A NOTE ON GOLDEN MEANS, NONLINEAR MATRIX EQUATIONS AND STRUCTURED DOUBLING ALGORITHMS

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Abstract. Several beautiful formulae for the solutions of some nonlinear matrix equations were proposed by Yongdo Lim in 2007, in terms of the matrix golden means. Numerically, these formulae will not be applicable when some matrices involved are ill-conditioned. In this note, we propose to partially fill in this gap of applicability with the structured doubling algorithm, under some favourable conditions. We also discuss how some pre-processing or scaling procedures can be applied to the matrix equations, to improve their condition. More generally, we also explore the possibility of computing the matrix golden mean using structured doubling algorithms. Some numerical examples will be presented for illustrative purposes.

1. INTRODUCTION

In [16], Lim generalized the concept of the golden means of positive numbers to the golden means of positive definite matrices and apply them to some algebraic and differential Riccati equations. In particular, explicit formulae for the solutions were given for the following matrix equations:

$$(1) \qquad X^2 \pm X - A^2 = 0$$

$$(2) \qquad BX^{-1}B - X \pm A = 0$$

$$(3) \qquad XA^{-1}X \pm X - B = 0$$

where $A > 0$ (i.e., A is positive definite) and $B \geq 0$ (i.e., B is semi-positive definite). Note that (1) is a special case of (3) and, without lose of generality, we need to consider only the solutions X_+ with the "+" sign in (2) and (3). The solutions X_- to the equations with the "−" sign satisfy $X_- = X_+ + A$ [16].

Compare to the state-of-the-art iterative procedures for the solution of the more general equations [2, 8, 9, 13, 17, 18], these golden mean formulae are beautiful and attractive, at least theoretically so. In this note, we shall consider (2) and (3) in the following form:

(4) $$BX^{-1}B - X - A = 0$$

(5) $$XA^{-1}X + X - (B - A) = 0$$

where $0 < A \leq B$ (i.e., $A > 0$ and $B - A \geq 0$). We shall refer to (4) as the nonlinear matrix equation (NME) and (5) the continuous-time algebraic Riccati equation (CARE).

In general, when A or B are ill-conditioned, $A \sharp B$ will be ill-conditioned to compute. In particular, when A or B are ill-conditioned for (4) or when A and B are large for (5), the solution in terms of the golden means will break down numerically. In such cases, we shall show how the structured doubling algorithm (SDA) [4, 17] may be applied effectively.

The plan for this note is as follows. In Section 2, Lim's results in [16] on the golden means are summarized and we give some new proofs. The possibility of computing the golden mean $A \sharp B$ by doubling is discussed in Section 3. The solutions of the "ill-conditioned" NME (4) and CARE (5) are respectively considered in Sections 4 and 5. The SDA algorithms are developed for these ill-conditioned cases and selected numerical examples are presented for illustrative purposes. The possibility of solving the equations (in equivalent forms) by cyclic reduction is considered briefly in Section 6 and some concluding remarks are made in Section 7.

Before we proceed, it is important to emphasize an obvious point – we are proposing an alternative method for computing the golden mean in general and solving (4) and (5) in particular, when the equations are "ill-conditioned" and computations involving the golden mean break down numerically. There may well be cases for which the golden mean yields "better" results than the SDA, or when both approaches fail. Different methods rewrite the matrix equations into different forms for which doubling can be applied, under different conditions. When these conditions break down simultaneously, there is little anyone can do.

2. Matrix Golden Means

In this section, we quote some relevant basic results on the matrix golden means from [16].

First of all, it is well known that every nonnegative number has a unique square root. The analog for matrices is the following lemma [12].

Lemma 2.1. *For every n-square matrix $A \geq 0$, there exist a unique $B \geq 0$ such that*

$$A = B^2.$$

If A is positive definite, then B is also a positive definite matrix. Furthermore, B can be written as a polynomial of A.

Such a matrix $B \geq 0$ is called the square root of A and denoted by $A^{1/2}$. Using Lemma 2.1, we can prove the following Lemma:

Lemma 2.2. *Let A and B be $n \times n$ complex matrices, then*

(6) $$A^*A = B^*B$$

if and only if there exist some unitary matrix W such that

(7) $$A = WB.$$

Proof. If $A = WB$ for some unitary matrix W, it is clearly that $A^*A = B^*W^*WB = B^*B$. Conversely, consider the singular value decomposition of A and B:

$$A = U_A \Sigma_A V_A^*,$$

$$B = U_B \Sigma_B V_B^*,$$

where U_A, V_A, U_B and V_B are $n \times n$ unitary matrices and $\Sigma_A, \Sigma_B \in \mathbb{R}^{n \times n}$ are diagonal matrices with nonegative main-diagonal entries. The condition (6) implies that

$$\Sigma_A^2 = V^* \Sigma_B^2 V,$$

where $V = V_B^* V_A$ is a unitary matrix, it follows from Lemma 2.1 that $\Sigma_A = V^* \Sigma_B V$. Thus,

$$A = U_A \Sigma_A V_A^* = U_A V_A^* V_B \Sigma_B V_B^* = WB,$$

where $W \equiv U_A V_A^* V_B U_B^*$ is unitary. ∎

The geometric mean (gm)

(8) $$A \sharp B \equiv A^{1/2}(A^{-1/2} B A^{-1/2})^{1/2} A^{1/2}$$

of positive definite matrices A and B has appeared in literature with various applications in matrix inequalities, inverse mean problems, semidefinite programming, geometry, statistical shape analysis and symmetric matrix word equations;

see [1, 3, 15, 16, 20] and the references therein. Note that $A\sharp B$ is the unique positive definite solution to the algebraic Riccati equation $XA^{-1}X = B$ (see Lemma 2.3 below). For the differential Riccati equation $\dot{X} = -XA^{-1}X + B$ with $X(0) > 0$, we have $\lim_{t\to\infty} X(t) = A\sharp B$.

First some basic properties of the gm are listed in the following lemmas:

Lemma 2.3. (Riccati). *Let A be positive definite and B be (semi-)positive definite. Then the geometric mean $A\sharp B$ is a unique (semi-)positive definite solution of the Riccati equation*

$$(9) \qquad XA^{-1}X = B.$$

Proof. We rewrite the Riccati equation (9) as $(A^{-1/2}X)^*(A^{-1/2}X) = (B^{1/2})^* B^{1/2}$, it follows from Lemma 2.2 that there exist an unitary matrix U such that $X = A^{1/2}UB^{1/2}$. Since X is a Hermitian matrix, thus $Y \equiv UB^{1/2}A^{-1/2} = A^{-1/2}B^{1/2}U^*$ and $X = A^{1/2}YA^{1/2}$. It is easy to see that

$$Y^2 = A^{-1/2}B^{1/2}U^*UB^{1/2}A^{-1/2} = A^{-1/2}BA^{-1/2}$$

and we have $Y = (A^{-1/2}BA^{-1/2})^{1/2} \geq 0$. We finally show that $X = A^{1/2}YA^{1/2} = A\sharp B \geq 0$. The uniqueness of the positive semi-definite solution of (9) can be obtained from Lemma 2.1. ■

Proposition 2.1. *The geometric mean has the following properties [16, Lemma 2.1]:*

(i) $A\sharp B = B\sharp A$.

(ii) $(A\sharp B)^{-1} = A^{-1}\sharp B^{-1}$.

(iii) $M(A\sharp B)M^\top = (MAM^\top)\sharp(MBM^\top)$ *for any nonsingular matrix M.*

(iv) $2(A^{-1} + B^{-1})^{-1} \leq A\sharp B \leq \frac{1}{2}(A + B)$ *for positive definite A, B.*

The golden ratios $\frac{1}{2}(1\pm\sqrt{5})$ are the roots of the quadratic equation $x^2 - x - 1 = 0$. For a generalization, consider the more general quadratic equation

$$\frac{x^2}{a} \mp x - (b - a) = 0 \ , \quad 0 < a \leq b$$

with the positive real solutions $\frac{1}{2}\left(a \pm \sqrt{4ab - 3a^2}\right)$. For matrices, we consider the Hermitian solution of the Riccati equation

$$(X - C)A^{-1}(X - C) = B,$$

where $A > 0$, $B \geq 0$ and C is a Hermitian matrix.

For the continuous-time Riccati equation and nonlinear matrix equation, the following two theorems give explicit formulae for their solutions. Similar results can be found in [16, §3]:

Theorem 2.1. *The CARE (5):*

$$XA^{-1}X + X - (B - A) = 0 , \quad 0 < A \leq B$$

has a unique positive definite solution

$$(10) \qquad X_{\text{Ric}} = A \bar{\natural} B \equiv \frac{1}{2} \left[-A + A\sharp(4B - 3A) \right].$$

Proof. We only show the uniqueness of the positive semi-definite solution (10). Suppose that X is a positive semi-definite solution of (5). Setting $Y = A^{-1/2}XA^{-1/2}$ and $\widetilde{B} = A^{-1/2}BA^{-1/2}$, we obtain the quadratic matrix equation

$$Y^2 + Y - (\widetilde{B} - 1) = 0.$$

With the help of $(Y + \frac{1}{2}I)^2 = \widetilde{B} - \frac{3}{4}I$ and Lemma 2.1, we have $X = A^{1/2}YA^{1/2} = A\bar{\natural}B$. ∎

Theorem 2.2. *The nonlinear matrix equation with the plus sign (NME-P):*

$$(11) \qquad BX^{-1}B + X - A = 0 , \quad A > 2B \geq 0$$

has the maximum positive definite solution

$$(12) \qquad X_{\text{Nmep}} = \frac{1}{2} \left[A + (A - 2B)\sharp(A + 2B) \right].$$

The nonlinear matrix equation with the minus sign (NME-M):

$$(13) \qquad BX^{-1}B - X + A = 0 , \quad A > 0, B \geq 0$$

has the unique positive definite solution

$$(14) \qquad X_{\text{Nmem}} = \frac{1}{2} \left[A + A\sharp(A + 4BA^{-1}B) \right].$$

Proof.

1. For the NME-P (11), assume that X is a positive definite solution. Let R be $X^{-1}B$, we noted that $\sigma(R) = \sigma(X^{-1/2}BX^{-1/2})$ and therefore the spectrum of R are lies in the closed right half planes. Since $A > 2B \geq 0$ and $X < A$,

we have $X = A - BX^{-1}B < A - BA^{-1}B = \frac{3}{4}A$. Let $\widetilde{X} = X - \frac{1}{2}A$, we rewrite (11) as

$$\begin{bmatrix} B & 0 \\ \frac{1}{2}A & -I \end{bmatrix} \begin{bmatrix} I \\ \widetilde{X} \end{bmatrix} = \begin{bmatrix} \frac{1}{2}A & I \\ B & 0 \end{bmatrix} \begin{bmatrix} I \\ \widetilde{X} \end{bmatrix} R,$$

then we have

$$\left(\begin{bmatrix} B & 0 \\ \frac{1}{2}A & -I \end{bmatrix}, \begin{bmatrix} \frac{1}{2}A & I \\ B & 0 \end{bmatrix} \right) \sim \left(\begin{bmatrix} 2B & 0 \\ \frac{1}{2}A+B & -I \end{bmatrix}, \begin{bmatrix} A & 2I \\ \frac{1}{2}A+B & I \end{bmatrix} \right)$$

$$\sim \left(\begin{bmatrix} B - \frac{1}{2}A & I \\ \frac{1}{2}A+B & -I \end{bmatrix}, \begin{bmatrix} \frac{1}{2}A-B & I \\ \frac{1}{2}A+B & I \end{bmatrix} \right)$$

$$\sim \left(\begin{bmatrix} I & -(\frac{1}{2}A-B)^{-1} \\ -(\frac{1}{2}A+B) & I \end{bmatrix}, \begin{bmatrix} -I & -(\frac{1}{2}A-B)^{-1} \\ -(\frac{1}{2}A+B) & -I \end{bmatrix} \right).$$

Here, the notation "$(A_1, B_1) \sim (A_2, B_2)$" indicates that there exist non-singular matrices P and Q such that $(A_1, B_1) = (PA_2Q, PB_2Q)$. Let $\mathcal{H} \equiv \begin{bmatrix} 0 & -(\frac{1}{2}A-B)^{-1} \\ -(\frac{1}{2}A+B) & 0 \end{bmatrix}$, we obtain

(15) $$(\mathcal{H} + I) \begin{bmatrix} I \\ \widetilde{X} \end{bmatrix} (\widetilde{R} - I) = (\mathcal{H} - I) \begin{bmatrix} I \\ \widetilde{X} \end{bmatrix} (\widetilde{R} + I),$$

where $\widetilde{R} = (R+I)^{-1}(R-I)$. Rewrite (15) as a Riccati equation in the form of (9):

$$\widetilde{X} \left(\frac{1}{2}A - B \right)^{-1} \widetilde{X} = \frac{1}{2}A + B,$$

we get a positive definite solution $X_{\text{Nmep}} = \frac{1}{2}A + \widetilde{X} = \frac{1}{2}[A + (A-2B)\sharp(A+2B)]$. Since $X_{\text{Nmep}}^{-1/2}BX_{\text{Nmep}}^{-1/2} < \frac{1}{2}A^{-1/2}BA^{-1/2} < I$, it follows from [7] that X is the maximum positive definite solution of (11).

2. For the NME-M (13), let $Y = A^{-1/2}XA^{-1/2}$, $\widetilde{B} = A^{-1/2}BA^{-1/2}$. The NME-M (13) becomes
$$Y - \widetilde{B}Y^{-1}\widetilde{B} = I.$$

Consider the matrix function $f(Y) \equiv I + \widetilde{B}Y^{-1}\widetilde{B}$ and we obtain

$$\begin{aligned} Y &= f(Y) = f(f(Y)) \\ &= I + \widetilde{B}(I + \widetilde{B}Y^{-1}\widetilde{B})^{-1}\widetilde{B} \\ &= I + \widetilde{B}(I - \widetilde{B}Y^{-1}(I + \widetilde{B}^2 Y^{-1})^{-1}\widetilde{B})\widetilde{B} \\ &\qquad \text{(using the Sherman-Morrison-Woodbury formula)} \\ &= I + \widetilde{B}^2 - \widetilde{B}^2(Y + \widetilde{B}^2)^{-1}\widetilde{B}^2. \end{aligned}$$

We get a matrix equation in the NME-P form. From (12), we have

$$Y + \widetilde{B}^2 = \frac{1}{2}\left[I + 2\widetilde{B}^2 + I\sharp(I + 4\widetilde{B}^2)\right],$$

where $\widetilde{B}^2 = A^{-1/2}BA^{-1}BA^{-1/2}$. Thus

$$\begin{aligned}X_{\mathrm{Nmem}} &= \frac{1}{2}A^{1/2}\left[I + I\sharp(I + 4A^{-1/2}BA^{-1}BA^{-1/2})\right]A^{1/2}\\ &= \frac{1}{2}\left[A + A\sharp(A + 4BA^{-1}B)\right].\end{aligned}$$

From [8], the positive definite solution X_{Nmem} is the unique maximum positive definite solution of (13). ∎

These results can be generalized further to the (matrix) golden means (GM) (when $0 < A \le B$):

(16) $A\natural B \equiv \frac{1}{2}\left[A + A\sharp(4B - 3A)\right]$, $A\bar\natural B \equiv \frac{1}{2}\left[-A + A\sharp(4B - 3A)\right]$

Some basic properties of GMs are listed in the following lemma [16, Proposition 4.2]:

Lemma 2.4. *Suppose that A and B are positive definite matrices with $A \le B$. Then*

 (*i*) $M(A\natural B)M^\top = (MAM^\top)\natural(MBM^\top)$ *and* $M(A\bar\natural B)M^\top = (MAM^\top)\bar\natural(MBM^\top)$ *for any compatible nonsingular matrix M.*

 (*ii*) $A\natural B = A\sharp B$ *if and only if $A = B$.*

 (*iii*) $A\natural B = \frac{1}{2}A^{1/2}\left[I + (4A^{-1/2}BA^{-1/2} - 3I)^{1/2}\right]A^{1/2}.$

 (*iv*) *If $A < B$, then $A\natural B = \frac{1}{2}\left\{A + (B - A)\sharp\left[4A + A(B - A)^{-1}A\right]\right\}.$*

 (*v*) (*The harmonic-geometric golden mean inequality*)

$$A \le 2(A^{-1} + B^{-1})^{-1} \le A\sharp B \le A\natural B \le B$$

 (*vi*) *If $B \ge 3A$ (or $B \le 3A$), then $A\natural B \le \frac{1}{2}(A + B)$ (or $A\natural B \ge \frac{1}{2}(A + B)$).*

 (*vii*) $(A\natural B)\sharp(A\bar\natural B) = A\sharp(B - A).$

 (*viii*) $A\natural B = A\sharp(B + A\bar\natural B)$ *and* $A\bar\natural B = A\sharp(B - A\natural B).$

We shall see later that the alternative formulae in (iii) and (iv) are numerically worse than (16). For other results on the gm and GM, please consult [16] and the references therein.

3. Golden Mean by Doubling

The GMs in (16) requires the square-roots of various positive definite matrices. The accuracy of this computation is governed by the following theorem:

Theorem 3.3. [10]. *Let $A \in \mathbb{R}^{n \times n}$ be a positive definite matrix, $X = A^{1/2}$ and $\overline{X}$ be an approximation to a square root of A. then*

$$(17) \qquad \|X - \overline{X}\|_F \leq \left(\frac{\|X\|_F^2}{\min\limits_{1 \leq i,j \leq n} |\mu_i + \mu_j|} cn \right) u,$$

where c is a constant of order 1, u is machine unit roundoff, and $\{\mu_i\}$ are the eigenvalues of X.

Consequently, the square-root $A^{1/2}$ will be numerically inaccurate and unstable when A is ill-conditioned.

Another possibility is to apply the structured doubling algorithm [17], which can be applied to the following standard symplectic forms (SSF) [4, 5, 17]:

(SSF-1):
$$\mathcal{M} = \begin{bmatrix} A & 0 \\ -H & I \end{bmatrix}, \quad \mathcal{L} = \begin{bmatrix} I & G \\ 0 & A^\top \end{bmatrix}, \quad H, G \geq 0$$

(SSF-2):
$$\mathcal{M} = \begin{bmatrix} A & 0 \\ Q & -I \end{bmatrix}, \quad \mathcal{L} = \begin{bmatrix} -P & I \\ A^\top & 0 \end{bmatrix}, \quad Q, Q - P \geq 0$$

From Section 2 or [16], the GM $A \sharp B$ equals the solution X of the Riccati equation

$$(18) \qquad X A^{-1} X = B,$$

where $A > 0$ and $B \geq 0$. We found two feasible ways to compute the GM using doubling.

3.1. SSF1

From [17], the associated Hamiltonian matrix of (18) is

$$\mathcal{H} \equiv \begin{bmatrix} 0 & A^{-1} \\ B & 0 \end{bmatrix}.$$

With the Cayley transformation for some positive number γ, we obtain the matrix pencil

$$(\mathcal{H} - \gamma I, \mathcal{H} + \gamma I) = \left(\begin{bmatrix} -\gamma I & A^{-1} \\ B & -\gamma I \end{bmatrix}, \begin{bmatrix} \gamma I & A^{-1} \\ B & \gamma I \end{bmatrix} \right),$$

note that the spectrum of (M, L) and (PMQ, PLQ) are identical for nonsingular P and Q. Pivoting at the identity matrix at the (2,2)-position in the first matrix, simple elementary row operations produce

$$(\mathcal{H} - \gamma I, \mathcal{H} + \gamma I) \sim \left(\begin{bmatrix} \frac{1}{\gamma} A^{-1} B - \gamma I & 0 \\ -\frac{1}{\gamma} B & I \end{bmatrix}, \begin{bmatrix} \frac{1}{\gamma} A^{-1} B + \gamma I & 2A^{-1} \\ -\frac{1}{\gamma} B & -I \end{bmatrix} \right).$$

Let $C \equiv \frac{1}{\gamma} A^{-1} B + \gamma I$ be a nonsingular matrix with $\sigma(A^{-1}B) \subseteq \mathbb{C}^+$. Multiply the first row-block by C^{-1} and apply elementary pivoting at the identity matrix at the (1,1)-position in the second matrix, we obtain

$$(\mathcal{H} - \gamma I, \mathcal{H} + \gamma I) \sim \left(\begin{bmatrix} I - 2\gamma C^{-1} & 0 \\ -\frac{1}{\gamma} B & I \end{bmatrix}, \begin{bmatrix} I & 2C^{-1}A^{-1} \\ -\frac{1}{\gamma} B & -I \end{bmatrix} \right)$$

$$\sim \left(\begin{bmatrix} I - 2\gamma C^{-1} & 0 \\ -2BC^{-1} & I \end{bmatrix}, \begin{bmatrix} I & 2C^{-1}A^{-1} \\ 0 & I - 2\gamma C^{-\top} \end{bmatrix} \right).$$

As BC^{-1}, $C^{-1}A^{-1} > 0$, the final matrix pencil is in SSF1 form and the associated SDA [17] can be applied for the solution of (18). However, this approach requires the inversion of C which may lead to numerical difficulties. The preferred approach can be formulated in terms of the SSF2 form.

3.2. SSF2

There are two possibilities in terms of the SSF2 form. Similar to Section 3.1, elementary row/column operations are applied to obtain matrix pencils which preserve the spectrum of the original pencil.

(a) Apply Cayley transformation for some positive number γ, we have

$$(\mathcal{H} - \gamma I, \mathcal{H} + \gamma I)$$

$$= \left(\begin{bmatrix} -\gamma I & A^{-1} \\ B & -\gamma I \end{bmatrix}, \begin{bmatrix} \gamma I & A^{-1} \\ B & \gamma I \end{bmatrix} \right) \sim \left(\begin{bmatrix} -\gamma A & I \\ \frac{1}{\gamma} B & -I \end{bmatrix}, \begin{bmatrix} \gamma A & I \\ \frac{1}{\gamma} B & I \end{bmatrix} \right)$$

$$\sim \left(\begin{bmatrix} \frac{1}{\gamma} B - \gamma A & 0 \\ \frac{1}{\gamma} B & -I \end{bmatrix}, \begin{bmatrix} \frac{1}{\gamma} B + \gamma A & 2I \\ \frac{1}{\gamma} B & I \end{bmatrix} \right)$$

$$\sim \left(\begin{bmatrix} \frac{1}{2}(\frac{1}{\gamma} B - \gamma A) & 0 \\ \frac{1}{2}(\frac{1}{\gamma} B + \gamma A) & -I \end{bmatrix}, \begin{bmatrix} \frac{1}{2}(\frac{1}{\gamma} B + \gamma A) & I \\ \frac{1}{2}(\frac{1}{\gamma} B - \gamma A) & 0 \end{bmatrix} \right).$$

The final matrix pencil is in SSF2 form and the associated SDA can be applied for solving (18). From [17], the SDA requires the positivity of $Q_0 - P_0 =$

$\frac{1}{\gamma}B + \gamma A > 0$, which is obvious. This is the preferred approach (denoted by GMSDA) for the solution of (18) and the computation of GMs, because of its nice numerical behaviour. The parameter γ is chosen to balance the ill-condition of A and B in $Q_0 - P_0 = \frac{1}{\gamma}B + \gamma A$. When B (A) is more ill-coniditoned, we increase (decrease) γ.

(b) The geometric mean satisfies

$$A\sharp B \equiv A^{1/2}(A^{-1/2}BA^{-1/2})^{1/2}A^{1/2} \geq \sigma_{min}(A^{-1/2}B^{1/2})A$$

which is a unique (semi-) p.s.d. solution of the Riccati equation $XA^{-1}X = B$, i.e., $X \geq \sigma_{min}(A^{-1/2}B^{1/2})A$. Assume that $B > 0$ and let $X_1 = X - aA$, with $a > 0$ to be determined. Rewrite (18) as

(19)
$$X_1 A^{-1} X_1 + 2aX_1 = B - a^2 A$$

with

$$0 < a < \sigma_{min}(A^{-1/2}B^{1/2}) = \lambda_{min}^{1/2}(A^{-1}B) = \sqrt{\min_{x\neq 0}\frac{x^\top Bx}{x^\top Ax}} \ .$$

The associated Hamiltonian matrix of (19) is

$$\mathcal{H}_1 \equiv \begin{bmatrix} aI & A^{-1} \\ B - a^2 A & -aI \end{bmatrix}.$$

Apply Cayley transformation with $\gamma = a$, we have

$$(\mathcal{H} - aI, \mathcal{H} + aI) = \left(\begin{bmatrix} 0 & A^{-1} \\ B - a^2 A & -2aI \end{bmatrix}, \begin{bmatrix} 2aI & A^{-1} \\ B - a^2 A & 0 \end{bmatrix} \right)$$

$$\sim \left(\begin{bmatrix} 0 & I \\ \frac{1}{2a}(B - a^2 A) & -I \end{bmatrix}, \begin{bmatrix} 2aA & I \\ \frac{1}{2a}(B - a^2 A) & 0 \end{bmatrix} \right).$$

Let $D \equiv \frac{1}{2a}(B - a^2 A) > 0$, then

$$(\mathcal{H} - aI, \mathcal{H} + aI) \sim \left(\begin{bmatrix} 0 & I \\ D & -I \end{bmatrix}, \begin{bmatrix} 2aA & I \\ D & 0 \end{bmatrix} \right) \sim \left(\begin{bmatrix} D & 0 \\ D & -I \end{bmatrix}, \begin{bmatrix} D + 2aA & I \\ D & 0 \end{bmatrix} \right).$$

We arrive at an SSF2 form, with $Q_0 - P_0 = 2(D + aA) = \frac{1}{a}(B + a^2 A) > 0$. This approach requires the estimation of a and the inversion of A, so the previous approach in (a) is preferred. Numerically, (a) and (b) behave similarly.

Some numerical experiments have been conducted to illustrate the feasibility of computing GMs using using approach (a) in terms of the SSF2 form

(denoted by SDA). In Example 3.1 below, SDA is compared the formulae in (8), realized by the MATALB command `sqrtm` for square roots of matrices (denoted by GM). Example 3.2 illustrates the fact that increasing a does not affect the condition of A or the error in A^{-1}, unlike the error in $A^{1/2}$.

Example 3.1. Let $A = B \equiv 1.e6 * gallery('randcorr', 5)$, From Table 1, we see that the absolute residual from SSF2 are smaller than those from GM by up to 4 digits.

Table 1. Results for Example 3.1.

	SDA	GM
Res	$3.28e - 16$	$1.43e - 12$
ITs	4	$*$

Example 3.2. *Let* $A = 10^a gallery('randcorr', 5)$, $B = sqrtm(A)$, Inverr $\equiv \|A/A - I_5\|$ *and* Sqrtmerr $\equiv \|B * B - A\|$. We list a comparison of absolute error for the Inverr and Sqrtmerr as increasing power a in Table 2.

Table 2. Results for Example 3.2.

a	Inverr	Sqrtmerr	cond(A)
0	2.2648e-016	2.1328e-015	3.8671e+001
2	2.8495e-015	3.5945e-013	4.0025e+002
4	3.3506e-016	2.2687e-011	1.1946e+001
6	6.3090e-016	2.2648e-009	1.7206e+001

From our numerical experience, the SDA is a feasible alternative to (18) (realized by square roots of matrices) in computing GMs, especially for A with large elements.

4. NONLINEAR MATRIX EQUATIONS

See [2, 6, 7, 8, 9, 13, 17, 18] for details of nonlinear matrix equations, their solution and applications.

Before pressing further, we want to know whether it is possible to improve the condition of A before square-rooting it, thus reducing the stability problem for the formulae (10), (12) and (14).

Let us consider the NME (4):

$$BX^{-1}B - X \pm A = 0$$

Pre- and post-multiply the equations with nonsingular $Q^\top$ and Q respectively, we obtain the equivalent equations

$$Q^\top BQ \cdot Q^{-1}X^{-1}Q^{-\top} \cdot Q^\top BQ - Q^\top XQ \pm Q^\top AQ = 0$$

Some obvious choices include $Q = B^{-1/2}$, $Q = A^{-1/2}$ and the diagonal scaling $Q = \mathrm{diag}\{d_1, \cdots, d_n\}$ with $d_i = \sqrt{\sum_{k=1}^{n} a_{ik}^2}$. For diagonal scaling, let D_n denotes the set of nonsingular diagonal matrices. We list the following well known results.

Theorem 4.1. (Van der Sluis) [11] . *Let $A \in \mathbb{R}^{n \times n}$ be symmetric positive definite and let $D_* = \mathrm{diag}\left\{a_{ii}^{-1/2}\right\}$, then*

$$\kappa_2(D_* A D_*) \leq n \min_{D \in D_n} (DAD).$$

Theorem 4.2. (Bauer) [11]. *Let $A \in \mathbb{R}^{n \times n}$ be nonsingular and suppose that $|A| \, |A^{-1}|$ is irreducible. Then*

$$\min_{D_1, D_2 \in D_n} \kappa_\infty(D_1 A D_2) = \rho(|A| \, |A^{-1}|).$$

The minimum is attained for $D_1 = \mathrm{diag}(x)^{-1}$ and $D_2 = \mathrm{diag}(|A^{-1} x|)$, where $x > 0$ is a right Perron vector.

Unfortunately, our numerical experiments show that the contribution of scaling towards lessening the condition of A and B is unclear. Ill-condition sometimes shifts or spreads out to other parts of the equation and does not help the overall accuracy of the solution. More work need to be done on the scaling of NMEs.

We shall consider two cases when either A or B is ill-conditioned in (4). Scaling may help when both matrices are ill-conditioned but both the SDA and GM approaches will encounter difficulty for such as case.

4.1. Ill-conditioned B

For (4) in the form

$$X - BX^{-1}B = A$$

where B is ill-conditioned, let

$$\mathcal{M} = \begin{bmatrix} B & 0 \\ -A & I \end{bmatrix}, \quad \mathcal{L} = \begin{bmatrix} 0 & I \\ B & 0 \end{bmatrix}.$$

It is easy to show that X is a solution to the NME (4) if and only if

$$\mathcal{M} \begin{bmatrix} I \\ X \end{bmatrix} = \mathcal{L} \begin{bmatrix} I \\ X \end{bmatrix} S,$$

where $S = X^{-1}B$. After the doubling transformation, block Gaussian elimination, and column permutation [17], we obtain

$$\begin{bmatrix} \widehat{B} & 0 \\ \widehat{A} + \widehat{P} & -I \end{bmatrix} \begin{bmatrix} I \\ X + \widehat{P} \end{bmatrix} = \begin{bmatrix} 0 & I \\ \widehat{B} & 0 \end{bmatrix} \begin{bmatrix} I \\ X + \widehat{P} \end{bmatrix} S^2,$$

which involves the SSF-2 form, where $\widehat{B} = BA^{-1}B$, $\widehat{A} = A + BA^{-1}B$, and $\widehat{P} = BA^{-1}B$. The SDA-2 in [17] can then be applied.

SDA$_1$ Algorithm

Set $A_0 = BA^{-1}B$, $B_0 = B + 2A_0$, $P_0 = 0$, $\widehat{P} = A_0$;
Compute until convergence
  $A_{k+1} = A_k(Q_k - P_k)^{-1}A_k$, $Q_{k+1} = Q_k - A_{k+1}$, $P_{k+1} = P_k + A_{k+1}$.
Output: $X = Q_{k+1} - \widehat{P}$.

It requires about $\frac{7}{6}n^3$ flops for each iteration.

Example 4.1. Let A and B be random 20×20 positive definition matrices of $O(1)$. Construct $B \leftarrow B - 0.999999 * \lambda_{min}(B) * I$ and $A \leftarrow 10^3 A$ so that $\lambda_{min}(B) \cong 0$ and $A = O(10^3)$. In GMSDA (approach (a) in Section 3.2), we choose $r = 1e3$ such that the initial matrix $Q_0 - P_0$ of inner iteration SDA2 is well condition, namely, $Q_0 - P_0 = \frac{1}{\gamma}B + \gamma A \cong A$. From Table 3, we see that the absolute residuals from SDA (SDA$_1$ Algorithm) and GMSDA ((14) realized by GMSDA as in approach (a) in Section 3.2) are smaller than those from GM ((14) realized by the MATLAB command sqrtm for square roots of matrices) by up to 2 digits, and Res(SDA)/Res(GMSDA)$= O(1)$.

Table 3. Results for Example 4.1.

	SDA	GM	GMSDA
Res	$6.24e-15$	$1.07e-13$	$4.43e-15$
ITs	4	*	4 (inner)

4.2. Ill-conditioned A

For the NME (4) when A is ill-conditioned, rewrite it as

$$X = f(X) = A + BX^{-1}B.$$

It was noted in [2] that if X solves (4), then it also obeys the Riccati equation

$$X = f(f(X)) = A + B(A + BX^{-1}B)^{-1}B = A + X(I + B^{-1}AB^{-1}X)^{-1}.$$

The associated symplectic pencil is:

$$\mathcal{M} = \begin{bmatrix} I & 0 \\ -A & I \end{bmatrix}, \quad \mathcal{L} = \begin{bmatrix} I & B^{-1}AB^{-1} \\ 0 & I \end{bmatrix}.$$

in SSF-1 form and the corresponding SDA-1 algorithm can be applied [4, 17].

SDA$_2$ Algorithm

Set $A_0 = I_n$, $H_0 = A$, $G_0 = B^{-1}AB^{-1}$;

Compute until convergence

$$A_{k+1} = A_k(I_n + G_kH_k)^{-1}A_k, \ G_{k+1} = G_k + A_kG_k(I_n + H_kG_k)^{-1}A_k,$$

$$H_{k+1} = H_k + A_k(I_n + H_kG_k)^{-1}H_kA_k.$$

Output: $X = H_{k+1}$.

It requires about $\frac{23}{3}n^3$ flops for each iteration.

Example 4.2. Let A and B be random 20×20 positive definition matrices with well condition, and construct $A \leftarrow A - 0.999999 * \lambda_{min}(A) * I$ so that $\lambda_{min}(A) \cong 0$. In GMSDA, we choose $r = 1e-3$ such that the initial matrix $Q_0 - P_0$ of inner iteration SDA2 is well condition, namely, $Q_0 - P_0 = \frac{1}{\gamma}B + \gamma A \cong B$. From Table 4, we see that the absolute residuals from SDA (SDA$_2$ Algorithm) are smaller than those from GM ((14) realized by sqrtm) by up to 6 digits, and Res(SDA)/Res(GMSDA)= $O(10^{-3})$.

Table 4. Results for Example 4.1.

	SDA	GM	GMSDA
Res	$2.33e - 11$	$8.79e - 5$	$1.19e - 8$
ITs	24	*	6 (inner)

5. CONTINUOUS-TIME ALGEBRAIC RICCATI EQUATION

The study of continuous-time algebraic Riccati equations is well-developed; see [4, 5, 9, 14, 17] and the references therein. For our special case (5), we first try to consider whether pre-conditioning or scaling can be helpful in the solution of the ARE by GM.

For the CARE (5):

$$XA^{-1}X + X - (B - A) = 0$$

pre- and post-multiply the equations with nonsingular $Q^{\top}$ and Q respectively, we obtain the equivalent equation

$$Q^{\top}XQ \cdot Q^{-1}A^{-1}Q^{-\top} \cdot Q^{\top}XQ + Q^{\top}XQ - Q^{\top}(B - A)Q = 0.$$

Similar choices for Q as in Section 5 can be made. Again, we found experimentally that scaling does not improve the GM method markedly.

Now consider (5) where $O(A)$ and $O(B)$ are large, thus affecting the square-roots when computing the GMs. Rewrite (5) as

$$-X(2A^{-1})X - X - X + 2(B - A) = 0.$$

The associated Hamiltonian matrix is

$$\mathcal{H} \equiv \begin{bmatrix} I & 2A^{-1} \\ 2(B - A) & -I \end{bmatrix}.$$

Apply Cayley transformation with $\gamma = 1$, we have

$$(\mathcal{H} - I, \mathcal{H} + I) = \left(\begin{bmatrix} 0 & 2A^{-1} \\ 2(B - A) & -2I \end{bmatrix}, \begin{bmatrix} 2I & 2A^{-1} \\ 2(B - A) & 0 \end{bmatrix} \right)$$

$$\sim \left(\begin{bmatrix} 0 & A^{-1} \\ (B - A) & -I \end{bmatrix}, \begin{bmatrix} I & A^{-1} \\ (B - A) & 0 \end{bmatrix} \right) \sim \left(\begin{bmatrix} 0 & I \\ (B - A) & -I \end{bmatrix}, \begin{bmatrix} A & I \\ (B - A) & 0 \end{bmatrix} \right)$$

$$\sim \left(\begin{bmatrix} (B - A) & 0 \\ (B - A) & -I \end{bmatrix}, \begin{bmatrix} B & I \\ (B - A) & 0 \end{bmatrix} \right).$$

We arrive at an SSF-2 form and the SDA-2 algorithm [17] can be applied, as shown in the following Algorithm.

SDA$_3$ Algorithm

`Set` $A_0 = B - A$, $Q_0 = B - A$, $P_0 = -B$;

`Compute until convergence`

$$A_{k+1} = A_k(Q_k - P_k)^{-1}A_k, \ Q_{k+1} = Q_k - A_{k+1}, \ P_{k+1} = P_k + A_{k+1}.$$

`Output:` $X = Q_{k+1}.$

It requires about $\frac{7}{6}n^3$ flops for each iteration.

Example 5.1. We choose $D_A = \text{diag}([10^6 \, rand(1,5), rand(1,5)))$, $D_B = \text{diag}([rand(1,10)])$ and a nonsingular matrix $U \in \mathbb{R}^{10 \times 10}$. Construct $A = UD_AU^{-1}$ and $B = A + UD_BU^{-1}$. In GMSDA, we are given $r = 1e - 3$, and the initial matrix $Q_0 - P_0$ of inner iteration SDA-2 is more better condition than A since $\text{cond}(Q_0 - P_0) = \frac{\lambda_{max}(\frac{1}{\gamma}B + \gamma A)}{\lambda_{min}(\frac{1}{\gamma}B + \gamma A)} \cong O(1)$. From Table , we see that the absolute residuals from SDA (SDA$_3$ Algorithm) are smaller than those from GM ((10) realized by `sqrtm`) by up to 3 digits, and Res(SDA)/Res(GMSDA)$= O(10^{-1})$.

Table 5. Results for Example 5.1.

	SDA	GM	GMSDA
Res	$2.33e - 10$	$4.39e - 7$	$3.19e - 9$
ITs	5	$*$	6 (inner)

6. CYCLIC REDUCTION

In this section, we shall explore the possibility of solving (4) and (5) by cyclic reduction (CR) [9, 18].

Consider the ARE (3) with $\tilde{X} \equiv A^{-1}X$ (assuming that A is nonsingular), in the form

$$\tilde{X}^2 \pm \tilde{X} - A^{-1}B = 0$$

This is not suitable for CR as $A^{-1}B$ is not symmetric. Assuming that $B > 0$ and A is nonsingular, a more careful transformation will be

$$B^{-1/2}XB^{-1/2} \cdot B^{1/2}A^{-1}B^{1/2} \cdot B^{-1/2}XB^{-1/2} \pm B^{-1/2}XB^{-1/2} - I = 0$$

producing

$$\Leftrightarrow \tilde{X}\tilde{A}^{-1}\tilde{X} \pm \tilde{X} - I = 0$$

with $\tilde{X} \equiv B^{-1/2}XB^{-1/2}$ and $\tilde{A} \equiv B^{-1/2}AB^{-1/2}$. With $A > 0$, another possibility is

$$A^{-1/2}XA^{-1/2} \cdot A^{-1/2}XA^{-1/2} \pm A^{-1/2}XA^{-1/2} - A^{-1/2}BA^{-1/2} = 0$$

$$\Leftrightarrow \tilde{X}^2 \pm \tilde{X} - \tilde{B} = 0$$

with $\tilde{X} \equiv A^{-1/2}XA^{-1/2}$ and $\tilde{B} \equiv A^{-1/2}BA^{-1/2}$.

For the NME (4):

$$BX^{-1}B - X \pm A = 0$$

it can be transformed, assuming $B > 0$, to

$$B^{1/2}X^{-1}B^{1/2} - B^{-1/2}XB^{-1/2} \pm B^{-1/2}AB^{-1/2} = 0$$

$$\Leftrightarrow \tilde{X}^{-1} - \tilde{X} \pm \tilde{A} = 0 \Leftrightarrow I - \tilde{X}^2 \pm \tilde{A}\tilde{X} = 0$$

which is suitable to be treated by CR. Another possibility, assuming $A > 0$, is

$$A^{-1/2}BA^{-1/2} \cdot A^{1/2}X^{-1}A^{1/2} \cdot A^{-1/2}BA^{-1/2} - A^{-1/2}XA^{-1/2} \pm I = 0$$

$$\Leftrightarrow \tilde{B}\tilde{X}^{-1}\tilde{B} - \tilde{X} \pm I = 0$$

with $\tilde{X} \equiv A^{-1/2}XA^{-1/2}$ and $\tilde{B} \equiv A^{-1/2}BA^{-1/2}$.

Yet another possibility will be, for $B > 0$:

$$B^{1/2}X^{-1}B^{1/2} \cdot B^{1/2}X^{-1}B^{1/2} - I \pm B^{-1/2}AB^{-1/2} \cdot B^{1/2}X^{-1}B^{1/2} = 0$$

or

$$Y^2 - I \pm \tilde{A}Y = 0$$

with $Y \equiv B^{1/2}X^{-1}B^{1/2}$ and $\tilde{A} \equiv B^{-1/2}AB^{-1/2}$.

Consequently, we can apply CR to some of the equivalent matrix quadratics but the transformations require well-conditioned A or B. As a result, CR will have the same pitfalls as the GM formulae or SDA when the NMEs are ill-conditioned. Also, we have previously applied CR to similar problems and found its efficiency and accuracy similar to that of SDA. Consequently, we shall not pursuit the application of CR further in this note.

7. Conclusions

We have proposed some structured doubling algorithms for the computation of golden means and the solution of the nonlinear matrix equation (4) and the algebraic Riccati equation (5). Under adverse conditions, the doubling algorithms perform better than the matrix square root approach for the computation of matrix golden means, or the golden-mean based formulae for the matrix equations (4) and (5).

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