A modified large-scale structure-preserving doubling algorithm for a large-scale Riccati equation from transport theory *

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Abstract

We consider the large scale nonsymmetric algebraic Riccati equation arising in transport theory, where the $n \times n$ coefficient matrices B, C are symmetric and low-ranked and A, Eare rank one updates of nonsingular diagonal matrices. By introducing a balancing strategy and setting appropriate initial matrices carefully, we can simplify the large-scale structurepreserving doubling algorithm (SDA_ls) for this special equation. We give modified largescale structure-preserving doubling algorithm, which can reduce the flop operations of original SDA_ls by half. Numerical experiments illustrate the effectiveness of our method.

Keywords: large-scale nonsymmetric algebraic Riccati equation, large-scale structure-preserving doubling algorithm, balancing strategy, appropriate initial matrices, transport theory.

1 Introduction

In nuclear physics, we need to solve the nonsymmetric algebraic Riccati equation (NARE):

$$XCX - XE - AX + B = 0 \tag{1.1}$$

and its dual equation

$$YBY - YA - EY + C = 0, (1.2)$$

where $A, B, C, E \in \mathbb{R}^{n \times n}$ are matrices given by

$$A = \Delta - eq^T, B = ee^T, C = qq^T, E = D - qe^T,$$
(1.3)

with

$$\begin{cases}
e = (1, 1, \dots, 1)^T, \\
q = (q_1, q_2, \dots, q_n)^T, \quad q_i = \frac{c_i}{2\omega_i}, \\
\Delta = \operatorname{diag}(\delta_1, \delta_2, \dots, \delta_n), \quad \delta_i = \frac{1}{c\omega_i(1+\alpha)}, \\
D = \operatorname{diag}(d_1, d_2, \dots, d_n), \quad d_i = \frac{1}{c\omega_i(1-\alpha)},
\end{cases}$$
(1.4)

and $0 < c \le 1, 0 \le \alpha < 1, 0 < \omega_n < \dots < \omega_2 < \omega_1, \sum_{i=1}^n c_i = 1, c_i > 0, i = 1, 2, \dots, n.$

These matrices and vectors rely on the parameters c, α , ω_i and c_i . For the further physical meaning of these parameters, please see [13] and the references therein. In this paper, NARE (1.1) is always referred to the nonsymmetric algebraic Riccati equation (1.1) associated with the special structure given by (1.3) and (1.4). In applications from transport theory, the minimal nonnegative

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solution of NARE (1.1) is of interest. The numerical algorithms about this minimal nonnegative solution have been studied by many authors in the past decade, and various direct and iterative methods have been proposed. The minimal nonnegative solution is associated with the matrix

$$H = \left[\begin{array}{cc} E & -C \\ B & -A \end{array} \right].$$

The solution of NARE (1.1) can be expressed in closed form in terms of the eigenvalues and eigenvectors of H; see [14] and [17]. Available iteration algorithms are the Newton's method [3, 5, 6, 16, 10], the fixed-point iteration method [2, 4, 8, 14, 15] and the structure-preserving doubling algorithm [7, 9, 1, 18].

In [9] the authors introduced a structure-preserving transformation and developed a structurepreserving doubling algorithm (SDA) approximating quadratically to the minimal nonnegative solution of NARE(1.1) and its dual equation. For medium size problems without the special structure SDA is very effective. In [18], the authors propose a large-scale structure-preserving doubling algorithm (SDA_ls) based on the sparse-plus-low-rank coefficient matrix structure, which has O(n) computational complexity and memory requirement per iteration and could be applied to large-scale NARE satisfying the sparse-like structure.

In this paper, we further utilize the special structure of coefficient matrices of NARE (1.1) and improve the large-scale structure-preserving doubling algorithm. There are four matrix sequences $\{E_k\}, \{F_k\}, \{H_k\}$ and $\{G_k\}$ when using SDA. After an appropriate balancing of the coefficient matrices, we design appropriate initial matrices of SDA_ls, which can reduce the flop operations of SDA_ls by half. Our modified SDA_ls maintains the same quadratic convergence rate as original SDA_ls and is more efficient on large-scale NARE (1.1). The main contribution of this paper is that we show how to reduce the flop operations of SDA_ls by half through introducing a balancing strategy and setting the appropriate initial matrices for SDA_ls. We prove our result theoretically.

The rest of this paper is organized as follows. In section 2 some preliminaries are presented. In section 3 we give the balancing strategy and the appropriate initial matrices for SDA_ls, showing how to reduce the flop operations by half at each iteration step. In section 4 we present some numerical examples, which show that our modified SDA_ls is much faster than original SDA_ls applied to NARE (1.1). Throughout the paper, the Hadamard product of A and B is defined by $A \circ B = (a_{ij}b_{ij})$, I is used to denote the identity matrix of appropriate dimension, \oplus is used to denote the direct sum of square matrices.

2 Preliminaries

2.1 Structure-Preserving Doubling Algorithm

The structure-preserving doubling algorithm [9] is quadratically convergent to computing the minimal positive solution of NARE(1.1). The algorithm can be described as follows.

Choose $\gamma \geq \max \{e_{ii}, a_{ii} : i = 1, \cdots, n\}$; let

$$W = A + \gamma I - B(E + \gamma I)^{-1}C, V = E + \gamma I - C(A + \gamma I)^{-1}B,$$

and

$$E_0 = I - 2\gamma V^{-1}, \qquad F_0 = I - 2\gamma W^{-1}, G_0 = 2\gamma (E + \gamma I)^{-1} C W^{-1}, \quad H_0 = 2\gamma W^{-1} B (E + \gamma I)^{-1}.$$
(2.1)

where A, B, C, E are coefficient matrices of (1.1) and e_{ii} and a_{ii} are the i - th diagonal elements of the matrices E and A, respectively.

For $k \ge 0$, calculate

$$\begin{aligned}
E_{k+1} &= E_k (I - G_k H_k)^{-1} E_k, \\
F_{k+1} &= F_k (I - H_k G_k)^{-1} F_k, \\
G_{k+1} &= G_k + E_k (I - G_k H_k)^{-1} G_k F_k, \\
H_{k+1} &= H_k + F_k (I - H_k G_k)^{-1} H_k E_k.
\end{aligned}$$
(2.2)

Let

$$K = \left[\begin{array}{cc} E & -C \\ -B & A \end{array} \right]$$

be a nonsingular *M*-matrix. If $\lambda_1, \lambda_2, \ldots, \lambda_{2n}$ are the eigenvalues of *H* ordered by nonincreasing real parts, then the eigenvalues of *K* are $\lambda_1, \ldots, \lambda_n, -\lambda_{n+1}, \ldots, -\lambda_{2n}[5]$.

From [7, 12], We have the following convergence result.

Lemma 2.1. If the matrix sequences $\{E_k\}, \{F_k\}, \{H_k\}$ and $\{G_k\}$ are generated by (2.2), and K is nonsingular, then $\lim_{k\to\infty} E_k = \lim_{k\to\infty} F_k = 0$, $\lim_{k\to\infty} G_k = Y$, and $\lim_{k\to\infty} H_k = X$ with quadratic convergence rate, where X and Y are the minimal nonnegative solutions of NARE (1.1) and its dual equation (1.2), respectively.

2.2 Large-scale SDA

To develop a large-scale SDA [18], The authors assume that E, A are sparselike (with the products $A^{-1}u, A^{-T}u, E^{-1}u, E^{-T}u$ computable in O(n) complexity where u is a vector) and $B, C \in \mathbb{R}^{n \times n}$ have the full low-ranked decompositions

$$B = B_1 B_2^T, C = C_1 C_2^T, (2.3)$$

where $B_1, C_1 \in \mathbb{R}^{n \times r}$ and $B_2, C_2 \in \mathbb{R}^{r \times n}$ with $r \ll n$. The authors apply the Sherman-Morrison-Woodbury formula to avoid the invention of large matrices and use low ranked matrices to represent iterates. The basic large-scale SDA (SDA_ls) is as follows.

For $k = 1, 2, \cdots$, SDA_ls is organized so that the iterates have the recursive forms

$$H_{k}^{\tau} = Q_{1k}^{\tau} \Sigma_{k}^{\tau} Q_{2k}^{\tau T}, \qquad G_{k}^{\tau} = P_{1k}^{\tau} \Gamma_{k}^{\tau} P_{2k}^{\tau T}, E_{k}^{\tau} = E_{k-1}^{\tau 2} + E_{1k}^{\tau} E_{2k}^{\tau T}, \quad F_{k}^{\tau} = F_{k-1}^{\tau 2} + F_{1k}^{\tau} F_{2k}^{\tau T},$$
(2.4)

where Q_{ik}^{τ} and P_{ik}^{τ} are column orthogonal with widths being m_k and l_k (i = 1, 2) respectively. Note that E_k^{τ} and F_k^{τ} are not formed explicitly.

For the initial matrices (2.1), we have

$$E_0 = I - 2\gamma V^{-1}, F_0 = I - 2\gamma W^{-1}, H_0 = Q_{10} \Sigma_0 Q_{20}^T, G_0 = P_{10} \Gamma_0 P_{20}^T, F_0 = P_{10} \Gamma_0 P_{20}^T, F_0$$

where

$$Q_{10} \equiv 2\gamma W^{-1} B_1, \quad Q_{20} \equiv (E + \gamma I)^{-T} B_2, \quad \Sigma_0 \equiv I,$$
 (2.5)

$$P_{10} \equiv 2\gamma (E + \gamma I)^{-1} C_1, \qquad P_{20} \equiv W^{-T} C_2, \qquad \Gamma_0 \equiv I.$$
 (2.6)

Note that efficient linear solvers with O(n) complexity for large scale A, E and $A + \gamma I, E + \gamma I$ are available. Utilizing Shermann-Morrison-Woodbury (SMW) formula $W^{-1}u$ and $V^{-1}u$ can be computed with O(n) complexity too. Then we compute the economic QR decompositions

$$Q_{10} = \hat{Q}_{10}R_{1q}, Q_{20} = \hat{Q}_{20}R_{2q}, P_{10} = \hat{P}_{10}R_{1p}, P_{20} = \hat{P}_{20}R_{2p},$$
(2.7)

where $\hat{Q}_{10}, \hat{Q}_{20}, \hat{P}_{10}, \hat{P}_{20}$ are column orthogonal and $R_{1q}, R_{2q}, R_{1p}, R_{2p}$ are upper triangular matrices with positive diagonal entries. Then we compute the SVDs

$$R_{1q}\Sigma_0 R_{2q}^T = [U_{10}^{\tau}, U_{10}^{\epsilon}] (\Sigma_0^{\tau} \oplus \Sigma_0^{\epsilon}) [U_{20}^{\tau}, U_{20}^{\epsilon}]^T, \|\Sigma_0^{\epsilon}\| < \epsilon_0,$$

$$R_{1p}\Gamma_0 R_{2p}^T = [V_{10}^{\tau}, V_{10}^{\epsilon}] (\Gamma_0^{\tau} \oplus \Gamma_0^{\epsilon}) [V_{20}^{\tau}, V_{20}^{\epsilon}]^T, \|\Gamma_0^{\epsilon}\| < \epsilon_0,$$
(2.8)

where $[U_{i0}^{\tau}, U_{i0}^{\epsilon}]$ and $[V_{20}^{\tau}, V_{20}^{\epsilon}]$ (i = 1, 2) are orthogonal, $\Sigma_0^{\tau} \oplus \Sigma_0^{\epsilon}$ and $\Gamma_0^{\tau} \oplus \Gamma_0^{\epsilon}$ are nonnegative diagonal. By setting

$$Q_{10}^{\tau} = \hat{Q}_{10} U_{10}^{\tau}, Q_{20}^{\tau} = \hat{Q}_{20} U_{20}^{\tau}, P_{10}^{\tau} = \hat{P}_{10} V_{10}^{\tau}, P_{20}^{\tau} = \hat{P}_{20} V_{20}^{\tau},$$
(2.9)

we get the truncated initial matrices for large-scale SDA (SDA_ls)

$$E_0^{\tau} = E_0, F_0^{\tau} = F_0, H_0^{\tau} = Q_{10}^{\tau} \Sigma_0^{\tau} Q_{20}^{\tau T}, G_0^{\tau} = P_{10}^{\tau} \Gamma_0^{\tau} P_{20}^{\tau T}.$$
 (2.10)

Then we compute

$$\begin{split} \check{\Sigma}_{k}^{\tau} &= \Sigma_{k}^{\tau} + \Sigma_{k}^{\tau} Q_{2k}^{\tau T} P_{1k}^{\tau} \Gamma_{k}^{\tau} (I - P_{2k}^{\tau T} H_{k}^{\tau} P_{1k}^{\tau} \Gamma_{k}^{\tau})^{-1} P_{2k}^{\tau T} Q_{1k}^{\tau} \Sigma_{k}^{\tau}, \\ \check{\Gamma}_{k}^{\tau} &= \Gamma_{k}^{\tau} + (I - \Gamma_{k}^{\tau} P_{2k}^{\tau T} H_{k}^{\tau} P_{1k}^{\tau})^{-1} \Gamma_{k}^{\tau} P_{2k}^{\tau T} H_{k}^{t} P_{1k}^{\tau} \Gamma_{k}^{\tau}, \end{split}$$

$$(2.11)$$

and

$$F_{1,k+1}^{\tau} = F_k^{\tau} Q_{1k}^{\tau} (I - \Sigma_k^{\tau} Q_{2k}^{\tau T} G_k^{\tau} Q_{1k}^{\tau})^{-1} \Sigma_k^{\tau} Q_{2k}^{\tau T} P_{1k}^{\tau} \Gamma_k^{\tau}, \quad F_{2,k+1}^{\tau} = F_k^{\tau T} P_{2k}^{\tau},$$

$$E_{1,k+1}^{\tau} = E_k^{\tau} P_{1k}^{\tau} (I - \Gamma_k^{\tau} P_{2k}^{\tau T} H_k^{\tau} P_{1k}^{\tau})^{-1} \Gamma_k^{\tau} P_{2k}^{\tau T} Q_{1k}^{\tau} \Sigma_k^{\tau}, \quad E_{2,k+1}^{\tau} = E_k^{\tau T} Q_{2k}^{\tau}.$$
(2.12)

From the economic QR decompositions

$$[Q_{1k}^{\tau}, F_k^{\tau} Q_{1k}^{\tau}] = [Q_{1k}^{\tau}, \hat{Q}_{1k}] \begin{bmatrix} I & S_{1q} \\ 0 & R_{1q} \end{bmatrix}, [Q_{2k}^{\tau}, E_k^{\tau} Q_{2k}^{\tau}] = [Q_{2k}^{\tau}, \hat{Q}_{2k}] \begin{bmatrix} I & S_{2q} \\ 0 & R_{2q} \end{bmatrix},$$
(2.13)

$$[P_{1k}^{\tau}, E_k^{\tau} P_{1k}^{\tau}] = [P_{1k}^{\tau}, \hat{P}_{1k}] \begin{bmatrix} I & S_{1p} \\ 0 & R_{1p} \end{bmatrix}, [P_{2k}^{\tau}, F_k^{\tau} P_{2k}^{\tau}] = [P_{2k}^{\tau}, \hat{P}_{2k}] \begin{bmatrix} I & S_{2p} \\ 0 & R_{2p} \end{bmatrix},$$
(2.14)

we compute

$$\hat{\Sigma}_{k+1} = \begin{bmatrix} I & S_{1q} \\ 0 & R_{1q} \end{bmatrix} \begin{bmatrix} \Sigma_k^{\tau} & 0 \\ 0 & \breve{\Sigma}_k^{\tau} \end{bmatrix} \begin{bmatrix} I & S_{2q} \\ 0 & R_{2q} \end{bmatrix}^T$$

$$\hat{\Gamma}_{k+1} = \begin{bmatrix} I & S_{1p} \\ 0 & R_{1p} \end{bmatrix} \begin{bmatrix} \Gamma_k^{\tau} & 0 \\ 0 & \breve{\Gamma}_k^{\tau} \end{bmatrix} \begin{bmatrix} I & S_{2p} \\ 0 & R_{2p} \end{bmatrix}^T,$$
(2.15)

then we compute the SVDs

$$\hat{\Sigma}_{k+1} = \begin{bmatrix} U_{1,k+1}^{\tau} & U_{1,k+1}^{\epsilon} \end{bmatrix} (\Sigma_{k+1}^{\tau} \oplus \Sigma_{k+1}^{\epsilon}) \begin{bmatrix} U_{2,k+1}^{\tau} & U_{2,k+1}^{\epsilon} \end{bmatrix}^{T}$$
$$\hat{\Gamma}_{k+1} = \begin{bmatrix} V_{1,k+1}^{\tau} & V_{1,k+1}^{\epsilon} \end{bmatrix} (\Gamma_{k+1}^{\tau} \oplus \Gamma_{k+1}^{\epsilon}) \begin{bmatrix} V_{2,k+1}^{\tau} & V_{2,k+1}^{\epsilon} \end{bmatrix}^{T}$$
(2.16)

with $\|\Sigma_{k+1}^{\epsilon}\| < \epsilon_{k+1}$ and $\|\Gamma_{k+1}^{\epsilon}\| < \epsilon_{k+1}$. The truncated matrices are

$$Q_{1,k+1}^{\tau} = [Q_{1k}^{\tau}, \hat{Q}_{1k}] U_{1,k+1}^{\tau}, \quad Q_{2,k+1}^{\tau} = [Q_{2k}^{\tau}, \hat{Q}_{2k}] U_{2,k+1}^{\tau},$$

$$P_{1,k+1}^{\tau} = [P_{1k}^{\tau}, \hat{P}_{1k}] V_{1,k+1}^{\tau}, \quad P_{2,k+1}^{\tau} = [P_{2k}^{\tau}, \hat{P}_{2k}] V_{2,k+1}^{\tau}.$$
(2.17)

We note that if QR decompositions and SVDs are not introduced to truncate Q_{ik} , $P_{ik}(i = 1, 2)$ in SDA_ls, then SDA_ls is mathematically equivalent to SDA (2.2) because (2.4) are derived from (2.2) by applying SMW formula:

$$\begin{array}{lll} (I - H_k^{\tau} G_k^{\tau})^{-1} &=& I + Q_{1k}^{\tau} (I - \Sigma_k^{\tau} Q_{2k}^{\tau T} G_k^{\tau} Q_{1k}^{\tau})^{-1} \Sigma_k^{\tau} Q_{2k}^{\tau T} G_k^{\tau}, \\ (I - G_k^{\tau} H_k^{\tau})^{-1} &=& I + P_{1k}^{\tau} (I - \Gamma_k^{\tau} P_{2k}^{\tau T} H_k^{\tau} P_{1k}^{\tau})^{-1} \Gamma_k^{\tau} P_{2k}^{\tau T} H_k^{\tau}. \end{array}$$

3 Balancing Strategy and Modified SDA_ls

In this section we introduce a balancing strategy, with which the matrix \widetilde{X}^T is the minimal positive solution of the dual equation if \widetilde{X} is the minimal positive solution of the algebraic Riccati equation.

Because the entries of the vector \boldsymbol{q} are positive, we may define

$$\Phi := \operatorname{diag}(\sqrt{q_1}, \cdots, \sqrt{q_n}), \phi := (\sqrt{q_1}, \cdots, \sqrt{q_n})^T.$$

Let

$$\begin{split} \tilde{X} &= \Phi X \Phi, \\ \tilde{A} &= \Phi A \Phi^{-1} = \Delta - \phi \phi^T, \\ \tilde{B} &= \Phi B \Phi = \phi \phi^T, \\ \tilde{C} &= \Phi^{-1} C \Phi^{-1} = \phi \phi^T = \tilde{B}, \\ \tilde{E} &= \Phi^{-1} E \Phi = D - \phi \phi^T. \end{split}$$

Then the algebraic Riccati equation of (1.1) can be equivalently expressed as

$$\tilde{X}\tilde{C}\tilde{X} - \tilde{X}\tilde{E} - \tilde{A}\tilde{X} + \tilde{B} = 0.$$
(3.1)

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Obviously, X is a solution of (1.1) if and only if $\tilde{X} = \Phi X \Phi$ is a solution of (3.1). Let

$$\begin{split} \tilde{K} &= \begin{bmatrix} \tilde{E} & -\tilde{C} \\ -\tilde{B} & \tilde{A} \end{bmatrix} \\ &= \begin{bmatrix} \Phi^{-1} & 0 \\ 0 & \Phi \end{bmatrix} K \begin{bmatrix} \Phi & 0 \\ 0 & \Phi^{-1} \end{bmatrix}. \end{split}$$

Then \tilde{K} is similar to K.

Choose $\tilde{\gamma} \ge \max{\{\tilde{e}_{ii}, \tilde{a}_{ii} : i = 1, \cdots, n\}};$ let

$$\tilde{W} = \tilde{A} + \tilde{\gamma}I - \tilde{B}(\tilde{E} + \tilde{\gamma}I)^{-1}\tilde{C}, \tilde{V} = \tilde{E} + \tilde{\gamma}I - \tilde{C}(\tilde{A} + \tilde{\gamma}I)^{-1}\tilde{B}$$

and

$$\tilde{E}_{0} = I - 2\tilde{\gamma}\tilde{V}^{-1}, \qquad \tilde{F}_{0} = I - 2\tilde{\gamma}\tilde{W}^{-1},
\tilde{G}_{0} = 2\tilde{\gamma}(\tilde{E} + \tilde{\gamma}I)^{-1}\tilde{C}\tilde{W}^{-1}, \qquad \tilde{H}_{0} = 2\tilde{\gamma}\tilde{W}^{-1}\tilde{B}(\tilde{E} + \tilde{\gamma}I)^{-1},$$
(3.2)

where $\tilde{A}, \tilde{B}, \tilde{C}$ and \tilde{E} are coefficient matrices of (3.1) and \tilde{e}_{ii} and \tilde{a}_{ii} are the i-th diagonal elements of the matrices \tilde{E} and \tilde{A} , respectively.

For $k \ge 0$, calculate

$$\tilde{E}_{k+1} = \tilde{E}_k (I - \tilde{G}_k \tilde{H}_k)^{-1} \tilde{E}_k,
\tilde{F}_{k+1} = \tilde{F}_k (I - \tilde{H}_k \tilde{G}_k)^{-1} \tilde{F}_k,
\tilde{G}_{k+1} = \tilde{G}_k + \tilde{E}_k (I - \tilde{G}_k \tilde{H}_k)^{-1} \tilde{G}_k \tilde{F}_k,
\tilde{H}_{k+1} = \tilde{H}_k + \tilde{F}_k (I - \tilde{H}_k \tilde{G}_k)^{-1} \tilde{H}_k \tilde{E}_k.$$
(3.3)

For the initial matrices of SDA_ls for NARE (3.1), if we set

$$E_0 = I - 2\tilde{\gamma}\tilde{V}^{-1}, F_0 = I - 2\tilde{\gamma}\tilde{W}^{-1}, H_0 = Q_{10}\Sigma_0 Q_{20}^T, G_0 = P_{10}\Gamma_0 P_{20}^T, F_0 = P_{10}\Gamma_0$$

where

$$Q_{10} \equiv \sqrt{2\tilde{\gamma}}\tilde{W}^{-1}\phi, \quad Q_{20} \equiv \sqrt{2\tilde{\gamma}}(\tilde{E} + \tilde{\gamma}I)^{-T}\phi, \quad \Sigma_0 \equiv I,$$
$$P_{10} \equiv \sqrt{2\tilde{\gamma}}(\tilde{E} + \tilde{\gamma}I)^{-1}\phi, \qquad P_{20} \equiv \sqrt{2\tilde{\gamma}}\tilde{W}^{-T}\phi, \qquad \Gamma_0 \equiv I,$$

then the flop operations of large scale structure preserving doubling algorithm can be reduced by half. We show this in Theorem 3.1.

Theorem 3.1. For the initial matrices of SDA_ls applied to NARE (3.1), if

$$E_0 = I - 2\tilde{\gamma}\tilde{V}^{-1}, F_0 = I - 2\tilde{\gamma}\tilde{W}^{-1}, H_0 = Q_{10}\Sigma_0 Q_{20}^T, G_0 = P_{10}\Gamma_0 P_{20}^T,$$

where

$$Q_{10} \equiv \sqrt{2\tilde{\gamma}}\tilde{W}^{-1}\phi, \quad Q_{20} \equiv \sqrt{2\tilde{\gamma}}(\tilde{E} + \tilde{\gamma}I)^{-T}\phi, \quad \Sigma_0 \equiv I, \tag{3.4}$$

$$P_{10} \equiv \sqrt{2\tilde{\gamma}}(\tilde{E} + \tilde{\gamma}I)^{-1}\phi, \qquad P_{20} \equiv \sqrt{2\tilde{\gamma}}\tilde{W}^{-T}\phi, \qquad \Gamma_0 \equiv I,$$
(3.5)

then for SDA_ls

$$Q_{1k}^{\tau} = P_{2k}^{\tau}, \quad Q_{2k}^{\tau} = P_{1k}^{\tau}, \quad \Sigma_k^{\tau} = \Gamma_k^{\tau}, \tag{3.6}$$

$$E_{k}^{\tau} = E_{k}^{\tau T} \quad F_{k}^{\tau} = F_{k}^{\tau T}, \quad H_{k}^{\tau} = G_{k}^{\tau T}, \tag{3.7}$$

$$E_k^{\tau} P_{1k}^{\tau} = E_k^{\tau T} Q_{2k}^{\tau}, F_k^{\tau} Q_{1k}^{\tau} = F_k^{\tau T} P_{2k}^{\tau}$$
(3.8)

hold true for $k = 1, 2, \cdots$.

Proof. We prove the result by mathematical induction.

After being balanced, Since $\tilde{B} = \tilde{C}$, $\tilde{A}^T = \tilde{A}$ and $\tilde{E}^T = \tilde{E}$, we have

$$\tilde{W}^T = \tilde{W}, \tilde{V}^T = \tilde{V},$$

and, thus,

$$E_0^T = E_0, F_0^T = F_0, H_0 = G_0^T.$$

From

$$\begin{aligned} Q_{10} &\equiv \sqrt{2\tilde{\gamma}}\tilde{W}^{-1}\phi, \quad Q_{20} \equiv \sqrt{2\tilde{\gamma}}(\tilde{E}+\tilde{\gamma}I)^{-T}\phi, \quad \Sigma_0 \equiv I, \\ P_{10} &\equiv \sqrt{2\tilde{\gamma}}(\tilde{E}+\tilde{\gamma}I)^{-1}\phi, \qquad P_{20} \equiv \sqrt{2\tilde{\gamma}}W^{-T}\phi, \qquad \Gamma_0 \equiv I, \end{aligned}$$

we get

$$Q_{10} = P_{20}, Q_{20} = P_{10}, \Sigma_0 = \Gamma_0^T.$$

Then from the initial process of SDA_ls, i.e. (2.7),(2.8), (2.9), (2.10), we can verify that

$$\begin{aligned} & Q_{10}^{\tau} = P_{20}^{\tau}, \quad Q_{20}^{\tau} = P_{10}^{\tau}, \quad \Sigma_{0}^{\tau} = \Gamma_{0}^{\tau T}, \\ & E_{0}^{\tau} = E_{0}^{\tau T} \quad F_{0}^{\tau} = F_{0}^{\tau T}, \quad H_{0}^{\tau} = G_{0}^{\tau T}, \end{aligned}$$

 $\quad \text{and} \quad$

$$E_0^{\tau} P_{10}^{\tau} = E_0^{\tau T} Q_{20}^{\tau}, F_0^{\tau} Q_{10}^{\tau} = F_0^{\tau T} P_{20}^{\tau}$$

Hence the result is true for k = 0. Assume that the result holds true for k = l, and we consider the case of k = l + 1. Note that at each local step of SDA_ls, the local truncation is done only on matrices Q_{ik} and P_{ik} (i=1,2), so the following iteration processes of SDA_ls

$$E_{l+1}^{\tau} = E_l^{\tau 2} + E_{1,l+1}^{\tau} E_{2,l+1}^{\tau T}, F_{l+1}^{\tau} = F_l^{\tau 2} + F_{1,l+1}^{\tau} F_{2,l+1}^{\tau T},$$

are mathematically equivalent to applying SMW formula to

$$E_{l+1}^{\tau} = E_l^{\tau} (I - G_l^{\tau} H_l^{\tau})^{-1} E_l^{\tau}, F_{l+1}^{\tau} = F_l^{\tau} (I - H_l G_l^{\tau})^{-1} F_l).$$
(3.9)

From the assumption of induction we know

$$E_l^{\tau} = E_l^{\tau T}, \quad F_l^{\tau} = F_l^{\tau T}, \quad H_l^{\tau} = G_l^{\tau T},$$

so from (3.9) we get

$$E_{l+1}^{\tau} = E_{l+1}^{\tau T}, F_{l+1}^{\tau} = F_{l+1}^{\tau T}.$$

By direct calculations we can verify that

$$\breve{\Sigma}_l^\tau = \breve{\Gamma}_l^{\tau T}$$

holds in the iteration step (2.11) and we have

$$[Q_{1l}^{\tau}, F_l^{\tau} Q_{1l}^{\tau}] = [P_{2l}^{\tau}, F_l^{\tau} P_{2l}^{\tau}], [Q_{2l}^{\tau}, E_l^{\tau} Q_{2l}^{\tau}] = [P_{1l}^{\tau}, E_l^{\tau} P_{1l}^{\tau}]$$

in iteration step (2.13) because of assumption of induction, so we get

$$\hat{\Sigma}_{l+1} = \hat{\Gamma}_{l+1}^T$$

in the iteration step (2.15). Then from (2.16) we get

$$\Sigma_{l+1}^{\tau} = \Gamma_{l+1}^{\tau T}$$

and from (2.17) we get

$$Q_{1,l+1}^{\tau} = P_{2,l+1}^{\tau}, Q_{2,l+1}^{\tau} = P_{1,l+1}^{\tau},$$

and thus

$$H_{l+1}^{\tau} = G_{l+1}^{\tau T}$$

Combining with

$$E_{l+1}^{\tau} = E_{l+1}^{\tau T}, F_{l+1}^{\tau} = F_{l+1}^{\tau T},$$

we see that

$$E_{l+1}^{\tau}P_{1,l+1}^{\tau} = E_{l+1}^{\tau T}Q_{2,l+1}^{\tau}, F_{l+1}^{\tau}Q_{1,l+1}^{\tau} = F_{l+1}^{\tau T}P_{2,l+1}^{\tau}.$$

So we know that the conclusion holds true for k = l+1. By induction we have proved the result. \Box

Based on the above discussion, we present the modified SDA_ls algorithm for NARE (1.1) as follows.

Modified SDA_ls for NARE (1.1)

1. Set $\phi := (\sqrt{q_1}, \cdots, \sqrt{q_n})^T$ and let

$$A = \Delta - \phi \phi^T, B = \phi \phi^T, C = \phi \phi^T, E = D - \phi \phi^T.$$

2. k := 0, compute W^{-1}, V^{-1} and E_0, F_0 implicitly and set

$$Q_{10} \equiv \sqrt{2\gamma} W^{-1} \phi, Q_{20} \equiv \sqrt{2\gamma} (E+\gamma)^{-T} \phi, \Sigma_0 \equiv I.$$

Compute economic QR decompositions

$$Q_{10} = \hat{Q}_{10} R_{1q}, Q_{20} = \hat{Q}_{20} R_{2q}$$

and compute the SVDs

$$R_{1q}\Sigma_0 R_{2q}^T = [U_{10}^{\tau}, U_{10}^{\epsilon}](\Sigma_0^{\tau} \oplus \Sigma_0^{\epsilon})[U_{20}^{\tau}, U_{20}^{\epsilon}]^T, \|\Sigma_0^{\epsilon}\| < \epsilon_0.$$

Set

$$\begin{aligned} Q_{10}^{\tau} &= \dot{Q}_{10} U_{10}^{\tau}, Q_{20}^{\tau} = \dot{Q}_{20} U_{20}^{\tau}, \\ E_0^{\tau} &= E_0, F_0^{\tau} = F_0, H_0^{\tau} = Q_{10}^{\tau} \Sigma_0^{\tau} Q_{20}^{\tau T}. \end{aligned}$$

Table 1: Flop operations for the kth iteration in SDA_ls

Computation	Flops
$\check{\Sigma}_k^ au,\check{\Gamma}_k^ au$	$4m_km_kn$
$E_k^\tau P_{1k}^\tau, E_k^{\tau T} Q_{2k}^\tau$	$2[2^{k}(c_{\gamma}+4\sum_{j=1}^{k}2^{-i}m_{j}]m_{k}n$
$F_k^ au Q_{1k}^ au, F_k^{ au T} P_{2k}^ au$	$2[2^{k}(c_{\gamma}+4\sum_{j=1}^{k}2^{-i}m_{j}]m_{k}n$
$F_{1,k+1}^{\tau}, E_{1,k+1}^{\tau}$	$4m_km_kn$
Orthogonalize $F_k^{\tau} Q_{1k}^{\tau}, F_k^{\tau T} P_{2k}^{\tau}, E_k^{\tau} P_{1k}^{\tau}, E_k^{\tau T} Q_{2k}^{\tau}$	$2[6(m_k^2 + m_k^2) + 2m_k]n$
$Q_{i,k+1}^{\tau}, P_{i,k+1}^{\tau} (i=1,2)$	$16(m_k m_{k+1})n$

3. For $k \ge 0$, calculate

$$\breve{\Sigma}_k^{\tau} = \Sigma_k^{\tau} + \Sigma_k^{\tau} Q_{2k}^{\tau T} Q_{2k}^{\tau} \Gamma_k^{\tau} (I - Q_{1k}^{\tau T} H_k^{\tau} Q_{2k}^{\tau} \Gamma_k^{\tau})^{-1} Q_{1k}^{\tau T} Q_{1k}^{\tau} \Sigma_k^{\tau},$$

and

$$\begin{split} F_{2,k+1}^{\tau} &= F_k^{\tau} Q_{1k}^{\tau}, \quad F_{1,k+1}^{\tau} = F_{2,k+1}^{\tau} (I - \Gamma_k^{\tau} Q_{2k}^{\tau T} H_k^{\tau T} Q_{1k}^{\tau})^{-1} \Sigma_k^{\tau} Q_{2k}^{\tau T} P_{1k}^{\tau} \Gamma_k^{\tau} \\ E_{2,k+1}^{\tau} &= E_k^{\tau} Q_{2k}^{\tau}, \quad E_{1,k+1}^{\tau} = E_{2,k+1}^{\tau} (I - \Gamma_k^{\tau} Q_{1k}^{\tau T} H_k^{\tau} P_{1k}^{\tau})^{-1} \Gamma_k^{\tau} Q_{1k}^{\tau T} Q_{1k}^{\tau} \Sigma_k^{\tau}. \end{split}$$

Compute economic QR decompositions

$$[Q_{1k}^{\tau}, F_k^{\tau} Q_{1k}^{\tau}] = [Q_{1k}^{\tau}, \hat{Q}_{1k}] \begin{bmatrix} I & S_{1q} \\ 0 & R_{1q} \end{bmatrix}, [Q_{2k}^{\tau}, E_k^{\tau} Q_{2k}^{\tau}] = [Q_{2k}^{\tau}, \hat{Q}_{2k}] \begin{bmatrix} I & S_{2q} \\ 0 & R_{2q} \end{bmatrix}$$

and

$$\hat{\Sigma}_{k+1} = \begin{bmatrix} I & S_{1q} \\ 0 & R_{1q} \end{bmatrix} \begin{bmatrix} \Sigma_k^{\tau} & 0 \\ 0 & \breve{\Sigma}_k^{\tau} \end{bmatrix} \begin{bmatrix} I & S_{2q} \\ 0 & R_{2q} \end{bmatrix}^T.$$

Then compute the SVDs

$$\hat{\Sigma}_{k+1} = \begin{bmatrix} U_{1,k+1}^{\tau} & U_{1,k+1}^{\epsilon} \end{bmatrix} (\Sigma_{k+1}^{\tau} \oplus \Sigma_{k+1}^{\epsilon}) \begin{bmatrix} U_{2,k+1}^{\tau}, U_{2,k+1}^{\epsilon} \end{bmatrix}^T$$

with $\|\Sigma_{k+1}^{\epsilon}\| < \epsilon_{k+1}$ and the truncated matrices

$$Q_{1,k+1}^{\tau} = [Q_{1k}^{\tau}, \hat{Q}_{1k}]U_{1,k+1}^{\tau}, Q_{2,k+1}^{\tau} = [Q_{2k}^{\tau}, \hat{Q}_{2k}]U_{2,k+1}^{\tau}$$

and form

$$E_k^{\tau} = E_{k-1}^{\tau 2} + E_{1k}^{\tau} E_{2k}^{\tau T}, F_k^{\tau} = F_{k-1}^{\tau 2} + F_{1k}^{\tau} F_{2k}^{\tau T}$$

implicitly.

4. If the stoping criterion is satisfied, then return

$$X = (\Phi^{-1}Q_{1k}^{\tau})\Sigma_k^{\tau}(Q_{2k}^{\tau T}\Phi^{-1}),$$

where $\phi^{-1} = \left(\frac{1}{\sqrt{q_1}}, \cdots, \frac{1}{\sqrt{q_n}}\right)^T$; else go to step 3.

We compare the operation counts for the kth iteration in SDA_ls and modified SDA_ls. From Table 1 and Table 2, we see clearly the flops of modified SDA_ls are roughly half of that of SDA_ls.

Table 2: Flop operations for the kth iteration in modified SDA_ls

Computation	Flops
$\check{\Sigma}_k^ au$	$2m_km_kn$
$E_k^{ au}Q_{2k}^{ au}$	$[2^k(c_{\gamma}+4\sum_{j=1}^k 2^{-i}m_j]m_kn$
$F_k^{ au}Q_{1k}^{ au}$	$[2^k(c_{\gamma} + 4\sum_{j=1}^k 2^{-i}m_j]m_kn$
$F_{1,k+1}^{\tau}, E_{1,k+1}^{\tau}$	$4m_km_kn$
Orthogonalize $F_k^{\tau} Q_{1k}^{\tau}, E_k^{\tau} Q_{2k}^{\tau}$	$[6(m_k^2 + m_k^2) + 2m_k]n$
$Q_{i,k+1}^{\tau}(i=1,2)$	$8(m_km_{k+1})n$

4 Numerical Experiments

5 Conclusions

We have presented a balancing strategy and specially chosen initial matrices for the large-scale structure-preserving doubling algorithm applied to NARE (1.1). We prove the flop operations of SDA_ls at each iteration step can be reduced by half for this special equation. Computationally it is an interesting scheme that helps reducing flop operations and computing the solution faster. Numerical experiments show that modified SDA_ls for NARE (1.1) is very effective and outperforms SDA_ls.

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