A decoupled form of the structure-preserving doubling algorithm with low-rank structures

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Abstract

The structure-preserving doubling algorithm (SDA) is a fairly efficient method for solving problems closely related to Hamiltonian (or Hamiltonian-like) matrices, such as computing the required solutions to algebraic Riccati equations. However, for large-scale problems in $\mathbb{C}^n$ (also $\mathbb{R}^n$), the SDA with an $O(n^3)$ computational complexity does not work well. In this paper, we propose a new decoupled form of the SDA (we name it as dSDA), building on the associated Krylov subspaces thus leading to the inherent low-rank structures. Importantly, the approach decouples the original two to four iteration formulae. The resulting dSDA is much more efficient since only one quantity (instead of the original two to four) is computed iteratively. For large-scale problems, further efficiency is gained from the low-rank structures. This paper presents the theoretical aspects of the dSDA. A practical algorithm dSDA with truncation and many illustrative numerical results will appear in a second paper.

Keywords. structure-preserving doubling algorithm, low-rank structure, decoupled form

1 Introduction

The doubling algorithm (DA), in some sense, skips many items in the iteration process and only computes the $k$-th iterates with $k = 2^j, j = 0, 1, 2, \ldots$. The DA idea can at least be traced back to, to the best of our knowledge, the nineteen seventies — in [12, 13, 28] the DA was adopted to solve the matrix Riccati differential equations. In 1978 Anderson [1] compendiously surveyed the existing DAs at that time and firstly introduced the structure-preserving doubling algorithm (SDA) for algebraic Riccati equations. In the last two decades or more, an enormous amount of research efforts goes into the remarkable method, including theories, numerical algorithms and efficient implementation; please consult [10, 23, 4, 8] and the references therein. In [10], Chu et al. revisited the SDA and applied successively it to the periodic discrete-time algebraic Riccati equations. Since then, the SDA has been generalized for many matrix equations, such as the continuous-time algebraic equations [9, 24, 23], the M-matrix algebraic Riccati equations [20, 42, 43, 16].

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and the $H^*$-matrix algebraic Riccati equations [33]. Some related eigenvalue problems, such as the palindromic quadratic eigenvalue problems [19, 36, 35] and the Bethe-Salpeter eigenvalue problems [21], have also been treated.

The classical SDA possesses an $O(n^3)$ computational complexity for problems in $\mathbb{R}^n$ or $\mathbb{C}^n$, and is best suited for moderate values of $n$, with its global and quadratic convergence [32]; for the linear convergence in the critical case, please consult [24]. However, for large-scale problems, the original SDA obviously does not work efficiently, because of its computational complexity, or the high costs in memory requirement and execution time.

In this paper we emphasize on the numerical solution of large-scale algebraic Riccati equations (AREs) with low-rank structures by the SDA. We consider the discrete-time algebraic Riccati equations (DAREs), the continuous-time algebraic Riccati equations (CAREs) and the M-matrix algebraic Riccati equations (MARE). For these AREs, the SDA has three or four coupled recursions (see (4) and (7) in Section 2). For large-scale problems however, one recursion has been applied implicitly (because of the loss of sparsity), leading to a flop count with an exponentially increasing constant thus inefficiency. We propose a new form of the SDA (namely dSDA), which decouples the three (see (4)) or four (see (7)) recursions. Because of the decoupling, the dSDA computes more efficiently, with only one recursion for the desired numerical solution.

Our main contributions are summarized as follows:

1. We decouple the three recursions (4) and four recursions (7) in the original SDA and develop the dSDA. On the surface, the new method is closely related to the Krylov subspace projection methods but the dSDA inherits the sound theoretical foundation of the SDA.

2. The original SDA has three (or four) iteration formulae (4) (or (7)) for $A_k$ (or $E_k$ and $F_k$), $G_k$ and $H_k$ in the $k$-th iteration. The dSDA for large-scale AREs no longer requires $A_k$ (or $E_k$ and $F_k$), thus eliminating the $2^k$ factor in the flop count and improving the efficiency tremendously. We only compute $H_k$, the desired approximate solution of the ARE.

This paper presents the theoretical aspects of the dSDA. A practical algorithm dSDA, with truncation and the illustrative numerical results will appear in a second paper.

**Notations** The null matrix is 0 and the $n$-by-$n$ identity matrix is denoted by $I_n$, with its subscript ignored when the size is clear; $(\cdot)^H$ and $(\cdot)^T$ take the conjugate transpose and the transpose of matrices, respectively. The complex conjugate of a matrix $A$ is $\bar{A}$. The 2-norm is denoted by $\| \cdot \|$. By $M \oplus N$, we denote $\begin{bmatrix} M & 0 \\ 0 & N \end{bmatrix}$.

**Organization** We revisit the SDA for the DAREs, CAREs and MAREs in Section 2, and then develop the dSDA for these AREs in Section 3; the SDA is also extended for the Bethe-Salpeter eigenvalue problems (BSEPs). Some numerical results are presented in Section 4, and some conclusions are drawn in Section 5.

The Sherman-Morrison-Woodbury formula (SMWF):

$$ (M + UDV^T)^{-1} = M^{-1} - M^{-1}U(D^{-1} + V^TM^{-1}U)^{-1}V^TM^{-1}, $$

with the inverse sign indicating invertibility, will be applied occasionally.
2 Structure-preserving doubling algorithm

Consider the linear time-invariant control system in continuous-time:
\[
\dot{x}(t) = Ax(t) + Bu(t), \quad y(t) = Cx(t),
\]
where \( A \in \mathbb{R}^{n \times n} \), \( B \in \mathbb{R}^{n \times m} \) and \( C \in \mathbb{R}^{l \times n} \) with \( m, l \leq n \), \( x(t) \) is the state vector and \( u(t) \) is the control vector. The linear-quadratic (LQ) optimal control minimizes the cost functional \( J(x,u) = \int_0^\infty [x(t)^\top H x(t) + u(t)^\top R u(t)] \, dt \), with \( H = C^\top C \geq 0 \) and \( R > 0 \). Here, a symmetric matrix \( M > 0 \) (\( \geq 0 \)) when all its eigenvalues are positive (non-negative). Also, \( M > N \) (\( M \geq N \)) if and only if \( M - N > 0 \) (\( \geq 0 \)). With \( G \equiv BR^{-1}B^\top \geq 0 \), the optimal control \( u(t) = -R^{-1}B^\top X x(t) \) can be expressed in terms of the unique Hermitian positive semi-definite (psd) stabilizing solution \( X \) of the CARE [4, 9, 29, 38]:
\[
C(X) \equiv A^\top X + XA - XGX + H = 0. \tag{2}
\]
In the paper we shall assume without loss of generality that \( B \) and \( C^\top \) are of full column rank and \( R = I_m \), for the sake of simpler notations in later development.

Analogously, for the LQ optimal control of the linear time-invariant control system in discrete-time:
\[
x_{k+1} = Ax_k + Bu_k, \quad k = 0, 1, 2, \ldots,
\]
the corresponding optimal control \( u_k = -(R + B^\top XB)^{-1}B^\top X Ax_k \) can be expressed in terms of the unique psd stabilizing solution \( X \) of the discrete-time algebraic Riccati equation (DARE) [4, 10, 29, 38]:
\[
D(X) \equiv -X + A^\top X(I + GX)^{-1}A + H = 0. \tag{3}
\]
Let \( A_0 \equiv A, G_0 \equiv G \), and \( H_0 \equiv H \). Assuming that \( I_n + G_k H_k \) are nonsingular for \( k = 0, 1, \ldots \), the SDA for DAREs has three iterative recursions:
\[
A_{k+1} = A_k(I_n + G_k H_k)^{-1} A_k, \quad G_{k+1} = G_k + A_k(I_n + G_k H_k)^{-1} G_k A_k^\top, \quad H_{k+1} = H_k + A_k^\top H_k(I_n + G_k H_k)^{-1} A_k. \tag{4}
\]

We have \( A_k \rightarrow 0 \), \( G_k \rightarrow Y \) (the solution to the dual DARE) and \( H_k \rightarrow X \), all quadratically [38] except for the critical case [24].

After the Cayley transform with nonsingular \( A_\gamma := A - \gamma I \) (\( \gamma > 0 \)) and \( K_\gamma := A_\gamma^\top + HA_\gamma^{-1}G \), the SDA for CAREs [9] shares the same formulae (4), with the alternative starting points:
\[
A_0 = I_n + 2\gamma K_\gamma^{-\top}, \quad G_0 = 2\gamma A_\gamma^{-1}G K_\gamma^{-1}, \quad H_0 = 2\gamma K_\gamma^{-1}HA_\gamma^{-1}. \tag{5}
\]

Unlikely to the doubling formulae (4) for DAREs and CAREs, the SDA has four coupled iteration recursions for the MARE:
\[
XCX - XD - AX + B = 0, \tag{6}
\]
A \in \mathbb{R}^{m \times m}, B, X \in \mathbb{R}^{m \times n}, C \in \mathbb{R}^{n \times m} and D \in \mathbb{R}^{n \times n}. With a_{ii} and d_{jj} respectively being the diagonal entries of A and D, for \( \gamma \geq \max_{i,j} \{ a_{ii}, d_{jj} \} \), let

\[ A_\gamma := A + \gamma I_n, \quad D_\gamma := D + \gamma I_n, \]
\[ W_\gamma := A_\gamma - BD_\gamma^{-1}C, \quad V_\gamma := D_\gamma - CA_\gamma^{-1}B, \]
\[ F_0 = I_m - 2\gamma W_\gamma^{-1}, \quad E_0 = I_n - 2\gamma V_\gamma^{-1}, \]
\[ H_0 = 2\gamma W_\gamma^{-1}BD_\gamma^{-1}, \quad G_0 = 2\gamma D_\gamma^{-1}CW_\gamma^{-1}. \]

Assuming that \( I_m - H_kG_k \) and \( I_n - G_kH_k \) are nonsingular for \( k = 0, 1, \ldots \), the SDA for MAREs has the form:

\[ F_{k+1} = F_k(I_m - H_kG_k)^{-1}F_k, \quad E_{k+1} = E_k(I_n - G_kH_k)^{-1}E_k, \]
\[ H_{k+1} = H_k + F_k(I_m - H_kG_k)^{-1}H_kE_k, \quad G_{k+1} = G_k + E_k(I_n - G_kH_k)^{-1}G_kF_k, \]

(7)

where \( E_k, F_k \to 0 \) and \( H_k \to X, G_k \to Y \) \((Y \) is the unique minimal nonnegative solution to the dual MARE\) as \( k \to \infty \).

MAREs have been considered widely in [16, 33, 43, 42, 20, 30, 2, 6, 5, 7, 14, 17, 18, 27, 37, 41, 15, 34], usually with \( M = \begin{bmatrix} D & -C \\ -B & A \end{bmatrix} \) being a nonsingular or an irreducible singular \( M \)-matrix for the solvability of (6). Actually, (6) has a unique minimal nonnegative solution in such conditions. Here, a matrix is nonnegative if all its entries are nonnegative and \( X \) is the minimal nonnegative solution if \( \bar{X} - X \) is nonnegative for all solutions \( \bar{X} \).

3 Decoupled form of SDA

For the classical SDA, when the initial iterates possess low-rank structures, the three coupled iterates (four for MAREs or two for BSEP\( s\) can be decoupled. This leads to the decoupled form in the dSDA shown in this section. This section contains many tedious but necessary details and the SMWF (1) will be used repeatedly.

3.1 dSDA for DAREs

3.1.1 New formulation for the first step

With the initial values \( A_0 = A, G_0 = BB^T \) and \( H_0 = C^TC \), where \( I_n + G_0H_0 \) is nonsingular, we are going to reformulate \( A_1, G_1 \) and \( H_1 \). By the SMWF (1), with \( Y_0 := B^TC, U_0 := B, V_0 := C^T, E_0 := I_m + Y_0^TY_0, F_0 := I_l + Y_0^TY_0 \) and \( K_0 := E_0^{-1}Y_0 = Y_0F_0^{-1} \), we have

\[ (I_n + G_0H_0)^{-1} = (I_n + BB^TC^TC)^{-1} = I_n - B(I_m + B^TC^TC)^{-1}B^TC^TC \]
\[ = I_n - U_0(I_m + Y_0^YT_0)^{-1}Y_0V_0^T \equiv I_n - U_0K_0V_0^T. \]

Similarly, with the symmetric \( I_m - K_0Y_0^T = E_0^{-1} \) and \( I_l - Y_0^TK_0 = F_0^{-1} \), it holds that

\[ (I_n + G_0H_0)^{-1}G_0 = (I_n - U_0E_0^{-1}Y_0V_0^TY_0^TU_0^T)U_0E_0^{-1}U_0^T \equiv U_0E_0^{-1}U_0^T, \]
\[ H_0(I_n + G_0H_0)^{-1} = V_0V_0^T(I_n - U_0E_0^{-1}Y_0V_0^TY_0^TU_0^T) \equiv V_0F_0^{-1}V_0^T. \]
With $U_1 := A_0 U_0$, $V_1 := A_1^T V_0$, $M_1^A := 0 \oplus K_0$, $M_1^G := I_m \oplus E_0^{-1}$, $M_1^H := I_t \oplus F_0^{-1}$, $\tilde{U}_1 := [U_0, U_1]$ and $\tilde{V}_1 := [V_0, V_1]$, some simple calculations produce

$$A_1 = A_0 (I_n + G_0 H_0)^{-1} A_0 = A_0 (I_n - U_0 K_0 V_0^T) A_0 = A_0^2 - \tilde{U}_1 M_1^A \tilde{V}_1^T,$$

$$G_1 = G_0 + A_0 (I_n + G_0 H_0)^{-1} G_0 A_0^T = U_0 U_0^T + A_0 (U_0 E_0^{-1} U_0^T) A_0^T \equiv \tilde{U}_1 M_1^G \tilde{V}_1^T,$$

$$H_1 = H_0 + A_0^T H_0 (I_n + G_0 H_0)^{-1} A_0^T = V_0 V_0^T + A_0^T (V_0 F_0^{-1} V_o^T) A_0^T \equiv \tilde{V}_1 M_1^H \tilde{V}_1^T.$$

Moreover, with $Y_1 := \begin{bmatrix} 0 & 0 \\ 0 & Y_0 \end{bmatrix} \in \mathbb{R}^{2m \times 2l}$, it is easy to see that

$$M_1^A = M_1^G Y_1 = Y_1 M_1^H, \quad (M_1^G)^{-1} = I_{2m} + Y_1 Y_1^T, \quad (M_1^H)^{-1} = I_{2l} + Y_1^T Y_1, \quad (8)$$

implying that

$$A_1 = A_0^2 - \tilde{U}_1 (I_{2m} + Y_1 Y_1^T)^{-1} Y_1 \tilde{V}_1^T,$$

$$G_1 = \tilde{U}_1 (I_{2m} + Y_1 Y_1^T)^{-1} \tilde{U}_1^T, \quad H_1 = \tilde{V}_1 (I_{2l} + Y_1^T Y_1)^{-1} \tilde{V}_1^T.$$

### 3.1.2 New formulation for the second step

For the 2nd iteration, with

$$T_1 := \tilde{U}_1 \tilde{V}_1, \quad K_1 := (I_{2m} + M_1^G T_1 M_1^H T_1^T)^{-1} M_1^G T_1 M_1^H,$$

and $I_n + G_1 H_1$ being nonsingular, then by the SMWF (1) we deduce that

$$(I_n + G_1 H_1)^{-1} = (I_n + \tilde{U}_1 M_1^G \tilde{V}_1 M_1^H \tilde{V}_1^T)^{-1} = I_n - \tilde{U}_1 K_1 \tilde{V}_1^T.$$

Define $E_1 := (M_1^G)^{-1} + T_1 M_1^H T_1^T$ and $F_1 := (M_1^H)^{-1} + T_1^T M_1^G T_1$, then manipulations produce

$$(I_n + G_1 H_1)^{-1} G_1 = (I_n - \tilde{U}_1 K_1 \tilde{V}_1^T) \tilde{U}_1 M_1^G \tilde{U}_1^T$$

$$= \tilde{U}_1 \left\{ M_1^G - (I_{2m} + M_1^G T_1 M_1^H T_1^T)^{-1} M_1^G T_1 M_1^H T_1^T M_1^G \right\} \tilde{U}_1^T$$

$$= \tilde{U}_1 \left\{ I_{2m} - (I_{2m} + M_1^G T_1 M_1^H T_1^T)^{-1} M_1^G T_1 M_1^H T_1^T \right\} M_1^G \tilde{U}_1^T \equiv \tilde{U}_1 E_1^{-1} \tilde{U}_1^T,$$

and

$$H_1 (I_n + G_1 H_1)^{-1} = \tilde{V}_1 M_1^H \tilde{V}_1^T \left\{ I_n - \tilde{U}_1 K_1 \tilde{V}_1^T \right\}$$

$$= \tilde{V}_1 M_1^H \left\{ I_{2l} - T_1^T \left( I_{2m} + M_1^G T_1 M_1^H T_1^T \right)^{-1} M_1^G T_1 M_1^H \right\} \tilde{V}_1^T \equiv \tilde{V}_1 F_1^{-1} \tilde{V}_1^T.$$
By denoting $U_2 := A_2^0U_0$, $U_3 := A_2^0U_0$, $V_2 := (A_2^0)^TV_0$, $V_3 := (A_2^0)^TV_0$, $\hat{U}_2 := [U_0, U_1, U_2, U_3]$ and $\hat{V}_2 := [V_0, V_1, V_2, V_3]$, we obtain

$$A_2 = A_1(I_n + G_1H_1)^{-1}A_1 = \left\{ A_2^0 - \hat{U}_1 M_1^A \hat{V}_1^T \right\} \left\{ I_n - \hat{U}_1 K_1 \hat{V}_1^T \right\} \left\{ A_2^0 - \hat{U}_1 M_1^A \hat{V}_1^T \right\}$$

$$= A_2^0 - \hat{U}_2 \left[ -M_1^A T_1^T (I_{2m} - K_1 T_1^T) M_1^A \begin{bmatrix} I_{2l} & 0 \\ -T_1^T M_1^A & I_{2l} \end{bmatrix} \right] \hat{V}_2^T$$

$$= A_2^0 - \hat{U}_2 \begin{bmatrix} I_{2m} & -M_1^A T_1^T \\ 0 & I_{2m} \end{bmatrix} \begin{bmatrix} M_1^G + M_1^A T_1^T E_1^{-1} T_1 (M_1^A)^T -M_1^A T_1^T E_1^{-1} \\ -E_1^{-1} T_1 (M_1^A)^T & E_1^{-1} \end{bmatrix} \begin{bmatrix} I_{2m} & 0 \\ -T_1 (M_1^A)^T & I_{2m} \end{bmatrix} \hat{V}_2^T := A_2^0 - \hat{U}_2 M_2^A \hat{V}_2^T,$$

$$G_2 = G_1 + A_1(I_n + G_1H_1)^{-1}A_1^T$$

$$= \hat{U}_1 M_1^G \hat{V}_1^T + \left\{ A_2^0 - \hat{U}_1 M_1^A \hat{V}_1^T \right\} \hat{U}_1 E_1^{-1} \hat{V}_1^T \left\{ (A_2^0)^T - \hat{V}_1 (M_1^A)^T \hat{V}_1^T \right\}$$

$$= \hat{U}_2 \begin{bmatrix} M_1^G + M_1^A T_1^T E_1^{-1} T_1 (M_1^A)^T -M_1^A T_1^T E_1^{-1} \\ -E_1^{-1} T_1 (M_1^A)^T & E_1^{-1} \end{bmatrix} \begin{bmatrix} I_{2m} & 0 \\ -T_1 (M_1^A)^T & I_{2m} \end{bmatrix} \hat{V}_2^T := \hat{U}_2 M_2^G \hat{V}_2^T,$$

and

$$H_2 = H_1 + A_1^T H_1 (I_n + G_1H_1)^{-1} A_1^T$$

$$= \hat{V}_1 M_1^H \hat{V}_1^T + \left\{ (A_2^0)^T - \hat{V}_1 (M_1^A)^T \hat{V}_1^T \right\} \hat{V}_1 F_1^{-1} \hat{V}_1^T \left\{ (A_2^0)^T - \hat{V}_1 (M_1^A)^T \hat{V}_1^T \right\}$$

$$= \hat{V}_2 \begin{bmatrix} M_1^H + (M_1^A)^T T_1 F_1^{-1} T_1^T M_1^A - (M_1^A)^T T_1 F_1^{-1} \\ -F_1^{-1} T_1^T M_1^A & F_1^{-1} \end{bmatrix} \begin{bmatrix} I_{2m} & 0 \\ -T_1^T M_1^A & I_{2m} \end{bmatrix} \hat{V}_2^T := \hat{V}_2 M_2^H \hat{V}_2^T.$$

By (8), and the definitions of $E_1$, $F_1$ and $K_1$, we then have

$$(M_2^G)^{-1} M_2^A = \begin{bmatrix} I_{2m} & 0 \\ T_1 (M_1^A)^T & I_{2m} \end{bmatrix} \left( (M_2^G)^{-1} \right)^{-1} \begin{bmatrix} I_{2l} & 0 \\ -T_1^T M_1^A & I_{2l} \end{bmatrix} \begin{bmatrix} I_{2m} & 0 \\ T_1 M_1^A & K_1 \end{bmatrix} \begin{bmatrix} I_{2l} & 0 \\ -T_1^T M_1^A & I_{2l} \end{bmatrix}$$

$$= \begin{bmatrix} I_{2m} & 0 \\ 0 & Y_1 \end{bmatrix} = Y_2 \in \mathbb{R}^{4m \times 4l},$$

and

$$M_2^A (M_2^H)^{-1} = \begin{bmatrix} I_{2m} & 0 \\ 0 & I_{2m} \end{bmatrix} \begin{bmatrix} M_1^A T_1^T M_1^A & M_1^A \\ M_1^A & K_1 \end{bmatrix} \left( (M_1^H)^{-1} \right)^{-1} \begin{bmatrix} I_{2l} & 0 \\ 0 & I_{2l} \end{bmatrix} = Y_2,$$
implying that $M_2^A = M_2^G Y_2 = Y_2 M_2^H$. Furthermore, it follows from (8), the definition of $E_1$ and $M_2^H + Y_1^T M_2^A = I_{2l}$ that

$$(M_2^G)^{-1} = \begin{bmatrix} I_{2m} & 0 \\ T_1 (M_1^A)^T I_{2m} & 0 \end{bmatrix} \begin{bmatrix} (M_1^G)^{-1} & 0 \\ 0 & E_1 \end{bmatrix} \begin{bmatrix} I_{2m} & M_1^A T_1^T \\ 0 & I_{2m} \end{bmatrix} = \begin{bmatrix} (M_1^G)^{-1} & Y_1 T_1^T \\ T_1 Y_1^T (M_1^G)^{-1} + T_1 (M_1^H + Y_1^T M_1^A) T_1^T & (M_1^G)^{-1} + T_1 T_1^T \end{bmatrix},$$

indicating that

$$(M_2^G)^{-1} - Y_2 Y_2^T = \begin{bmatrix} (M_1^G)^{-1} - Y_1 Y_1^T \\ 0 \end{bmatrix} (M_1^G)^{-1} - Y_1 Y_1^T \equiv I_{4m}.$$

Similarly, $(M_1^H)^{-1} - Y_2 Y_2^T = I_{4l}$. Consequently, we have the following result.

**Lemma 3.1.** For the SDA in (4), with $I_n + G_1 H_1$ being nonsingular, we have the following decoupled forms:

$$A_2 = A_0^2 - \hat{U}_2 (I_{4m} + Y_2 Y_2^T)^{-1} Y_2 \hat{V}_2^T, \quad G_2 = \hat{U}_2 (I_{4m} + Y_2 Y_2^T)^{-1} \hat{U}_2^T, \quad H_2 = \hat{V}_2 (I_{4l} + Y_2^T Y_2)^{-1} \hat{V}_2^T.$$

### 3.1.3 Decoupled recursions for DAREs

Similarly and recursively, we have the following result for $A_k, G_k$ and $H_k$.

**Theorem 3.1** (Decoupled formulae of the dSDA for DAREs). Let $U_j := A_0 U_{j-1}$ ($U_0 = B$) and $V_j := A_0^2 V_{j-1}$ ($V_0 = C^T$) for $j \geq 1$. Assume that $I_n + G_k H_k$ are nonsingular for $k \geq 0$. For all $k \geq 2$, the SDA (4) produces

$$A_k = A_0^{2k} - \hat{U}_k (I_{2^k m} + Y_k Y_k^T)^{-1} Y_k \hat{V}_k^T,$$

$$G_k = \hat{U}_k (I_{2^k m} + Y_k Y_k^T)^{-1} \hat{U}_k^T, \quad H_k = \hat{V}_k (I_{2^k l} + Y_k^T Y_k)^{-1} \hat{V}_k^T,$$

where $Y_k := \begin{bmatrix} 0 \\ Y_{k-1} \end{bmatrix} \in \mathbb{R}^{2^k m \times 2^k l}$, $\hat{U}_k := [U_0, U_1, \cdots, U_{2^k-1}]$, $\hat{V}_k := [V_0, V_1, \cdots, V_{2^k-1}]$ and $T_{k-1} := \begin{bmatrix} \hat{U}_k^T \\ \hat{V}_k \\ \vdots \\ \hat{V}_{k-1}^T \end{bmatrix}$ with $Y_1 = \begin{bmatrix} 0 \\ 0 \\ B^T C^T \end{bmatrix} \in \mathbb{R}^{2^m \times 2^l}$.

**Proof.** We will prove the result by induction. By Lemma 3.1 the result is valid for $k = 2$. Now assume that the result holds for $j > 2$, then by the SMWF (1) we have

$$(I_n + G_j H_j)^{-1} = I_n - \hat{U}_j K^{-1} T_j \hat{N} \hat{V}_{j-1}^T,$$

$$(I_n + G_j H_j)^{-1} G_j = \hat{U}_j K^{-1} \hat{U}_{j-1}^T, \quad H_j (I_n + G_j H_j)^{-1} = \hat{V}_j L^{-1} \hat{V}_{j-1}^T,$$

where $M = (I_{2^j m} + Y_j Y_j^T)^{-1}$, $N = (I_{2^j l} + Y_j^T Y_j)^{-1}$, $K = I_{2^j m} + Y_j Y_j^T + T_j \hat{N} T_j^T$, $L = I_{2^j l} + Y_j^T Y_j + T_j^T M T_j$. Define $Z_1 := (I_{2^j m} + Y_j Y_j^T)^{-1} Y_j T_j^T$ and $Z_2 := (I_{2^j l} + Y_j^T Y_j)^{-1} Y_j^T T_j^T$. 


then by (4) it holds that
\[ A_{j+1} = A_0^{j+1} - \tilde{U}_{j+1} \begin{bmatrix} I_{2m} & -Z_1 & Z_1MY_j & MY_j \\ 0 & 0 & K^{-1}T_jN & -Z_2^T \\ I_{2m} & 0 & -K^{-1}Z_1^T & K^{-1} \\ I_{2m} & I_{2m} & I_{2m} & I_{2m} \end{bmatrix} \tilde{V}_{j+1}^T, \]
\[ G_{j+1} = \tilde{U}_{j+1} \begin{bmatrix} M + Z_1K^{-1}Z_1^T & -Z_1K^{-1} \\ -K^{-1}Z_1^T & K^{-1} \end{bmatrix} \tilde{V}_{j+1}^T \]
\[ = \tilde{U}_{j+1} \begin{bmatrix} I_{2m} & -Z_1 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} M & 0 \\ 0 & K \end{bmatrix} \begin{bmatrix} I_{2m} & 0 \\ -Z_1^T & I_{2m} \end{bmatrix} \tilde{U}_{j+1}^T, \]
and
\[ H_{j+1} = \tilde{V}_{j+1} \begin{bmatrix} N + Z_2L^{-1}Z_2^T & -Z_2L^{-1} \\ -L^{-1}Z_2^T & L^{-1} \end{bmatrix} \tilde{V}_{j+1}^T, \]
\[ = \tilde{V}_{j+1} \begin{bmatrix} I_{2l} & -Z_2 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} N & 0 \\ 0 & L^{-1} \end{bmatrix} \begin{bmatrix} I_{2l} & 0 \\ -Z_2^T & I_{2l} \end{bmatrix} \tilde{V}_{j+1}^T. \]

Define \( Y_{j+1} := \begin{bmatrix} 0 & Y_j \\ Y_j & T_j \end{bmatrix} \in \mathbb{R}^{2^{j+1}m \times 2^{j+1}l} \), then we have
\[ \begin{bmatrix} I_{2m} & 0 \\ Z_1^T & I_{2m} \end{bmatrix} \begin{bmatrix} I_{2m} & Y_j^T \\ 0 & 0 \end{bmatrix} \begin{bmatrix} I_{2m} & Z_1 \\ 0 & I_{2m} \end{bmatrix} = I_{2^{j+1}m} + Y_{j+1}Y_{j+1}^T, \]
leading to \( G_{j+1} = \tilde{U}_{j+1} (I_{2^{j+1}m} + Y_{j+1}Y_{j+1}^T)^{-1} \tilde{U}_{j+1}^T \). Similarly, we can verify analogous formulae for \( A_{j+1} \) and \( H_{j+1} \). The proof by induction is complete. \( \Box \)

**Remark 3.1.** Theorem 3.1 decouples the original SDA (4), implying that only the iteration for \( H_k \) is required for the solution of the DARE (3). This eliminates the difficulty in [31], in which the implicit recursion in \( A_k \) increases the flop counts exponentially. The decoupled formulae are simple and elegant, with the updating recursion for \( Y_k \) nontrivial. The resulting \( dSDA \) is obviously equivalent to a projection method, with the corresponding Krylov subspace \( K_{2^{k-1}}(A^T, C^T) \equiv [C^T, A^TC^T, \ldots, (A^T)^{2^{k-1}}C^T] \) and the coefficient matrix \( (I + Y_k^TY_k)^{-1} \) being the solution of the corresponding projected equation. Note that the SDA (and the equivalent \( dSDA \)) has been proved to converge [32], assuming that \( I_n + G_kH_k \) are nonsingular for \( k \geq 0 \). In contrast, the projected equations in Krylov subspace methods are routinely assumed to be solvable [22, 25, 26, 39, 40]. However, with round-off errors, the Krylov subspaces may lose linear independence, requiring a remedy in a truncation process. Also, near convergence, new additions to the Krylov subspaces play lesser parts in the approximate solution, implying that the coefficient matrix \( (I + Y_k^TY_k)^{-1} \) has relatively smaller components in the lower right corner. Without truncation, the ill-conditioned coefficient matrix, as an inverse, will be difficult to compute as \( k \) increases. Limited by the article space, many practical compute issues will be treated in another paper, where we shall develop a novel truncation technique.

**Remark 3.2.** For the complex DARE:
\[ -X + A^H(X(I + GX)^{-1}A + H = 0, \]
the above decoupled form of the SDA proves valid, with the \( (\cdot)^T \) replaced by \( (\cdot)^H \). Such comment applies for the results in the subsequent sections.
3.2 dSDA for CAREs

Note that in (5), the starting points for CAREs are different from those for DAREs, and to get $A_0, G_0, H_0$ we need to compute $K_\gamma$ at first. For CAREs, alternatively with $U_0 := A_{\gamma}^{-1}B$, $V_0 := A_{\gamma}^{-\top}C^\top$ and $Y_0 := B^\top V_0$, then by the SMWF (1) we get

$$K_\gamma^{-1} = A_{\gamma}^{-\top} - V_0 (I + Y_0^T Y_0)^{-1} Y_0^T U_0^\top,$$

leading to

$$A_0 = (I_n + 2\gamma A_{\gamma}^{-1}) - 2\gamma U_0 Y_0 F_0^{-1} V_0^\top, \quad G_0 = 2\gamma U_0 E_0^{-1} U_0^\top, \quad H_0 = 2\gamma V_0 F_0^{-1} V_0^\top,$$

where $E_0 := I_m + Y_0 Y_0^\top, F_0 := I_t + Y_0^T Y_0$ satisfy $Y_0 F_0^{-1} = E_0^{-1} Y_0$ and $Y_0^T E_0^{-1} = F_0^{-1} Y_0^T$.

Defining $T_0 := U_0^T V_0, K := (E_0 + 4\gamma^2 T_0 F_0^{-1} T_0^\top)^{-1}$ and $L := (F_0 + 4\gamma^2 T_0^T E_0^{-1} T_0)^{-1}$, the SMWF (1) again implies

$$(I_n + G_0 H_0)^{-1} = (I_n + 4\gamma^2 U_0 E_0^{-1} T_0 F_0^{-1} V_0^\top)^{-1} = I_n - 4\gamma^2 U_0 K T_0 F_0^{-1} V_0^\top,$$

$$(I_n + G_0 H_0)^{-1} G_0 = 2\gamma (I_n + 4\gamma^2 U_0 E_0^{-1} T_0 F_0^{-1} V_0^\top)^{-1} U_0 E_0^{-1} U_0^\top = 2\gamma U_0 K U_0^\top,$$

$$(I_n + G_0 H_0)^{-1} H_0 = 2\gamma V_0 F_0^{-1} V_0^\top (I_n + 4\gamma^2 U_0 E_0^{-1} T_0 F_0^{-1} V_0^\top)^{-1} = 2\gamma V_0 L V_0^\top.$$

Denote $\tilde{A}_\gamma := (I_n + 2\gamma A_{\gamma}^{-1}), U_1 := \tilde{A}_\gamma U_0, V_1 := \tilde{A}_\gamma^\top V_0$ and $Y_1 := \begin{bmatrix} 0 & Y_0 \\ Y_0 & 2\gamma T_0 \end{bmatrix} \in \mathbb{R}^{2m \times 2l}$, with similar notations $\tilde{U}_1$ and $\tilde{V}_1$ as in the previous section (here $U_1 := \tilde{A}_\gamma U_0$ and $V_1 := \tilde{A}_\gamma^\top V_0$) and the help of (4), (9) and (10), some manipulations yield

$$G_1 = 2\gamma \tilde{U}_1 \begin{bmatrix} E_0^{-1} + 4\gamma^2 Y_0 F_0^{-1} T_0 K T_0 F_0^{-1} Y_0^\top & -2\gamma Y_0 F_0^{-1} T_0^\top K \\ -2\gamma K T_0 F_0^{-1} Y_0^\top & K \end{bmatrix} \tilde{U}_1^\top$$

$$= 2\gamma \tilde{U}_1 \begin{bmatrix} E_0 & 2\gamma Y_0 T_0^\top \\ 2\gamma T_0 Y_0^\top & E_0 + 4\gamma^2 T_0^T T_0 \end{bmatrix}^{-1} \tilde{U}_1^\top \equiv 2\gamma \tilde{U}_1 (I_{2m} + Y_1 Y_1^\top)^{-1} \tilde{U}_1^\top,$$

$$H_1 = 2\gamma \tilde{V}_1 \begin{bmatrix} F_0^{-1} + 4\gamma^2 F_0^{-1} Y_0^T T_0 L T_0^\top Y_0 F_0^{-1} & -2\gamma F_0^{-1} Y_0^T T_0 L \\ -2\gamma L T_0^\top Y_0 F_0^{-1} & L \end{bmatrix} \tilde{V}_1^\top$$

$$= 2\gamma \tilde{V}_1 \begin{bmatrix} F_0 & 2\gamma Y_0^T T_0 \\ 2\gamma T_0^\top Y_0 & F_0 + 4\gamma^2 T_0^T T_0 \end{bmatrix}^{-1} \tilde{V}_1^\top \equiv 2\gamma \tilde{V}_1 (I_{2l} + Y_1 Y_1^\top)^{-1} \tilde{V}_1^\top,$$

$$A_1 = \tilde{A}_\gamma^2 - 2\gamma \tilde{U}_1 \begin{bmatrix} -2\gamma Y_0 F_0^{-1} T_0^\top K Y_0 & Y_0 L \\ K Y_0 & 2\gamma K T_0 F_0^{-1} \end{bmatrix} \tilde{V}_1^\top$$

$$= \tilde{A}_\gamma^2 - 2\gamma \tilde{U}_1 Y_1 \begin{bmatrix} F_0^{-1} + 4\gamma^2 F_0^{-1} Y_0^T T_0 L T_0^\top Y_0 F_0^{-1} & -2\gamma F_0^{-1} Y_0^T T_0 L \\ -2\gamma L T_0^\top Y_0 F_0^{-1} & L \end{bmatrix} \tilde{V}_1^\top$$

$$= \tilde{A}_\gamma^2 - 2\gamma \tilde{U}_1 Y_1 (I_{2l} + Y_1 Y_1^\top)^{-1} \tilde{V}_1^\top \equiv \tilde{A}_\gamma^2 - 2\gamma \tilde{U}_1 (I_{2m} + Y_1 Y_1^\top)^{-1} Y_1 \tilde{V}_1^\top.$$

Obviously, $A_1, G_1$ and $H_1$ are decoupled. Rewriting the symbols in the recursions, we subsequently get the following decoupled result for the SDA.
Z.-C. Guo, E.K.-W. Chu, X. Liang and W.-W. Lin

\textbf{Theorem 3.2} (Decoupled formulae of the dSDA for CAREs). Denote \( U_j := \tilde{A}_j U_{j-1} \) and \( V_j := \tilde{A}_j^T V_{j-1} \) for \( j \geq 1 \). Assume that \( I_n + G_k H_k \) are nonsingular for \( k \geq 0 \). For all \( k \geq 1 \), the SDA produces

\[
A_k = \tilde{A}_k^2 - 2\gamma \tilde{U}_k \left( I_{2^k m} + Y_k Y_k^T \right)^{-1} Y_k \tilde{V}_k^T,
\]
\[
G_k = 2\gamma \tilde{U}_k \left( I_{2^k m} + Y_k Y_k^T \right)^{-1} \tilde{U}_k^T,
\]
\[
H_k = 2\gamma \tilde{V}_k \left( I_{2^k l} + Y_k^T Y_k \right)^{-1} \tilde{V}_k^T,
\]

(12)

where \( Y_k = \begin{bmatrix} 0 & Y_{k-1} \\ Y_{k-1} & 2\gamma T_{k-1} \end{bmatrix} \in \mathbb{R}^{2^k m \times 2^k l} \), \( \tilde{U}_k := [U_0, U_1, \ldots, U_{2^k-1}] \), \( \tilde{V}_k := [V_0, V_1, \ldots, V_{2^k-1}] \) and \( T_k := \tilde{U}_k^T \tilde{V}_k \), with \( U_0 = A_\gamma^{-1} B \), \( V_0 = A_\gamma^{-T} C^T \), \( Y_0 = B^T A_\gamma^{-T} C^T \) and \( T_0 = U_0^T V_0 \).

As the dSDA for DAREs, the three formulae in the iteration are all decoupled. To solve CAREs while monitoring \( \|H_k - H_{k-1}\| \) or the normalized residual for convergence control, there is no need to compute \( A_k \) or \( G_k \). Comments analogous to those in Remarks 3.1 and 3.2 for the dSDA for DAREs also hold for the dSDA for CAREs in Theorem 3.2, with \( \tilde{A}_\gamma \) in place of \( A \).

Theoretically, we can employ the decoupled formulae (12) to compute \( H_k \) which approximates the solution \( X \) for the CAREs. However, without truncation the size of \( Y_k \) will grow exponentially and the lower right corner of the kernel \( (I + Y_k Y_k^T)^{-1} \) will diminish fast. Hence, how to incorporate truncation in the dSDA is a crucial issue. We shall solve the associated problems in a companion paper, in which a practical dSDA with truncation strategy will be presented and analyzed. For a taste of what is to come, the truncation strategy is summarized in the follow diagram.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{truncation_diagram.png}
\caption{Truncation in dSDA}
\end{figure}

On the first row, we have \( H_k \) from the dSDA without truncation. After \( H_1 \) is computed, it may be truncated to \( H_1^{(1)} \) and then it may generate \( H_k^{(1)} \) by the dSDA without truncation. In
general, $H_j^{(k)}$ generates $H_j^{(k)}$ ($j > k$) by the dSDA without truncation, and $H_j^{(k)}$ is truncated to $H_j^{(k+1)}$. Notice that $H_j^{(k)}$ ($j > k$) on any row enjoy the support of the rich existing theory of the dSDA (also SDA). In the companion paper, we shall analyzed the dSDA with truncation extending the results of the dSDA (and SDA). We shall also produce the formula for the short-cut from $H_j^{(k)}$ to $H_j^{(k+1)}$, without going through $H_j^{(k+1)}$.

3.3 Bethe-Salpeter eigenvalue problem

In [21], the SDA is extended to solve the (discretized) BSEP, a Hamiltonian-like eigenvalues problem, where only two iterative formulae are computed instead of three in CAREs. The question is whether the proposed dSDA can be generalized to the BSEP. We give the results in this section.

Consider the following discretized BSEP:

$$Hx = \lambda x,$$

for $x \neq 0$, where $A, B \in \mathbb{C}^{n \times n}$ satisfy $A^H = A$, $B^T = B$. For problem (13) any eigenvalue $\lambda$ appears in quadruplets $\{\pm \lambda, \pm \overline{\lambda}\}$ (except for the degenerate cases when $\lambda$ is purely real or imaginary) and thus shows Hamiltonian-like structure. When applying the SDA to the BSEP (13), by assuming that $I_n - T_kF_k$ are nonsingular for $k \geq 0$ it generates the following iterations:

$$E_{k+1} = E_k(I_n - T_kF_k)^{-1}E_k, \quad F_{k+1} = F_k + T_kF_k(I_n - T_kF_k)^{-1}E_k,$$

where $E_0 = I_n - 2\alpha \overline{R}^{-1}(\alpha I_n - A)^{-1}$ and $F_0 = -2\alpha(\alpha I_n - A)^{-1}\overline{BR}^{-1}(\alpha I_n - A)^{-1}$, with $R = I_n - (\alpha I_n - A)^{-1}\overline{B}(\alpha I_n - A)^{-1}B$.

When initially $B = L_B L_B^T$ with $L_B \in \mathbb{C}^{n \times p}$ and $p \leq n$, by defining $V_0 := (\alpha I_n - A)^{-1}L_B$, $Y_0 := L_B^T(\alpha I_n - A)^{-1}B > 0$ and $A_0 := I_n - 2\alpha(\alpha I_n - A)^{-1}$, we have

$$R^{-1} = I_n + \overline{V}_0(I_p - Y_0 Y_0^T)^{-1}Y_0 L_B^H,$$

$$E_0 = A_0 - 2\alpha \overline{V}_0(I_p - Y_0 Y_0^T)^{-1}Y_0 V_0^T, \quad F_0 = -2\alpha V_0(I_p - Y_0 Y_0^T)^{-1}V_0^T.$$

Denote $T_0 := V_0^H V_0$ and since $Y_0$ is Hermitian, we get

$$(I - T_0 F_0)^{-1} = I + 4\alpha^2 \overline{V}_0 \{I_p - 4\alpha^2(I_p - Y_0 Y_0^T)^{-1}T_0(I_p - Y_0 Y_0^T)^{-1}T_0\}^{-1}\cdot(I_p - Y_0 Y_0^T)^{-1}T_0(I_p - Y_0 Y_0^T)^{-1}T_0^T,$$

$$F_0(I - T_0 F_0)^{-1} = -2\alpha V_0 \{I_p - Y_0 Y_0^T - 4\alpha^2 T_0(I_p - Y_0 Y_0^T)^{-1}T_0\}^{-1}V_0^T.$$

Furthermore, by defining $V_1 := \overline{V}_0 V_0$, $\overline{V}_1 := [V_0, V_1]$ and $Y_1 = \begin{bmatrix} 0 & Y_0 \\ Y_0 & -2\alpha T_0 \end{bmatrix}$, some manipulations similar to those in (11) yield

$$E_1 = A_0^2 - 2\alpha \overline{V}_1(I_{2p} - Y_1 Y_1^T)^{-1}Y_1 V_1^T, \quad F_1 = -2\alpha \overline{V}_1(I_{2p} - Y_1^T Y_1)^{-1}V_1^T.$$

From the above discussions, we know that the initial $E_0, F_0$ and the first iterates $E_1, F_1$ possess similar structures as those in the dSDA for CAREs. Thus with the similar manipulations, where the SMWF (1) is applied, we eventually deduce the dSDA for the BSEP, as stated in the following theorem without proof.
Theorem 3.3 (Decoupled formulae of the dSDA for the BSEP). Let \( V_j = \overline{A}_n V_{j-1} \) for \( j \geq 1 \). Assume that \( I_n - \overline{T}_k F_k \) are nonsingular for \( k \geq 0 \). Then for all \( k \geq 1 \) the SDA produces

\[
E_k = A\alpha - 2\alpha [V_0, V_1, \cdots, V_{2k-1}] (I - Y_k Y_k^T)^{-1} Y_k [V_0, V_1, \cdots, V_{2k-1}]^T,
\]

\[
F_k = -2\alpha [V_0, V_1, \cdots, V_{2k-1}] (I - Y_k Y_k^T)^{-1} [V_0, V_1, \cdots, V_{2k-1}]^T,
\]

where \( Y_k = \begin{bmatrix} 0 & Y_{k-1} \\ Y_{k-1} & -2\alpha T_{k-1} \end{bmatrix} \) with \( T_{k-1} = [V_0, V_1, \cdots, V_{2k-1}]^T [V_0, V_1, \cdots, V_{2k-1}] \).

Remark 3.3. Assume that there is no purely imaginary nor zero eigenvalues for \( H \) and let \( HX = X\Lambda \) with \( X \in \mathbb{C}^{2n \times n} \) and all eigenvalues of \( \Lambda \in \mathbb{C}^{n \times n} \) in the interior of the left-half plane. Write \( X = [X_1^T, X_2^T] \) with \( X_1 \in \mathbb{C}^{n \times n} \) and choose \( \alpha > 0 \), then it holds that \( \lim_{k \to \infty} E_k = 0 \) and \( \lim_{k \to \infty} F_k = -X_2 X_1^{-1} \). With some simple but tedious computations, we can further show that \( \lim_{k \to \infty} \sin \Theta(X_2 X_1^{-1}, F_k) = 0 \), where \( P \) is the projection matrix of \( [I, (X_2 X_1^{-1})^T] \) and

\[
\Theta(W, Z) = \arccos \left[ (I + ZZ^T)^{-1/2} (I - ZW) (I + WW^T)^{-1} (I - WW^T)^{-1} \right]^{-1/2}.
\]

Obviously, once obtaining \( F_k \) we can approximate all eigenvalues of \( \Lambda \) by those of

\[
H_k = [I, -F_k^H] H [I, -F_k^T]^T (I + F_k^H F_k)^{-1}.
\]

In [3] it was claimed, in quantum chemistry and modern material science, that the matrix \( B \) is of low-rank in some large-scale discretized BSEPs. Then by Theorem 3.3, \( F_k \) is of low-rank thus providing further possibilities for the solution of large-scale BSEPs.

3.4 dSDA for MAREs

Assume that \( B \) and \( C \) are of low rank and possess the full rank factorizations \( B = B_l B_r^T \) and \( C = C_l C_r^T \), where \( B_l \in \mathbb{R}^{m \times m}, B_r \in \mathbb{R}^{n \times m}, C_l \in \mathbb{R}^{n \times n}, C_r \in \mathbb{R}^{m \times n} \). Denote

\[
Y_0 := B_l^T D_\gamma^{-1} C_l, \quad Z_0 := C_r^T A_\gamma^{-1} B_l,
\]

\[
U_0 := A_\gamma^{-1} B_l, \quad V_0 := A_\gamma^{-1} C_r, \quad W_0 := D_\gamma^{-1} C_l, \quad Q_0 := D_\gamma^{-1} B_r,
\]

\[
T_0 := Q_0^T W_0 = B_l^T D_\gamma^{-2} C_l, \quad S_0 := V_0^T U_0 = C_r^T A_\gamma^{-2} B_l,
\]

\[
\tilde{A}_\gamma := I_m - 2\gamma A_\gamma^{-1}, \quad \tilde{D}_\gamma := I_n - 2\gamma D_\gamma^{-1},
\]

\[
M_0 := (I_m - Y_0 Z_0)^{-1}, \quad N_0 := (I_n - Z_0 Y_0)^{-1}.
\]

Note that \( M_0 Y_0 = Y_0 N_0 \) and \( N_0 Z_0 = Z_0 M_0 \). In terms of the matrices in (14), we apply the SMWF (1) and obtain

\[
W_\gamma^{-1} = A_\gamma^{-1} + U_0 M_0 Y_0 V_0^T, \quad W_\gamma^{-1} = D_\gamma^{-1} + W_0 N_0 Z_0 Q_0^T,
\]

\[
F_0 = \tilde{A}_\gamma - 2\gamma U_0 M_0 Y_0 V_0^T, \quad F_0 = \tilde{D}_\gamma - 2\gamma W_0 N_0 Z_0 Q_0^T,
\]

\[
H_0 = 2\gamma U_0 M_0 Q_0^T, \quad H_0 = 2\gamma W_0 N_0 V_0^T.
\]
Furthermore, let

\[ K := M_0^{-1} - 4\gamma^2T_0N_0S_0 \quad \text{and} \quad L := N_0^{-1} - 4\gamma^2S_0M_0T_0, \]

which satisfy

\[ S_0M_0K = LN_0S_0, \quad T_0N_0L = KM_0T_0, \quad (15) \]

routine manipulations produce

\[
(I_m - H_0G_0)^{-1} = I_m + 4\gamma^2U_0K^{-1}T_0N_0V_0^T, \quad (I_n - G_0H_0)^{-1} = I_n + 4\gamma^2W_0L^{-1}S_0M_0Q_0^T,
\]

\[
(I_m - H_0G_0)^{-1}H_0 = 2\gammaU_0K^{-1}Q_0^T, \quad (I_n - G_0H_0)^{-1}G_0 = 2\gammaW_0L^{-1}V_0^T,
\]

where the invertibility of \( K \) and \( L \) comes from that of \( I_m - H_0G_0 \) and \( I_n - G_0H_0 \). In fact, \( K \) and \( L \) are nonsingular if and only if \( I_m - H_0G_0 \) and \( I_n - G_0H_0 \) are nonsingular, respectively.

Since (15) indicates \( N_0S_0K^{-1} = L^{-1}S_0M_0 \) and \( K^{-1}T_0N_0 = M_0T_0L^{-1} \), then with

\[
U_1 := \tilde{A}_sU_0, \quad V_1 := \tilde{A}_y^Tv_0, \quad W_1 := \tilde{D}_sW_0, \quad Q_1 := \tilde{D}_y^TQ_0,
\]

\[
\hat{U}_1 := [U_0, U_1], \quad \hat{V}_1 := [V_0, V_1], \quad \hat{W}_1 := [W_0, W_1], \quad \hat{Q}_1 := [Q_0, Q_1],
\]

\[
Y_1 := \begin{bmatrix} 0 & Y_0 \\ Y_0 & -2\gammaT_0 \end{bmatrix}, \quad Z_1 := \begin{bmatrix} 0 & Z_0 \\ Z_0 & -2\gammaS_0 \end{bmatrix},
\]

the SDA (7) leads to

\[
F_1 = \tilde{A}_y^2 - 2\gamma\hat{U}_1 \begin{bmatrix} -2\gammaY_0N_0S_0K^{-1}Y_0 & Y_0L^{-1} \\ K^{-1}Y_0 & -2\gammaK^{-1}T_0N_0 \end{bmatrix} \hat{V}_1^T
\]

\[
= \tilde{A}_y^2 - 2\gamma\hat{U}_1Y_1 \begin{bmatrix} N_0 + 4\gamma^2N_0Z_0T_0L^{-1}S_0Y_0N_0 & -2\gammaN_0Z_0T_0L^{-1} \\ -2\gammaL^{-1}S_0Y_0N_0 & L^{-1} \end{bmatrix} \hat{V}_1^T
\]

\[
= \tilde{A}_y^2 - 2\gamma\hat{U}_1Y_1 (I_{2n_1} - Z_1Y_1)^{-1} \hat{V}_1^T \equiv \tilde{A}_y^2 - 2\gamma\hat{U}_1 (I_{2n_1} - Y_1Z_1)^{-1} Y_1 \hat{V}_1^T. \quad (16)
\]

Similarly, we have

\[
E_1 = \tilde{D}_y^2 - 2\gamma\hat{W}_1 \begin{bmatrix} -2\gammaZ_0M_0T_0L^{-1}Z_0 & Z_0K^{-1} \\ L^{-1}Z_0 & -2\gammaL^{-1}S_0M_0 \end{bmatrix} \hat{Q}_1^T
\]

\[
= \tilde{D}_y^2 - 2\gamma\hat{W}_1Z_1 \begin{bmatrix} M_0 + 4\gamma^2M_0Y_0S_0K^{-1}T_0Z_0M_0 & -2\gammaM_0Y_0S_0K^{-1} \\ -2\gammaK^{-1}T_0Z_0M_0 & K^{-1} \end{bmatrix} \hat{Q}_1^T
\]

\[
= \tilde{D}_y^2 - 2\gamma\hat{W}_1Z_1 (I_{2m_1} - Y_1Z_1)^{-1} \hat{Q}_1^T \equiv \tilde{D}_y^2 - 2\gamma\hat{W}_1 (I_{2m_1} - Y_1Z_1)^{-1} Z_1 \hat{Q}_1^T, \quad (17)
\]

\[
H_1 = 2\gamma\hat{U}_1 \begin{bmatrix} M_0 + 4\gamma^2M_0Y_0S_0K^{-1}T_0N_0Z_0 & -2\gammaM_0Y_0S_0K^{-1} \\ -2\gammaK^{-1}T_0N_0Z_0 & K^{-1} \end{bmatrix} \hat{Q}_1^T
\]

\[
= 2\gamma\hat{U}_1 (I_{2m_1} - Y_1Z_1)^{-1} \hat{Q}_1^T, \quad (18)
\]

\[
G_1 = 2\gamma\hat{W}_1 \begin{bmatrix} N_0 + 4\gamma^2N_0Z_0T_0L^{-1}S_0Y_0N_0 & -2\gammaN_0Z_0T_0L^{-1} \\ -2\gammaL^{-1}S_0Y_0N_0 & L^{-1} \end{bmatrix} \hat{V}_1^T
\]

\[
= 2\gamma\hat{W}_1 (I_{2m_1} - Y_1Z_1)^{-1} \hat{V}_1^T. \quad (19)
\]

**Remark 3.4.** Checking \((I_{2n_1} - Z_1Y_1)^{-1}\) and \((I_{2m_1} - Y_1Z_1)^{-1}\) respectively have the forms in (16) and (17) is easy but finding the formulae as well as the recursions for \(Y_j\) and \(Z_j\) in the first place is nontrivial!
By pursuing a similar process we subsequently obtain the following theorem.

**Theorem 3.4** (Decoupled formulae for the dSDA for MAREs). Define $U_0 := A^{-1}_γ B_l$, $V_0 := A^{-T}_γ C_r$, $W_0 := D^{-1}_γ C_l$, $Q_0 := D^{-T}_γ B_r$, $Y_0 := B^T_l D^{-1}_γ C_l$, $Z_0 := C^T_l A^{-1}_γ B_l$, $T_0 := Q^T_0 W_0$ and $S_0 := V^T_0 U_0$. For $j \geq 1$, denote $U_j := \bar{A}_j U_{j-1}$, $V_j := \bar{A}_T^j V_{j-1}$, $W_j := \bar{D}_j W_{j-1}$, $Q_j := \bar{D}_T^j Q_{j-1}$, $\bar{U}_j := [U_0, \ldots, U_{2^j-1}]$, $\bar{V}_j := [V_0, \ldots, V_{2^j-1}]$, $\bar{W}_j := [W_0, \ldots, W_{2^j-1}]$, $\bar{Q}_j := [Q_0, \ldots, Q_{2^j-1}]$, $T_j := \bar{Q}^T_j \bar{W}_j$, $S_j := \bar{V}^T_j \bar{U}_j$, $Y_j := \begin{bmatrix} 0 & 0 \\ \bar{Y}_{j-1} & -2\gamma \bar{T}_{j-1} \end{bmatrix}$, $Z_j := \begin{bmatrix} 0 & Z_{j-1} \\ Z_{j-1} & -2\gamma S_{j-1} \end{bmatrix}$.

Assume that $I_m - H_k G_k$ and $I_n - G_k H_k$ are nonsingular for $k \geq 0$. For all $k \geq 1$ it holds that

\[
F_k = \bar{A}^{2^k}_\gamma - 2\gamma \bar{U}_k (I_{2^k m_1} - Y_k Z_k)^{-1} Y_k \bar{V}^T_k, \quad E_k = \bar{D}^{2^k}_\gamma - 2\gamma \bar{W}_k (I_{2^k n_1} - Z_k Y_k)^{-1} Z_k \bar{Q}^T_k, \\
H_k = 2\gamma \bar{U}_k (I_{2^k m_1} - Y_k Z_k)^{-1} \bar{Q}^T_k, \quad G_k = 2\gamma \bar{W}_k (I_{2^k n_1} - Z_k Y_k)^{-1} \bar{V}^T_k.
\]

Again the four formulae in the SDA (7) are decoupled. There is no reason why we need to calculate $F_k$, $E_k$ or $G_k$, if we only want to solve MAREs and control convergence using $H_k - H_{k-1}$ or the normalized residual.

**Remark 3.5.** For the alternating-directional doubling algorithm (ADDA for abbreviation) proposed in [41], which is a variation of the SDA, the initial items contain two parameters as follows:

\[
A_\beta := A + \beta I_m, \quad D_\alpha := D + \alpha I_n, \\
W_{\alpha, \beta} := A_\beta - BD^{-1}_\alpha C, \quad V_{\alpha, \beta} := D_\alpha - C A^{-1}_\beta B, \\
F_0 = I_m - (\beta + \alpha) W^{-1}_{\alpha, \beta}, \quad E_0 = I_n - (\alpha + \beta) V^{-1}_{\alpha, \beta}, \\
H_0 = (\beta + \alpha) W^{-1}_{\alpha, \beta} BD^{-1}_\alpha, \quad G_0 = (\alpha + \beta) D^{-1}_\alpha CW^{-1}_{\alpha, \beta},
\]

where $\alpha \geq \max_a a_{ii}$, $\beta \geq \max_j d_{jj}$ with $a_{ii}$ and $d_{jj}$ respectively being the diagonal entries of $A$ and $D$. Similar to (14) we define

\[
Y_0 := B^T_l D^{-1}_\alpha C_l, \quad Z_0 := C^T_l A^{-1}_\beta B_l, \\
U_0 := A^{-1}_\beta B_l, \quad V_0 := A^{-T}_\beta C_r, \quad W_0 := D^{-1}_\alpha C_l, \quad Q_0 := D^{-T}_\alpha B_r, \\
\bar{A}_\beta := I_m - (\alpha + \beta) A^{-1}_\beta, \quad \bar{D}_\alpha := I_n - (\alpha + \beta) D^{-1}_\alpha,
\]

then applying the SMWF (1) yields

\[
F_0 = \bar{A}_\beta - (\alpha + \beta) U_0 (I_{m_1} - Y_0 Z_0)^{-1} Y_0 V_0^T, \quad E_0 = \bar{D}_\alpha - (\alpha + \beta) W_0 (I_{n_1} - Z_0 Y_0)^{-1} Z_0 Q_0^T, \\
H_0 = (\alpha + \beta) U_0 (I_{m_1} - Y_0 Z_0)^{-1} Q_0^T, \quad G_0 = (\alpha + \beta) W_0 (I_{n_1} - Z_0 Y_0)^{-1} V_0^T.
\]

Let $U_1 := \bar{A}_\beta U_0$, $V_1 := \bar{A}_T^\beta V_0$, $W_1 := \bar{D}_\alpha W_0$, $Q_1 := \bar{D}_T^\alpha Q_0$, $Y_1 := \begin{bmatrix} 0 & Y_0 \\ Y_0 & -T_0 \end{bmatrix}$, $Z_1 := \begin{bmatrix} 0 & Z_0 \\ Z_0 & -T_0 \end{bmatrix}$.
where $T_0 := Q_0^T W_0$ and $S_0 := V_0^T U_0$, and use similar notations $\hat{U}_1$, $\hat{V}_1$, $\hat{W}_1$ and $\hat{Q}_1$ as in Theorem 3.4, then by the manipulations analogy to (16), (17),(18) and (19), we get

$$ F_1 = \mathcal{A}_\beta^2 \alpha (\alpha + \beta) \hat{U}_1 (I_{2m_1} - Y_1 Z_1)^{-1} Y_1 \hat{V}_1^T, \quad E_1 = \mathcal{D}_\alpha^2 \beta (\alpha + \beta) \hat{W}_1 (I_{2n_1} - Z_1 Y_1)^{-1} Z_1 \hat{Q}_1^T, $$

$$ H_1 = (\alpha + \beta) \hat{U}_1 (I_{2m_1} - Y_1 Z_1)^{-1} \hat{Q}_1^T, \quad G_1 = (\alpha + \beta) \hat{W}_1 (I_{2n_1} - Z_1 Y_1)^{-1} \hat{V}_1^T. $$

Clearly, with low-rank structure $F_1$, $E_1$, $H_1$ and $G_1$ in the ADDA is decoupled. Furthermore, by performing many similar operations we will obtain the same results as those in Theorem 3.4, implying that the ADDA can be decoupled.

**Theorem 3.5** (Decoupled form of the ADDA for MAREs). Define $U_j := \mathcal{A}_\beta U_{j-1}$, $V_j := \mathcal{A}_\beta^2 V_{j-1}$, $W_j := \mathcal{D}_\alpha W_{j-1}$ and $Q_j := \mathcal{D}_\alpha^2 Q_{j-1}$ for $j \geq 1$. Assume that $I_m - H_k G_k$ and $I_n - G_k H_k$ are nonsingular for $k \geq 0$. For $k \geq 2$, denote $Q_k = [Q_0, Q_1, \cdots, Q_{2^{k-1}}]$, $U_k = [U_0, U_1, \cdots, U_{2^{k-1}}]$, $\hat{V}_k = [V_0, V_1, \cdots, V_{2^{k-1}}]$ and $\hat{W}_k = [W_0, W_1, \cdots, W_{2^{k-1}}]$, and let $Y_k = \begin{bmatrix} 0 & Y_{k-1} & - (\alpha + \beta) T_{k-1} \end{bmatrix}$ and $Z_k = \begin{bmatrix} 0 & Z_{k-1} & - (\alpha + \beta) S_{k-1} \end{bmatrix}$ with $T_{k-1} = \hat{Q}_1^T \hat{W}_{k-1}$ and $S_{k-1} = \hat{V}_1^T \hat{U}_{k-1}$. The ADDA produces the following decoupled form

$$ F_k = \mathcal{A}_\beta^2 \alpha (\alpha + \beta) \hat{U}_k (I_{2^k m_1} - Y_k Z_k)^{-1} Y_k \hat{V}_k^T, \quad E_k = \mathcal{D}_\alpha^2 \beta (\alpha + \beta) \hat{W}_k (I_{2^k n_1} - Z_k Y_k)^{-1} Z_k \hat{Q}_k^T, $$

$$ H_k = (\alpha + \beta) \hat{U}_k (I_{2^k m_1} - Y_k Z_k)^{-1} \hat{Q}_k^T, \quad G_k = (\alpha + \beta) \hat{W}_k (I_{2^k n_1} - Z_k Y_k)^{-1} \hat{V}_k^T. $$

### 4 Numerical example

In this section, we apply the proposed dSDA to one steel profile cooling model to illustrate its feasibility and also the fault, hence showing the necessity of truncation.

**Example 4.1.** We test the dSDA on one example on the cooling of steel rail profiles, which is available from morWiki [11] and whose size is 1357. In this example, $A \in \mathbb{R}^{1357 \times 1357}$ is negative definite, thus stable, and $B$ and $C^T$ respectively have 7 and 6 columns. To approximate the stabilizing solution, we solve the corresponding CARE (2). For stopping criteria, we use the normalized residual of the CARE:

$$ \rho(H_k) := \frac{\| A^T H_k + H_k A - H_k B B^T H_k + C^T C \|_F}{2 \| A^T H_k \|_F + \| H_k B B^T H_k \|_F + \| C^T C \|_F}. $$

We set the tolerance for $\rho(H_k)$ as $10^{-13}$ and the maximal number of iterations to 20.

Table 1 shows the variation of the normalized residual $\rho(H_k)$ and the numerical rank of $H_k$ as determined by MATLAB (or $r(H_k)$) along with the iteration index $k$. With 9 doubling iterations the dSDA produces a stabilizing approximation whose relative residual is $7.614 \times 10^{-15}$. Besides, the computed solution has a low rank of 191. The total execution time is 60.156 seconds when running on a 64-bit PC with an Intel Core i7 CPU at 2.70GHz and 16G RAM.

For comparison, we also apply the SDA with the same parameters. After 9 iterates it produces an accurate approximation of a low-rank 110. However, the execution time for the SDA is only 16.194 seconds. By comparing the numerical results from the SDA and the dSDA, we know that although the proposed dSDA is feasible, it is far from satisfactory. For instance, the columns of $\hat{V}_k$
doubles in each iterate, thus we compute with many insignificant and unnecessary basis vectors. In other words, the lower right corner of \((I + Y_k Y_k^T)^{-1}\) attenuates rapidly when the dSDA begins to converge although its size grows doubly, so we have to calculate many inconsequential values. In fact, the superfluous operations can be avoid when “truncation” is applied.

\[
\begin{array}{|c|c|c|c|}
\hline
k & \rho(H_k) & r(H_k) & k & \rho(H_k) & r(H_k) \\
\hline
1 & 3.287 \times 10^{-2} & 12 & 6 & 4.513 \times 10^{-10} & 160 \\
2 & 9.694 \times 10^{-4} & 24 & 7 & 1.157 \times 10^{-11} & 178 \\
3 & 2.635 \times 10^{-5} & 48 & 8 & 2.969 \times 10^{-13} & 191 \\
4 & 6.852 \times 10^{-7} & 96 & 9 & 7.614 \times 10^{-15} & 191 \\
5 & 1.759 \times 10^{-8} & 139 & & & \\
\hline
\end{array}
\]

Table 1: Normalized residuals and ranks

The example merely illustrates the validity of the dSDA. As the closely related Krylov subspace methods, it only makes sense for applications to large-scale problems, with truncation implemented (as in the dSDA).

5 Conclusions

In this paper, we present a decoupled form for the classical structure-preserving doubling algorithm, the dSDA. We only need to compute with one recursion and may apply the associated low-rank structures, solving large-scale problems efficiently. Due to the page limitation, we only present the theoretical development for the dSDA. The computation issues in practical applications, especially the truncation process to control the rank of the approximate solution, will be presented in a companion paper.

Acknowledgements

Part of the work was completed when the first three authors visited the ST Yau Research Centre at the National Chiao Tung University, Hsinchu, Taiwan. The first author is supported in part by NSFC-11901290 and Fundamental Research Funds for the Central Universities, and the third author is supported in part by NSFC-11901340.

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DSDA: a Decoupled Form for the SDA

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