|S\|_2$  is not too big. Indeed, we have by (10) that

$$\|S\|_2 - \sqrt{\frac{m}{n}} \leq \|\tilde{S}\|_2 \leq \|S\|_2 + \sqrt{\frac{m}{n}}.$$

Since  $Se \leq e$  by Theorem 1, we have  $\|S\|_\infty \leq 1$ . Thus,

$$\|S\|_2 \leq \sqrt{m}\|S\|_\infty \leq \sqrt{m}$$

and

$$\|\tilde{S}\|_2 \leq \|S\|_2 + \sqrt{\frac{m}{n}} \leq \sqrt{m}\left(1 + \frac{1}{\sqrt{n}}\right).$$

#### 4 A simplified Latouche–Ramaswami algorithm

Recall that the matrix  $M$  in (2) is an irreducible singular  $M$ -matrix with  $Me = 0$ . Ramaswami [22] made an interesting observation that the matrix equation (1) is closely related to a quadratic matrix equation arising in QBDs.

Choose a number  $\theta \geq \max_{1 \leq i \leq m+n} m_{ii}$ , where  $m_{ii}$  are the diagonal elements of  $M$ ; let  $P = I - \frac{1}{\theta}M$ . Then  $P$  is nonnegative with  $Pe = e$ , i.e.,  $P$  is a stochastic matrix. Let

$$P = \begin{bmatrix} P_{11} & P_{12} \\ P_{21} & P_{22} \end{bmatrix},$$

where the partitioning is conformable with that for the matrix  $M$ . Thus,

$$P_{11} = I - \frac{1}{\theta}M_{11}, \quad P_{12} = -\frac{1}{\theta}M_{12}, \quad P_{21} = -\frac{1}{\theta}M_{21}, \quad P_{22} = I - \frac{1}{\theta}M_{22}. \quad (13)$$

Ramaswami [22] constructed three matrices from the matrix  $P$ :

$$A_0 = \begin{bmatrix} P_{11} & 0 \\ \frac{1}{2}P_{21} & 0 \end{bmatrix}, \quad A_1 = \begin{bmatrix} 0 & P_{12} \\ 0 & \frac{1}{2}P_{22} \end{bmatrix}, \quad A_2 = \begin{bmatrix} 0 & 0 \\ 0 & \frac{1}{2}I \end{bmatrix}. \quad (14)$$

Note that the nonnegative matrices  $A_0, A_1, A_2$  are such that  $A = A_0 + A_1 + A_2$  is irreducible and  $Ae = e$ . We can associate a QBD process with the matrices  $A_0, A_1, A_2$ . Let  $\alpha$  be the stationary probability vector of  $A$ , i.e.,  $\alpha > 0$ ,  $\alpha^T e = 1$  and  $\alpha^T A = \alpha^T$ . The QBD is called positive recurrent if  $\alpha^T A_0 e > \alpha^T A_2 e$ , null recurrent if  $\alpha^T A_0 e = \alpha^T A_2 e$ , and transient if  $\alpha^T A_0 e < \alpha^T A_2 e$ .

By (13), we know that  $\alpha^T A = \alpha^T$  is equivalent to

$$\alpha^T \begin{bmatrix} M_{11} & M_{12} \\ \frac{1}{2}M_{21} & \frac{1}{2}M_{22} \end{bmatrix} = 0.$$

Thus,  $\alpha^T = [u_1^T \ 2u_2^T]/(u_1^T e + 2u_2^T e)$ . It then follows that  $\alpha^T A_0 e - \alpha^T A_2 e = (u_1^T e - u_2^T e)/(u_1^T e + 2u_2^T e)$ . In other words, the QBD is positive recurrent, null recurrent, or transient according as  $u_1^T e > u_2^T e$ ,  $u_1^T e = u_2^T e$ , or  $u_1^T e < u_2^T e$ .

The matrix equation

$$G = A_0 + A_1 G + A_2 G^2 \quad (15)$$

has a minimal nonnegative solution  $G$ . Likewise, the dual equation

$$F = A_2 + A_1F + A_0F^2. \quad (16)$$

has a minimal nonnegative solution  $F$ . Moreover, the following result is well known (see [19] and [21]).

**Theorem 6** *If the QBD is positive recurrent, then  $G$  is stochastic and  $F$  is substochastic with spectral radius  $\rho(F) < 1$ . If the QBD is transient, then  $F$  is stochastic and  $G$  is substochastic with  $\rho(G) < 1$ . If the QBD is null recurrent, then  $G$  and  $F$  are both stochastic.*

The following result is a slight different presentation of Theorem 4.1 of [22]. We provide an algebraic proof for completeness.

**Proposition 7** *The minimal nonnegative solution of (15) is*

$$G = \begin{bmatrix} P_{11} + P_{12}S & 0 \\ S & 0 \end{bmatrix},$$

where  $S$  is the minimal nonnegative solution of (1).

**PROOF.** Using block matrix multiplications and the relations (13), we can see that a matrix of the form

$$\begin{bmatrix} A & 0 \\ B & 0 \end{bmatrix}$$

is a solution of (15) if and only if  $A = P_{11} + P_{12}B$  and

$$BM_{12}B + BM_{11} + M_{22}B + M_{21} = 0.$$

This completes the proof.  $\square$

We will also need the following result.

**Proposition 8** *The minimal nonnegative solution of (16) is*

$$F = \begin{bmatrix} 0 & \hat{S} \\ 0 & (2I - P_{22} - P_{21}\hat{S})^{-1} \end{bmatrix}, \quad (17)$$

where  $\hat{S}$  is the minimal nonnegative solution of (3).

**PROOF.** Using block matrix multiplications, we see that

$$\begin{bmatrix} 0 & C \\ 0 & D \end{bmatrix}$$

is a solution of (16) if and only if

$$C = (P_{12} + P_{11}C)D \tag{18}$$

and

$$(2I - P_{22} - P_{21}C)D = I. \tag{19}$$

Equation (19) implies  $D(2I - P_{22} - P_{21}C) = I$ . So post-multiplying (18) by  $2I - P_{22} - P_{21}C$  gives

$$CP_{21}C + CP_{22} + P_{11}C + P_{12} = 2C,$$

which is equivalent to

$$CM_{21}C + CM_{22} + M_{11}C + M_{12} = 0$$

in view of (13). For the minimal solution  $\hat{S}$  of (3), we have  $\hat{S}e \leq e$  and  $(2I - P_{22} - P_{21}\hat{S})e \geq 2e - (P_{22} + P_{21})e = e$ . Thus,  $2I - P_{22} - P_{21}\hat{S}$  is a nonsingular  $M$ -matrix and  $(2I - P_{22} - P_{21}\hat{S})^{-1} \geq 0$  (see [4], for example). Therefore, the minimal nonnegative solution of (16) is given by (17).  $\square$

The solution  $G$  can be computed by the LR algorithm [18]:

**Algorithm 1** *Set*

$$\begin{aligned} L^{(0)} &= (I - A_1)^{-1}A_0; \\ H^{(0)} &= (I - A_1)^{-1}A_2; \\ G^{(0)} &= L^{(0)}; \\ T^{(0)} &= H^{(0)}. \end{aligned}$$

For  $k = 0, 1, \dots$ , compute

$$\begin{aligned}
U^{(k)} &= H^{(k)}L^{(k)} + L^{(k)}H^{(k)}; \\
L^{(k+1)} &= (I - U^{(k)})^{-1}(L^{(k)})^2; \\
H^{(k+1)} &= (I - U^{(k)})^{-1}(H^{(k)})^2; \\
G^{(k+1)} &= G^{(k)} + T^{(k)}L^{(k+1)}; \\
T^{(k+1)} &= T^{(k)}H^{(k+1)}.
\end{aligned}$$

It is shown in [18] that the matrices  $H^{(k)}$  and  $L^{(k)}$  are well defined and non-negative and that the (monotonically increasing) sequence  $\{G^{(k)}\}$  converges quadratically to the matrix  $G$  for positive recurrent QBDs and for transient QBDs. The convergence is expected to be linear with rate  $1/2$  for null recurrent QBDs (see [8]). We also note that a refined implementation of the LR algorithm has been given in [25] to have better numerical stability.

The computational work involved in each iteration of Algorithm 1 is about  $\frac{50}{3}(m+n)^3$  flops. However, in our case, the matrices  $A_0, A_1, A_2$  have very special structures, and it is possible to reduce the computational work significantly.

For this purpose, we partition the matrices  $L^{(k)}, H^{(k)}, G^{(k)}, T^{(k)}$  as

$$\begin{aligned}
L^{(k)} &= \begin{bmatrix} L_1^{(k)} & L_3^{(k)} \\ L_2^{(k)} & L_4^{(k)} \end{bmatrix}, & H^{(k)} &= \begin{bmatrix} H_1^{(k)} & H_3^{(k)} \\ H_2^{(k)} & H_4^{(k)} \end{bmatrix}, \\
G^{(k)} &= \begin{bmatrix} G_1^{(k)} & G_3^{(k)} \\ G_2^{(k)} & G_4^{(k)} \end{bmatrix}, & T^{(k)} &= \begin{bmatrix} T_1^{(k)} & T_3^{(k)} \\ T_2^{(k)} & T_4^{(k)} \end{bmatrix},
\end{aligned}$$

conformably with the partitioning of  $M$  (or that of  $A_0, A_1, A_2$ ). It is easily seen by block matrix computations that  $L_3^{(k)}, L_4^{(k)}, H_1^{(k)}, H_2^{(k)}, G_3^{(k)}, G_4^{(k)}, T_1^{(k)}, T_2^{(k)}$  are all zero matrices for each  $k \geq 0$ . Moreover, the matrices  $G_1^{(k)}$  and  $T_3^{(k)}$  are not needed in finding the solution  $S$ . The LR algorithm can thus be simplified to the following.

**Algorithm 2** *Set*

$$\begin{aligned}
\begin{bmatrix} L_1^{(0)} & H_3^{(0)} \\ L_2^{(0)} & H_4^{(0)} \end{bmatrix} &= \begin{bmatrix} I & -P_{12} \\ 0 & I - \frac{1}{2}P_{22} \end{bmatrix}^{-1} \begin{bmatrix} P_{11} & 0 \\ \frac{1}{2}P_{21} & \frac{1}{2}I \end{bmatrix}; \\
G_2^{(0)} &= L_2^{(0)}; \\
T_4^{(0)} &= H_4^{(0)}.
\end{aligned}$$

For  $k = 0, 1, \dots$ , compute

$$\begin{aligned}
U^{(k)} &= \begin{bmatrix} H_3^{(k)} & L_2^{(k)} & L_1^{(k)} & H_3^{(k)} \\ H_4^{(k)} & L_2^{(k)} & L_2^{(k)} & H_3^{(k)} \end{bmatrix}; \\
\begin{bmatrix} L_1^{(k+1)} & H_3^{(k+1)} \\ L_2^{(k+1)} & H_4^{(k+1)} \end{bmatrix} &= (I - U^{(k)})^{-1} \begin{bmatrix} (L_1^{(k)})^2 & H_3^{(k)} & H_4^{(k)} \\ L_2^{(k)} & L_1^{(k)} & (H_4^{(k)})^2 \end{bmatrix}; \\
G_2^{(k+1)} &= G_2^{(k)} + T_4^{(k)} L_2^{(k+1)}; \\
T_4^{(k+1)} &= T_4^{(k)} H_4^{(k+1)}.
\end{aligned}$$

The solution  $S$  is approximated by the sequence  $\{G_2^{(k)}\}$ . The computational work involved in each iteration of Algorithm 2 is about  $4m^3 + 8m^2n + 6mn^2 + 2n^3 + \frac{8}{3}(m+n)^3$  flops. When  $m = n$ , Algorithm 1 requires  $\frac{400}{3}n^3$  flops and Algorithm 2 requires  $\frac{124}{3}n^3$  flops. The simplified LR algorithm is also less expensive than Newton's method, which requires roughly  $60n^3$  flops each iteration when  $m = n$ .

In [8] it is shown, using the formulation in [5], that the LR algorithm can be obtained by using a cyclic reduction algorithm combined with proper block diagonal scaling. In particular, we have for each  $k \geq 0$

$$-L^{(k)} + G^{2^k} - H^{(k)}G^{2^{k+1}} = 0, \quad (20)$$

$$-H^{(k)} + F^{2^k} - L^{(k)}F^{2^{k+1}} = 0, \quad (21)$$

and

$$G = G^{(k)} + \left( \prod_{0 \leq i \leq k} H^{(i)} \right) G^{2^{k+1}}. \quad (22)$$

**Remark 9** *It is important to note that the derivation of the above three equations does not need any special properties of the matrices  $A_0, A_1, A_2, G$ , and  $F$ , as long as the LR algorithm is well defined and  $G$  and  $F$  are solutions of (15) and (16), respectively.*

Using the special properties of the matrices involved, we have the following error estimate (see [8]).

$$0 \leq G - G^{(k)} \leq F^{2^{k+1}-1} G^{2^{k+1}}, \quad k \geq 0. \quad (23)$$

It follows that

$$\limsup_{k \rightarrow \infty} \sqrt[2^{k+1}]{\|S - G_2^{(k)}\|_\infty} \leq \limsup_{k \rightarrow \infty} \sqrt[2^{k+1}]{\|G - G^{(k)}\|_\infty} \leq \rho(F)\rho(G). \quad (24)$$

The next result suggests that we should take  $\theta = \max_{1 \leq i \leq m+n} m_{ii}$  in (13) to have faster convergence for the (modified) LR algorithm.

**Proposition 10** *For  $\theta \geq \max_{1 \leq i \leq m+n} m_{ii}$ ,  $\rho(G)$  and  $\rho(F)$  are nondecreasing functions of  $\theta$ .*

**PROOF.** By Propositions 7 and 8, relation (13) and the Perron–Frobenius theorem,

$$\rho(G) = \rho(P_{11} + P_{12}S) = \rho\left(I - \frac{1}{\theta}(M_{11} + M_{12}S)\right) = 1 - \frac{1}{\theta}\lambda,$$

where  $\lambda \geq 0$  is the smallest real eigenvalue of  $M_{11} + M_{12}S$ , and

$$\begin{aligned} \rho(F) &= \rho((2I - P_{22} - P_{21}\hat{S})^{-1}) \\ &= \rho\left(\left(I + \frac{1}{\theta}(M_{22} + M_{21}\hat{S})\right)^{-1}\right) = \left(1 + \frac{1}{\theta}\mu\right)^{-1}, \end{aligned}$$

where  $\mu \geq 0$  is the smallest real eigenvalue of  $M_{22} + M_{21}\hat{S}$ . The result follows immediately.  $\square$

## 5 A shift technique for the Latouche–Ramaswami algorithm

We start with a nice property of the matrix  $G$  in Proposition 7.

**Proposition 11** *For the matrix  $G$ ,  $0 < \rho(G) \leq 1$  and  $\rho(G)$  is a simple eigenvalue of  $G$ . Moreover,  $\rho(G)$  is the only eigenvalue of  $G$  of modulus  $\rho(G)$ .*

**PROOF.** Since  $M_{11} + M_{12}S$  is irreducible,  $P_{11} + P_{12}S = I - \frac{1}{\theta}(M_{11} + M_{12}S)$  is also irreducible. Thus, by the Perron–Frobenius theorem,  $\rho(G) = \rho(P_{11} + P_{12}S) > 0$  and  $\rho(G)$  is a simple eigenvalue of  $G$ . That  $\rho(G) \leq 1$  is already known. Since  $P_{12} \neq 0$  and  $S > 0$ ,  $P_{11} + P_{12}S$  has at least one positive row. Thus,  $P_{11} + P_{12}S$  cannot be cyclic. So, it is primitive, i.e.,  $\rho(P_{11} + P_{12}S)$  is the only eigenvalue of  $P_{11} + P_{12}S$  with modulus  $\rho(P_{11} + P_{12}S)$  (see Section 2.2 of [24], for example).  $\square$

We now limit our attention to the case  $u_1^T e \geq u_2^T e$ . So the QBD associated with the matrices  $A_0, A_1, A_2$  in (14) is positive recurrent or null recurrent. We

know by Theorem 6 that  $G$  is stochastic. It follows from Proposition 11 that the only eigenvalue of  $G$  on the unit circle is the simple eigenvalue 1.

The shift technique introduced in [14] is  $H = G - ev^T$ , where  $v > 0$  and  $v^T e = 1$ . For our purposes here, we only require that  $v \geq 0$  and  $v^T e = 1$ . Then the eigenvalues of  $H$  are those of  $G$  except that in  $H$  the eigenvalue 1 of  $G$  is replaced by 0, and  $H$  is a solution of the new equation

$$H = B_0 + B_1 H + B_2 H^2, \quad (25)$$

where

$$B_0 = A_0(I - ev^T), \quad B_1 = A_1 + A_2 ev^T, \quad B_2 = A_2. \quad (26)$$

Let

$$A(\lambda) = -A_0 + (I - A_1)\lambda - A_2\lambda^2$$

be the matrix polynomial corresponding to (15), and let

$$B(\lambda) = -B_0 + (I - B_1)\lambda - B_2\lambda^2$$

be the matrix polynomial associated with (25). In general, the eigenvalues of a matrix polynomial  $L(\lambda) = L_0 + L_1\lambda + L_2\lambda^2$  are the zeros of  $\det(L(\lambda))$ . However, if 0 is an eigenvalue of  $\lambda^2 L(1/\lambda) = L_2 + L_1\lambda + L_0\lambda^2$  with multiplicity  $p$ , we also say that  $\infty$  is an eigenvalue of  $L(\lambda)$  with multiplicity  $p$ . Note that  $A(\lambda)$  and  $B(\lambda)$  have eigenvalues at  $\infty$  since  $A_2$  is singular.

The following result is a generalization of Theorem 3.1 in [14] and Lemma 2.1 in [10]. The proof of Lemma 2.1 of [10] carries over without change.

**Lemma 12** *The eigenvalues of  $B(\lambda)$  are obtained from the eigenvalues of  $A(\lambda)$  by replacing one eigenvalue 1 by 0.*

The next result is a special case of Theorem 4 in [6].

**Lemma 13** *Counting multiplicities for all eigenvalues and including eigenvalues at  $\infty$ , we have*

- (1) *If the QBD is positive recurrent, then  $A(\lambda)$  has  $m + n - 1$  eigenvalues inside the unit circle, one eigenvalue 1, and  $m + n$  eigenvalues outside the unit circle.*
- (2) *If the QBD is null recurrent, then  $A(\lambda)$  has  $m + n - 1$  eigenvalues inside the unit circle, two eigenvalues 1, and  $m + n - 1$  eigenvalues outside the unit circle.*

**Corollary 14** *If the QBD is positive recurrent then  $B(\lambda)$  has  $m + n$  eigenvalues inside the unit circle and no eigenvalues on the unit circle; if the QBD is null recurrent then  $B(\lambda)$  has  $m + n$  eigenvalues inside the unit circle, one (simple) eigenvalue 1 on the unit circle, and  $m + n - 1$  eigenvalues outside the unit circle.*

To find the solution  $H$  of (25), we can apply Algorithm 1 with the triple  $(A_0, A_1, A_2)$  replaced by the triple  $(B_0, B_1, B_2)$ . To avoid confusion, we will put a “hat” on each sequence generated. The matrix  $G$  can be recovered by  $\hat{G} = H + ev^T$ . Once again, we can get a simplified LR algorithm when  $(A_0, A_1, A_2)$  is replaced by  $(B_0, B_1, B_2)$ . To reduce computational work, the last  $m$  components of  $v$  are taken to be zero. We partition the matrix  $H$  and the vector  $v$  (conformably with the matrices  $A_0, A_1, A_2$ ) as

$$H = \begin{bmatrix} H_1 & 0 \\ H_2 & 0 \end{bmatrix}, \quad v = \begin{bmatrix} p \\ 0 \end{bmatrix}, \quad (27)$$

where  $p > 0$  and  $p^T e = 1$ .

The simplified LR algorithm with a shift is as follows.

**Algorithm 3** *Set*

$$\begin{bmatrix} L_1^{(0)} & H_3^{(0)} \\ L_2^{(0)} & H_4^{(0)} \end{bmatrix} = \begin{bmatrix} I & -P_{12} \\ -\frac{1}{2}ep^T & I - \frac{1}{2}P_{22} \end{bmatrix}^{-1} \begin{bmatrix} P_{11}(I - ep^T) & 0 \\ \frac{1}{2}P_{21}(I - ep^T) & \frac{1}{2}I \end{bmatrix},$$

*and proceed as in Algorithm 2.*

Thus, the computational work for each iteration of Algorithm 3 is about  $\frac{124}{3}n^3$  flops when  $m = n$ . If we took  $v > 0$ , we could still get a simplified LR algorithm, but the computational work each iteration would be about  $\frac{208}{3}n^3$  flops when  $m = n$ .

To avoid confusion, we will put a “hat” on each sequence generated by Algorithm 3. We expect the sequence  $\hat{G}_2^{(k)}$  produced by Algorithm 3 to approximate the matrix  $H_2$ . Once  $H_2$  is computed, the solution  $S$  of (1) is obtained by  $S = H_2 + ep^T$ .

As in [14] and [10], to study the convergence of the LR algorithm with a shift, we need to show that there is a matrix  $K$  with  $\rho(K) \leq 1$  such that

$$K = B_2 + B_1K + B_0K^2. \quad (28)$$

**Lemma 15** *When the QBD is positive recurrent,  $I - ev^T F$  is nonsingular and*

$$K = (I - ev^T F)F(I - ev^T F)^{-1} \quad (29)$$

*is a solution of (28).*

**PROOF.** We only need to show that  $I - ev^T F$  is nonsingular. The rest is shown as in [14]. By (17), (27) and Theorem 2 (2),  $v^T F e = p^T \hat{S} e < p^T e = 1$ . Therefore,  $(I - ev^T F)e > 0$  and  $I - ev^T F$  is a nonsingular  $M$ -matrix.  $\square$

When the QBD is null recurrent, we have  $F e = e$  by Theorem 6. As a result,  $(I - ev^T F)e = 0$  and  $I - ev^T F$  is singular. However, we can show that the matrix  $K$  in Lemma 15 is bounded independent of the nearness to null recurrency.

**Lemma 16** *If the QBD is positive recurrent, then for the matrix  $K$  in (29)*

$$\|K\|_\infty < 3 + \frac{2}{\min_{1 \leq i \leq n} p_i},$$

*where  $p_i$  is the  $i$ th component of  $p$ . In particular,  $\|K\|_\infty < 3 + 2n$  if  $p = \frac{1}{n}e$ .*

**PROOF.** As in the proof of Lemma 2.5 in [10], we get

$$\|K\|_\infty < 3 + 2 \frac{\|e - F e\|_\infty}{v^T(e - F e)}.$$

Since  $(2I - P_{22} - P_{21}\hat{S})e \geq e$ , we have  $(2I - P_{22} - P_{21}\hat{S})^{-1}e \leq e$  and  $\|(2I - P_{22} - P_{21}\hat{S})^{-1}\|_\infty \leq 1$ . Moreover,

$$\begin{aligned} & \|e - (2I - P_{22} - P_{21}\hat{S})^{-1}e\|_\infty \\ &= \|(2I - P_{22} - P_{21}\hat{S})^{-1}((2I - P_{22} - P_{21}\hat{S})e - (2I - P_{22} - P_{21})e)\|_\infty \\ &= \|(2I - P_{22} - P_{21}\hat{S})^{-1}P_{21}(e - \hat{S}e)\|_\infty \\ &\leq \|(2I - P_{22} - P_{21}\hat{S})^{-1}\|_\infty \|P_{21}\|_\infty \|e - \hat{S}e\|_\infty \\ &\leq \|e - \hat{S}e\|_\infty. \end{aligned}$$

Therefore,

$$\|e - Fe\|_\infty = \left\| \begin{bmatrix} e - \hat{S}e \\ e - (2I - P_{22} - P_{21}\hat{S})^{-1}e \end{bmatrix} \right\|_\infty = \|e - \hat{S}e\|_\infty.$$

Thus,

$$\frac{\|e - Fe\|_\infty}{v^T(e - Fe)} = \frac{\|e - \hat{S}e\|_\infty}{p^T(e - \hat{S}e)} \leq \frac{1}{\min_{1 \leq i \leq n} p_i}.$$

This completes the proof.  $\square$

When the QBD is positive recurrent, (28) has a solution given by (29). Note that  $\rho(K) = \rho(F) < 1$ . For the null recurrent case, we have the following result.

**Theorem 17** *If the QBD is null recurrent, then (28) has a solution  $K$  having one eigenvalue 1 and  $m + n - 1$  eigenvalues inside the unit circle.*

**PROOF.** For any  $\epsilon$  with  $0 < \epsilon < 1$ , define

$$A_0(\epsilon) = A_0, \quad A_1(\epsilon) = \begin{bmatrix} 0 & P_{12} \\ 0 & \frac{1}{2}(P_{22} + \epsilon I) \end{bmatrix}, \quad A_2(\epsilon) = \begin{bmatrix} 0 & 0 \\ 0 & \frac{1}{2}(1 - \epsilon)I \end{bmatrix}.$$

Since  $\alpha^T A_0(\epsilon)e > \alpha^T A_2(\epsilon)e$ , where  $\alpha$  is the stationary probability vector of  $A = A_0 + A_1 + A_2 = A_0(\epsilon) + A_1(\epsilon) + A_2(\epsilon)$ , the QBD corresponding to  $(A_0(\epsilon), A_1(\epsilon), A_2(\epsilon))$  is positive recurrent. We now define

$$B_0(\epsilon) = A_0(\epsilon)(I - ev^T), \quad B_1(\epsilon) = A_1(\epsilon) + A_2(\epsilon)ev^T, \quad B_2(\epsilon) = A_2(\epsilon)$$

and let  $F_\epsilon$  be the minimal nonnegative solution of

$$F_\epsilon = A_2(\epsilon) + A_1(\epsilon)F_\epsilon + A_0(\epsilon)F_\epsilon^2.$$

As in Proposition 8, we can show that

$$F_\epsilon = \begin{bmatrix} 0 & \hat{S}_\epsilon \\ 0 & (1 - \epsilon)((2 - \epsilon)I - P_{22} - P_{21}\hat{S}_\epsilon)^{-1} \end{bmatrix}, \quad (30)$$

where  $\hat{S}_\epsilon$  is the minimal nonnegative solution of

$$XM_{21}X + XM_{22} + (1 - \epsilon)M_{11}X + (1 - \epsilon)M_{12} = 0.$$

Since

$$\left[ \begin{array}{cc} 1 & \\ \frac{1}{1-\epsilon}u_1^T & u_2^T \end{array} \right] \left[ \begin{array}{cc} (1-\epsilon)M_{11} & (1-\epsilon)M_{12} \\ M_{21} & M_{22} \end{array} \right] = 0$$

and  $\frac{1}{1-\epsilon}u_1^T e > u_2^T e$ , we have  $\hat{S}_\epsilon e \leq e$  and  $\hat{S}_\epsilon e \neq e$  by Theorem 2(2). Thus, as in Lemma 15,  $I - ev^T F_\epsilon$  is nonsingular and  $K_\epsilon = (I - ev^T F_\epsilon)F_\epsilon(I - ev^T F_\epsilon)^{-1}$  is a solution of

$$K_\epsilon = B_2(\epsilon) + B_1(\epsilon)K_\epsilon + B_0(\epsilon)K_\epsilon^2.$$

Let the sequence  $\{\epsilon_n\}$  be such that  $0 < \epsilon_n < 1$  and  $\lim \epsilon_n = 0$ . Since the sequence  $\{K_{\epsilon_n}\}$  is bounded by Lemma 16, it has a limit point  $K$ . It is clear that this matrix  $K$  is a solution of (28). Since  $\rho(F_\epsilon) < 1$  by Theorem 6, we have  $\rho(K) \leq 1$ . Since the eigenvalues of the matrix polynomial

$$\hat{B}(\lambda) = -B_2 + (I - B_1)\lambda - B_0\lambda^2$$

are the reciprocals of the eigenvalues of  $B(\lambda)$  and the eigenvalues of  $K$  are part of the eigenvalues of  $\hat{B}(\lambda)$ , we know from Corollary 14 that  $K$  has  $m + n - 1$  eigenvalues inside the unit circle and one eigenvalue 1.  $\square$

We are now ready to study the convergence of Algorithm 1 when the triple  $(A_0, A_1, A_2)$  is replaced by  $(B_0, B_1, B_2)$ , assuming that no breakdown occurs, i.e., assuming that  $I - \hat{U}^{(k)}$  is invertible for each  $k \geq 0$ . Note that the matrix

$$I - B_1 = \left[ \begin{array}{cc} I & -P_{12} \\ -\frac{1}{2}ep^T & I - \frac{1}{2}P_{22} \end{array} \right]$$

in the initialization step is always invertible. In fact, for the irreducible matrix

$$C = \left[ \begin{array}{cc} P_{11} & P_{12} \\ \frac{1}{2}(P_{21} + ep^T) & \frac{1}{2}P_{22} \end{array} \right],$$

we have  $Ce = e$ . So, by the Perron–Frobenius theorem,  $\rho(B_1) < \rho(C) = 1$ .

Let  $K$  be the solution of (28) given by Lemma 15 for the positive recurrent case and given by Theorem 17 for the null recurrent case. Now, by (20)–(22) and Remark 9, we have for each  $k \geq 0$

$$-\hat{L}^{(k)} + H^{2^k} - \hat{H}^{(k)} H^{2^{k+1}} = 0, \quad (31)$$

$$-\hat{H}^{(k)} + K^{2^k} - \hat{L}^{(k)} K^{2^{k+1}} = 0, \quad (32)$$

and

$$H = \hat{G}^{(k)} + \left( \prod_{0 \leq i \leq k} \hat{H}^{(i)} \right) H^{2^{k+1}}. \quad (33)$$

From (31) and (32) we get

$$\hat{H}^{(k)} (I - H^{2^{k+1}} K^{2^{k+1}}) = (I - H^{2^k} K^{2^k}) K^{2^k}, \quad (34)$$

$$\hat{L}^{(k)} (I - K^{2^{k+1}} H^{2^{k+1}}) = (I - K^{2^k} H^{2^k}) H^{2^k}. \quad (35)$$

For any fixed  $\epsilon > 0$ , we let  $\|\cdot\|_\epsilon$  be a submultiplicative matrix norm such that  $\|K\|_\epsilon \leq \rho(K) + \epsilon$ . Since  $\lim_{k \rightarrow \infty} H^{2^k} = 0$  and  $\{K^{2^k}\}$  is bounded, we know from (34) that  $\|\hat{H}^{(k)}\|_\epsilon \leq c \|K^{2^k}\|_\epsilon \leq c(\rho(K) + \epsilon)^{2^k}$  for all  $k \geq 0$  and a constant  $c$ . Thus, by (33)

$$\|H - \hat{G}^{(k)}\|_\epsilon \leq c^{k+1} (\rho(K) + \epsilon)^{2^{k+1}-1} \|H^{2^{k+1}}\|_\epsilon.$$

Therefore,

$$\limsup_{k \rightarrow \infty} \sqrt[2^{k+1}]{\|H - \hat{G}^{(k)}\|_\infty} = \limsup_{k \rightarrow \infty} \sqrt[2^{k+1}]{\|H - \hat{G}^{(k)}\|_\epsilon} \leq (\rho(K) + \epsilon) \rho(H).$$

Since  $\epsilon > 0$  is arbitrary, we have

$$\limsup_{k \rightarrow \infty} \sqrt[2^{k+1}]{\|H - \hat{G}^{(k)}\|_\infty} \leq \rho(K) \rho(H) = \rho(F) \rho(H) < 1. \quad (36)$$

Therefore,  $\{\hat{G}^{(k)}\}$  converges to  $H$  quadratically.

Approximations  $\hat{S}^{(k)}$  to the matrix  $S$  can be obtained using  $\hat{S}^{(k)} = \hat{G}_2^{(k)} + e p^T$ , where  $\hat{G}_2^{(k)}$  are from Algorithm 3, and we have by (36)

$$\limsup_{k \rightarrow \infty} \sqrt[2^{k+1}]{\|S - \hat{S}^{(k)}\|_\infty} = \limsup_{k \rightarrow \infty} \sqrt[2^{k+1}]{\|H_2 - \hat{G}_2^{(k)}\|_\infty} \leq \rho(F) \rho(H) < 1.$$

For Algorithm 2,  $S^{(k)} = G_2^{(k)}$  are approximations to  $S$  and we see from (24) that

$$\limsup_{k \rightarrow \infty} \sqrt[2^{k+1}]{\|S - S^{(k)}\|_\infty} \leq \limsup_{k \rightarrow \infty} \sqrt[2^{k+1}]{\|G - G^{(k)}\|_\infty} \leq \rho(F)\rho(G) \leq 1.$$

Since  $\rho(H) < \rho(G)$ , the shift technique has improved the rate of convergence. In particular,  $\hat{S}^{(k)}$  converges to  $S$  quadratically for both positive recurrent and null recurrent QBDs (i.e., whenever  $u_1^T e \geq u_2^T e$ ).

Since  $He = (G - ev^T)e = 0$ , it follows from (33) that  $\hat{G}^{(k)}e = 0$  for each  $k \geq 0$ . Since  $\hat{G}^{(k)}$  has the form

$$\begin{bmatrix} \hat{G}_1^{(k)} & 0 \\ \hat{G}_2^{(k)} & 0 \end{bmatrix},$$

we have  $\hat{G}_2^{(k)}e = 0$  and  $\hat{S}^{(k)}e = e$  for each  $k \geq 0$ . This means that  $\|(\hat{S}^{(k)} - S)e\|_\infty = 0$  for each  $k \geq 0$ . On the other hand, we have  $S^{(k)} \leq S$  for Algorithm 2 and thus  $\|(S^{(k)} - S)e\|_\infty = \|S^{(k)} - S\|_\infty$ .

If the matrices  $I - \hat{U}^{(k)}$  are all invertible in Algorithm 3, we can show that  $I - \hat{U}^{(k)}$  converges to  $I$  quadratically. In fact, by (34) and (35) we have

$$\limsup_{k \rightarrow \infty} \sqrt[2^k]{\|\hat{U}^{(k)}\|} = \limsup_{k \rightarrow \infty} \sqrt[2^k]{\|\hat{H}^{(k)}\hat{L}^{(k)} + \hat{L}^{(k)}\hat{H}^{(k)}\|} \leq \rho(K)\rho(H) < 1.$$

Whether the matrices  $I - \hat{U}^{(k)}$  could be singular for small  $k$  remains an open question. We believe that breakdown in Algorithm 3 is extremely unlikely. If a breakdown were detected, we could simply abandon Algorithm 3 and apply Algorithm 2 instead.

## 6 Numerical results

In this section we present some numerical results to show the efficiency and accuracy of the modified Schur method the simplified LR algorithm with a shift (Algorithm 3).

For each of our test examples the exact solution  $S$  is not known. To check the accuracy of an approximate solution  $S'$ , we may compute the residual  $\|\mathcal{R}(S')\|$ , where  $\mathcal{R}(X) = XM_{12}X + XM_{11} + M_{22}X + M_{21}$  and  $\|\cdot\|$  is the  $\infty$ -norm throughout this section. However, the relation between  $\|\mathcal{R}(S')\|$  and  $\|S' - S\|$  is not always easy to determine. On the one hand, we have

$$\begin{aligned}
\|\mathcal{R}(S')\| &= \|\mathcal{R}(S') - \mathcal{R}(S)\| \\
&= \|S'M_{12}(S' - S) + (S' - S)M_{12}S + (S' - S)M_{11} + M_{22}(S' - S)\| \\
&\leq (\|S'\| \|M_{12}\| + \|M_{12}\| \|S\| + \|M_{11}\| + \|M_{22}\|) \|S' - S\|,
\end{aligned}$$

and thus a rough upper bound for  $\|\mathcal{R}(S')\|$  is  $(2\|M_{12}\| + \|M_{11}\| + \|M_{22}\|)\|S' - S\|$  since  $\|S'\|$  is close to  $\|S\|$  and  $\|S\| \leq 1$ . On the other hand, a very small residual does not imply a very small actual error when  $u_1^T e \approx u_2^T e$  since the Fréchet derivative of the Riccati function  $\mathcal{R}$  at the solution  $S$  is a singular map when  $u_1^T e = u_2^T e$  (see [7]).

When  $u_1^T e \geq u_2^T e$ , we may sometimes use  $\|S'e - e\|$  as an indicator for the accuracy of  $S'$ . Since  $Se = e$  in this case (see Theorem 2), we have  $\|S'e - e\| = \|(S' - S)e\| \leq \|S' - S\|$ . If  $S'$  is computed by Newton's method or basic fixed-point iterations starting with the zero matrix (see the discussions in [7]), or if  $S'$  is computed by Algorithm 2, we have  $S' \leq S$  and thus  $\|S'e - e\| = \|S' - S\|$ . When  $S'$  is computed by the (modified) Schur method, we do not generally have  $S' \leq S$  or  $S' \geq S$  and thus  $\|S'e - e\|$  is usually smaller than  $\|S' - S\|$ . In theory,  $\|S'e - e\|$  can be arbitrarily smaller than  $\|S' - S\|$ . In practice, however, it is unlikely that  $\|S'e - e\|$  is smaller than  $\|S' - S\|$  by a large factor. It should be emphasized that  $\|S'e - e\|$  is not an indicator for the accuracy of  $S'$  when  $S'$  is computed by Algorithm 3 since we always have  $\|S'e - e\| = 0$  (in exact arithmetic) in that case.

**Example 18** Consider (1) with  $n = m = 100$ ,  $M_{12} = M_{21} = -I$ , and

$$M_{11} = M_{22} = \begin{pmatrix} 2 & -1 & & \\ & 2 & \ddots & \\ & & \ddots & -1 \\ -1 & & & 2 \end{pmatrix}.$$

For this example, we have case (1) of Theorem 2. So zero is a double eigenvalue of  $R$ . For the Schur method, the two computed eigenvalues near the origin are  $0.24 \times 10^{-7}$  and  $-0.24 \times 10^{-7}$ . For the approximate solution  $S'$  obtained by the Schur method, we have  $\|\mathcal{R}(S')\| = 0.81 \times 10^{-13}$ . However, the accuracy of  $S'$  is not very high. Indeed, we find that  $\|S'e - e\| = 0.24 \times 10^{-7}$  and thus  $\|S' - S\| \geq 0.24 \times 10^{-7}$ . For the modified Schur method, the two eigenvalues near the origin are found to be 0,  $-0.10 \times 10^{-15}$  (the zero eigenvalue is obtained without computation). For the approximate solution  $S'$  obtained by the modified Schur method, we have  $\|\mathcal{R}(S')\| = 0.21 \times 10^{-12}$  and  $\|S'e - e\| = 0.25 \times 10^{-13}$ .

As judged by  $\|S'e - e\|$ , the modified Schur method provides a much more accurate approximate solution. Note, however, that we have a smaller residual for the Schur method. The sharp difference between  $\|\mathcal{R}(S')\|$  and  $\|S'e - e\|$

for the Schur method is not too surprising since the difference for Newton's method can be more dramatic. If  $S'$  is obtained after 22 Newton iterations starting with the zero matrix, we have  $\|\mathcal{R}(S')\| = 0.57 \times 10^{-13}$  and  $\|S' - S\| = \|S'e - e\| = 0.24 \times 10^{-6}$ .

For Newton's method, the convergence of the Newton sequence  $\{X_k\}$  is observed to be linear and we have an explanation for the sharp difference between the residual and the actual error. In fact, the results in [7,13] imply that

$$\lim_{k \rightarrow \infty} \frac{\|X_{k+1} - S\|}{\|X_k - S\|} = \frac{1}{2}, \quad \lim_{k \rightarrow \infty} \frac{\|\mathcal{R}(X_{k+1})\|}{\|\mathcal{R}(X_k)\|} = \frac{1}{4}.$$

Thus,  $\|\mathcal{R}(X_k)\| = O(\|X_k - S\|^2)$  as  $k \rightarrow \infty$ . So, it is quite natural to have  $\|\mathcal{R}(S')\| = 0.57 \times 10^{-13}$  and  $\|S' - S\| = 0.24 \times 10^{-6}$  for  $S' = X_{22}$ .

We also note that the performance of Newton's method can be improved by using a double Newton step (see discussions in [12,13]). If  $S'$  is obtained by six Newton iterations (with  $X_0 = 0$ ) followed by one double Newton step, then we have  $\|\mathcal{R}(S')\| = 0.46 \times 10^{-14}$ . The improvement in the accuracy of  $S'$  is much more significant than the decrease in the residual suggests. In fact, we find that  $\|S'e - e\| = 0.27 \times 10^{-14}$ . Unfortunately, the double Newton strategy works well only when  $u_1^T e$  and  $u_2^T e$  are equal or very close. Moreover, the computational work for the Schur method or the modified Schur method is no more than that for four Newton iterations.

Now we apply Algorithms 2 and 3 to this example. We use  $\theta = \max_{1 \leq i \leq m+n} m_{ii}$  for both algorithms and take  $p = \frac{1}{n}e$  for Algorithm 3. For Algorithm 2, we get after 22 iterations  $S' = S^{(22)}$  as an approximation for  $S$ . We have  $\|\mathcal{R}(S')\| = 0.57 \times 10^{-13}$  and  $\|S' - S\| = \|S'e - e\| = 0.24 \times 10^{-6}$ . For Algorithm 3, we get after 6 iterations  $S' = \hat{S}^{(6)}$  as an approximation for  $S$ . We have  $\|\mathcal{R}(S')\| = 0.22 \times 10^{-13}$ . We also compute  $\hat{S}^{(7)}$  and  $\hat{S}^{(8)}$ , and find that  $\|\hat{S}^{(6)} - \hat{S}^{(7)}\| = 0.11 \times 10^{-13}$  and  $\|\hat{S}^{(7)} - \hat{S}^{(8)}\| = 0$ . This suggests that  $\|\hat{S}^{(6)} - S\| \approx 0.11 \times 10^{-13}$ . So Algorithm 3 efficiently compute an accurate approximation.

**Example 19** *The example is obtained from Example 18 by changing the last diagonal element of  $M_{21}$  and  $M_{22}$  to  $-1 - \epsilon$  and  $2 + \epsilon$ , respectively. So we have  $u_1^T e \approx u_2^T e$ , but  $u_1^T e \neq u_2^T e$ .*

We first consider the case with  $\epsilon = 10^{-4}$ . For the Schur method, the two computed eigenvalues near the origin are  $0.20 \times 10^{-9}$  and  $-0.10 \times 10^{-5}$ . For the modified Schur method, the two eigenvalues near the origin are 0 and  $-0.10 \times 10^{-5}$ . So, by Theorem 2, this is a case with  $u_1^T e > u_2^T e$  and we have  $Se = e$  for the exact solution  $S$ . Let  $S'_a$  and  $S'_b$  be approximate solutions obtained by the Schur method and the modified Schur method, respectively. We have  $\|\mathcal{R}(S'_a)\| = 0.76 \times 10^{-13}$ ,  $\|S'_a e - e\| = 0.20 \times 10^{-9}$ ,  $\|\mathcal{R}(S'_b)\| = 0.23 \times$

$10^{-12}$ , and  $\|S'_b e - e\| = 0.25 \times 10^{-13}$ . Again,  $S'_b$  is much more accurate than  $S'_a$ , as judged by  $\|S'_a e - e\|$  and  $\|S'_b e - e\|$ . We also find that  $\|S'_a - S'_b\| = 0.20 \times 10^{-9}$ , which indicates that  $\|S'_a - S\| \approx \|S'_a e - e\|$  and  $\|S'_b - S\| \ll \|S'_a - S\|$ . For Algorithm 2, we have  $\|\mathcal{R}(S^{(22)})\| = 0.17 \times 10^{-13}$  and  $\|S^{(22)} - S\| = \|S^{(22)}e - e\| = 0.15 \times 10^{-7}$ . For Algorithm 3, we have  $\|\mathcal{R}(\hat{S}^{(6)})\| = 0.33 \times 10^{-13}$  and  $\|\hat{S}^{(6)} - S\| \approx 0.63 \times 10^{-13}$ . Again, Algorithm 3 efficiently compute an accurate approximation.

We next consider the case with  $\epsilon = -10^{-4}$ . For the Schur method, the two computed eigenvalues near the origin are  $0.10 \times 10^{-5}$  and  $0.16 \times 10^{-9}$ . For the modified Schur method, the two eigenvalues near the origin are  $0.10 \times 10^{-5}$  and 0. So, this is a case with  $u_1^T e < u_2^T e$  and we have  $Se \neq e$ . For this case, the residual is the only available measure for accuracy. We have  $\|\mathcal{R}(S'_a)\| = 0.77 \times 10^{-13}$  and  $\|\mathcal{R}(S'_b)\| = 0.21 \times 10^{-12}$ . As in the previous case, the residual for the Schur method is slightly smaller. However, we believe that  $S'_b$  is much more accurate than  $S'_a$ , as in the previous case. For Algorithm 2, we have  $\|\mathcal{R}(S^{(22)})\| = 0.17 \times 10^{-13}$ , but  $\|S^{(22)} - S\| \geq \|S^{(22)} - S^{(23)}\| = 0.15 \times 10^{-7}$ . The use of Algorithm 3 is not theoretically justified for this case. However, if we apply Algorithm 3 anyway, we get  $\|\mathcal{R}(\hat{S}^{(6)})\| = 0.40 \times 10^{-13}$  and  $\|\hat{S}^{(6)} - S\| \approx 0.63 \times 10^{-13}$ .

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