LEAST SQUARES SOLUTION OF MATRIX EQUATION $AXB^* + CYD^* = E$

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Abstract. We present an efficient algorithm for the least squares solution (X, Y) of the matrix equation $AXB^* + CYD^* = E$ with arbitrary coefficient matrices A, B, C, D and the right hand side E. This method determines the minimum residual solution (X, Y) with the least norm. It relies on the SVD and generalized SVD of the coefficient matrices, and has complexity proportional to the cost of these SVDs.

Key words. least norm solution, matrix equation, singular value decomposition

AMS subject classifications. 15A24, 65F20, 65F22, 65K10

1. Introduction. Let m, m_1, m_2; n, n_1, n_2 be six positive integers, and let $E \in \mathbb{C}^{m\times n}$, $A \in \mathbb{C}^{m\times m_1}$, $B \in \mathbb{C}^{n\times n_1}$, $C \in \mathbb{C}^{m\times m_2}$, and $D \in \mathbb{C}^{n\times n_2}$. We consider the linear matrix equation

$$AXB^* + CYD^* = E \tag{1.1}$$

for $X \in \mathbb{C}^{m_1\times n_1}$ and $Y \in \mathbb{C}^{m_2\times n_2}$. The least squares solution of (1.1) is essential to the inverse scattering problem for the Helmholtz equation, where E is the scattering matrix for a domain D partitioned into two non-overlapping subdomains D_1 and D_2, X and Y are the scattering matrices for the two subdomains. The determination of the two scattering matrices (X, Y) from the parent scattering matrix E is known as matrix splitting, and the least norm solution is crucial to the stability of splitting.

In terms of generalized inverse, generalized SVD, and canonical correlation decomposition (CCD), respectively, solution formulae for (1.1) are established in [3], [4], and [5], provided that (1.1) is consistent. Minimum residual solutions are also given in [5] via CCD if (1.1) is not consistent. It appear that there is no method that determines the least squares solution - the minimum residual solution with the least norm - at a cost proportional to that for the SVDs of the coefficient matrices A, B, C, D.

In this paper, we develop such an efficient method for the least squares solution of (1.1). In Section 2, we will start with the equivalent normal equation of (1.1) and construct minimum residual solutions to (1.1). Our approach differs from [5]; it only requires SVDs of the coefficient matrices A, B, C, D. The resulting formula for the minimum residual solutions also differs from the one of [5], and it enables us to construct the minimum norm solution in Section 3.

As is well-known, the use of the normal equation leads to the squaring of the condition number. This does not seem to cause any practical problem to our intended application where the linear equation (1.1) originates from an inverse scattering problem and thus has a high condition number; it must be regularized before its least norm solution. It appears that the squaring of a high condition number does not have adverse effects on the regularization.

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2. Minimum Residual Solutions. The pair (X, Y) is referred to as the minimum residual solution of (1.1) if it minimizes the Frobenius norm of the residual

$$\|AXB^* + CYD^* - E\|_F^2 \tag{2.1}$$

To construct the minimum residual solution of (1.1), we first consider its normal equation in Section 2.1. We then reduce the normal equation to the two equations (2.6) and (2.7) that are always consistent, and equivalent to (1.1). Finally, we solve (2.6) in Section 2.2, and (2.7) in Section 2.3.

2.1. The normal equation. In this section we will reformulate the minimum residual problem for the linear equation (1.1) as the solution of its normal equation. We will require the following two lemmas on the normal equation. Their proofs are straightforward, and are omitted.

LEMMA 2.1. *The normal equation of the linear equation (1.1) is*

$$\begin{aligned} A^*AXB^*B + A^*CYD^*B &= A^*EB, \\ C^*AXB^*D + C^*CYD^*D &= C^*ED, \end{aligned} \tag{2.2}$$

and it is always consistent.

LEMMA 2.2. *The pair (X, Y) is a minimum residual solution of the linear equation (1.1) if and only if it is a solution of the normal equation (2.2).* Therefore, the remainder of this section is devoted to the solution of the normal equation (2.2). Two steps are required to simplify (2.2).

Step 1. Take the reduced SVDs of the coefficient matrices A, B, C, D,

$$A = U_A D_A V_A^*,\ B = U_B D_B V_B^*,\ C = U_C D_C V_C^*,\ D = U_D D_D V_D^* \tag{2.3}$$

where D_A, D_B, D_C, D_D are square, diagonal matrices with full rank. Substituting (2.3) into (2.2), we obtain a system of equations, which is equivalent to (2.2),

$$\begin{aligned} D_A V_A^* X V_B D_B + (U_A^* U_C) D_C V_C^* Y V_D D_D (U_D^* U_B) &= U_A^* E U_B, \\ (U_C^* U_A) D_A V_A^* X V_B D_B (U_B^* U_D) + D_C V_C^* Y V_D D_D &= U_C^* E U_D \end{aligned} \tag{2.4}$$

REMARK 2.3. *The singular values of $U_A^* U_C$ and $U_B^* U_D$ are bounded by 1 because U_A, U_B, U_C, U_D all have orthonormal columns.*

Step 2. Take the full SVD of the matrices $U_A^* U_C$ and $U_B^* U_D$ in (2.4)

$$U_A^* U_C = U_{AC} D_{AC} V_{AC}^*, \quad U_B^* U_D = U_{BD} D_{BD} V_{BD}^*. \tag{2.5}$$

and we rewrite (2.4)

$$\begin{aligned} \tilde{X} + D_{AC} \tilde{Y} D_{BD}^* &= U_{AC}^* U_A^* E U_B U_{BD}, \\ D_{AC}^* \tilde{X} D_{BD} + \tilde{Y} &= V_{AC}^* U_C^* E U_D V_{BD} \end{aligned} \tag{2.6}$$

with new variables

$$\tilde{X} = U_{AC}^* D_A V_A^* X V_B D_B U_{BD}, \quad \tilde{Y} = V_{AC}^* D_C V_C^* Y V_D D_D V_{BD}. \tag{2.7}$$

REMARK 2.4. *The linear equations (2.6) and (2.7) for (X, Y) are equivalent to (2.4) because the procedures leading to (2.6) and (2.7) are reversible. Therefore, it remains that we solve equation (2.6) for $(\tilde{X}, \tilde{Y})$ and then equation (2.7) for (X, Y) in order to construct the minimum residual solutions of (1.1).*

2.2. Solution of equation (2.6) for $(\tilde{X}, \tilde{Y})$. The coefficient matrices of (2.6) are all diagonal (they may not be square), and therefore (2.6) is decoupled into 1-by-2, 2-by-2, and 1-by-1 scalar equations.

Let $n_a = rank(A)$, $n_b = rank(B)$, $n_c = rank(C)$, $n_d = rank(D)$, and let n_{ac} be the number of unit singular values in D_{AC}, n_{bd} be the number of unit singular values in D_{BD}. Note that matrix $\tilde{X}$ and the first equation in (2.6) both have dimensions n_a-by-n_b; matrix $\tilde{Y}$ and the second equation in (2.6) both have dimensions n_c-by-n_d. Depending on how the two equations in (2.6) overlay (see, for example, Figure 2.1 for a possible configuration), we group the decoupled equations into four cases.

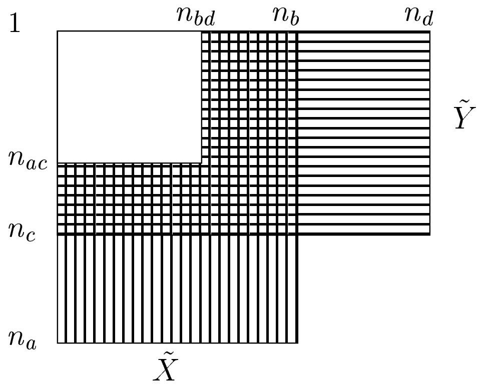

FIG. 2.1. *Overlaying the matrices $\tilde{X}$ and $\tilde{Y}$; $\tilde{X}$ is n_a-by-n_b, $\tilde{Y}$ is n_c-by-n_d.*

Case 1. The rectangular domain of entries (i, j) of dimensions n_{ac}-by-n_{bd} inside the overlapping area of $\tilde{X}$ and $\tilde{Y}$; see the unshaded area in Figure 2.1. In this area, the (i, j)-th entry of the matrices $\tilde{X}$, $\tilde{Y}$ are multiplied by the unit singular values $(D_{AC})_{ii}$ and $(D_{BD})_{jj}$, and the two equations in (2.6) are identical:

$$\tilde{X}_{ij} + \tilde{Y}_{ij} = (U_{AC}^* U_A^* E U_B U_{BD})_{ij} \tag{2.8}$$

for $1 \le i \le n_{ac}$, $1 \le j \le n_{bd}$.

Case 2. The overlapping area of $\tilde{X}$ and $\tilde{Y}$ that is doubly shaded in Figure 2.1 where $i \le \min(n_a, n_c)$ and $j \le \min(n_b, n_d)$ and $\{n_{ac} < i \quad \text{or} \quad n_{bd} < j\}$. In this area, at least one of the two singular values $(D_{AC})_{ii}, (D_{BD})_{jj}$ is less than 1 (see Remark 2.3 and Case 1), and the (i, j)-th entries of $\tilde{X}$, $\tilde{Y}$ are uniquely determined by the pair of equations

$$\begin{aligned} \tilde{X}_{ij} + (D_{AC})_{ii}(D_{BD})_{jj}\tilde{Y}_{ij} &= (U_{AC}^* U_A^* E U_B U_{BD})_{ij}, \\ (D_{AC})_{ii}(D_{BD})_{jj}\tilde{X}_{ij} + \tilde{Y}_{ij} &= (V_{AC}^* U_C^* E U_D V_{BD})_{ij} \end{aligned} \tag{2.9}$$

Case 3. The singly shaded area of $\tilde{X}$, if it exists at all, where $\tilde{X}_{ij}$ is given by

$$\tilde{X}_{ij} = (U_{AC}^* U_A^* E U_B U_{BD})_{ij} \tag{2.10}$$

for $\{\ n_c < i \le n_a,\ 1 \le j \le n_b\ \}$ or $\{\ 1 \le i \le n_a,\ n_d < j \le n_b\ \}$.

Case 4. The singly shaded area of $\tilde{Y}$, if it exists at all, where $(\tilde{Y})_{ij}$ is given by

$$\tilde{Y}_{ij} = (V_{AC}^* U_C^* E U_D V_{BD})_{ij} \tag{2.11}$$

for $\{\ n_a < i \le n_c,\ 1 \le j \le n_b\ \}$ or $\{\ 1 \le i \le n_a,\ n_b < j \le n_d\ \}$.

Evidently, matrices $\tilde{X}$, $\tilde{Y}$ each can be uniquely partitioned into 2-by-2 blocks

$$\tilde{X} = \begin{pmatrix} \Phi_{11} & \Phi_{12} \\ \Phi_{21} & \Phi_{22} \end{pmatrix}, \quad \tilde{Y} = \begin{pmatrix} \Psi_{11} & \Psi_{12} \\ \Psi_{21} & \Psi_{22} \end{pmatrix} \tag{2.12}$$

where the matrices Φ_{11}, Ψ_{11} are dimensioned n_{ac}-by-n_{bd}, and are solutions to (2.8) in Case 1. The general solutions to (2.8) are of the form

$$\Phi_{11} = R, \quad \Psi_{11} = [U_{AC}^* U_A^* E U_B U_{BD}]\,(1{:}n_{ac},\, 1{:}n_{bd}) - R, \tag{2.13}$$

where R is an arbitrary n_{ac}-by-n_{bd} matrix. We choose a special solution to be

$$\hat{\Phi}_{11} = 0, \quad \hat{\Psi}_{11} = [U_{AC}^* U_A^* E U_B U_{BD}]\,(1{:}n_{ac},\, 1{:}n_{bd}), \tag{2.14}$$

The remaining six blocks in (2.12) appear only in the equations (2.9)-(2.11), and are uniquely determined. Therefore,

$$\tilde{X}_s = \begin{pmatrix} \hat{\Phi}_{11} & \Phi_{12} \\ \Phi_{21} & \Phi_{22} \end{pmatrix}, \quad \tilde{Y}_s = \begin{pmatrix} \hat{\Psi}_{11} & \Psi_{12} \\ \Psi_{21} & \Psi_{22} \end{pmatrix} \tag{2.15}$$

is a special solution of equation (2.6), and

$$\tilde{X} = \begin{pmatrix} \hat{\Phi}_{11} & \Phi_{12} \\ \Phi_{21} & \Phi_{22} \end{pmatrix} + \begin{pmatrix} R & 0 \\ 0 & 0 \end{pmatrix}, \quad \tilde{Y} = \begin{pmatrix} \hat{\Psi}_{11} & \Psi_{12} \\ \Psi_{21} & \Psi_{22} \end{pmatrix} - \begin{pmatrix} R & 0 \\ 0 & 0 \end{pmatrix} \tag{2.16}$$

is the general solution.

2.3. Solution of equation (2.7) for (X, Y). With $(\tilde{X}, \tilde{Y})$ obtained in Section 2.2, we solve equation (2.7) for (X, Y). Since $U_{AC}, U_{BD}, V_{AC}, V_{BD}$ are unitary and D_A, D_B, D_C, D_D are invertible, (2.7) can be rewritten

$$\begin{aligned} V_A^* X V_B &= D_A^{-1} U_{AC} \tilde{X} U_{BD}^* D_B^{-1} \\ V_C^* Y V_D &= D_C^{-1} V_{AC} \tilde{Y} V_{BD}^* D_D^{-1}. \end{aligned} \tag{2.17}$$

The following lemma from [3] is directly useful for the solution of (2.17).

Lemma 2.5. *Let A^+ and B^+ be pseudo-inverses of A and B. The linear equation*

$$AZB = C \tag{2.18}$$

for matrix Z is consistent if and only if

$$AA^+CB^+B = C. \tag{2.19}$$

Furthermore, if (2.18) is consistent, its general solution is given by

$$Z = A^+CB^+ + U - A^+AUBB^+ \tag{2.20}$$

with U an arbitrary matrix. Finally,

$$\|Z\|_F^2 = \|A^+CB^+\|_F^2 + \|U - A^+AUBB^+\|_F^2 \tag{2.21}$$

To apply Lemma 2.5 for the solution of (2.17), we note that

$$(V_A^*)^+ = V_A, \ (V_B)^+ = V_B^*, \ (V_C^*)^+ = V_C, \ (V_D)^+ = V_D^*,$$

and that (2.17) is trivially consistent. It follows immediately from (2.20) that the solutions of (2.17) are

$$\begin{aligned} X &= V_A D_A^{-1} U_{AC} \tilde{X} U_{BD}^* D_B^{-1} V_B^* + R_X - V_A V_A^* R_X V_B V_B^*, \\ Y &= V_C D_C^{-1} V_{AC} \tilde{Y} V_{BD}^* D_D^{-1} V_D^* + R_Y - V_C V_C^* R_Y V_D V_D^*, \end{aligned} \tag{2.22}$$

where arbitrary matrices R_X is n_a-by-n_b, R_Y is n_c-by-n_d.

THEOREM 2.6. *Let $(\tilde{X}_s, \tilde{Y}_s)$ be the special solution (2.15) to (2.6). Furthermore, let*

$$C_1 = -D_A^{-1} U_{AC}\, \tilde{X}_s\, U_{BD}^* D_B^{-1}, \quad C_2 = D_C^{-1} V_{AC}\, \tilde{Y}_s\, V_{BD} D_D^{-1}. \tag{2.23}$$

Finally, let

$$\begin{aligned} \tilde{U}_{AC} &= U_{AC}(:, 1{:}n_{ac}), \quad \tilde{U}_{BD} = U_{BD}(:, 1{:}n_{bd}), \\ \tilde{V}_{AC} &= V_{AC}(:, 1{:}n_{ac}), \quad \tilde{V}_{BD} = V_{BD}(:, 1{:}n_{bd}). \end{aligned}$$

Then the minimum residual solutions of (1.1) are given by the formula

$$\begin{aligned} X &= V_A(D_A^{-1} \tilde{U}_{AC}\, R\, \tilde{U}_{BD}^* D_B^{-1} - C_1) V_B^* + R_X - V_A V_A^* R_X V_B V_B^*, \\ Y &= V_C(C_2 - D_C^{-1} \tilde{V}_{AC}\, R\, \tilde{V}_{BD}^* D_D^{-1}) V_D^* + R_Y - V_C V_C^* R_Y V_D V_D^*. \end{aligned} \tag{2.24}$$

where arbitrary matrices R_X is n_a-by-n_b, R_Y is n_c-by-n_d, and R is n_{ac}-by-n_{bd}.

3. The Least Norm Solution. Denote by $\mathcal{C}$ the set of minimum residual solutions of (1.1); see Theorem 2.6. A pair $(X, Y) \in \mathcal{C}$ is referred to as a least norm solution if it minimizes

$$\|X\|_F^2 + \|Y\|_F^2 \tag{3.1}$$

over $\mathcal{C}$. Since the Frobenius norm of a matrix is the standard 2-norm of the vector formed by the its columns, there is a unique least norm solution to (1.1). In this section, we construct the least norm solution by minimizing (3.1) over the three arbitrary matrices R_X, R_Y, and R in (2.24).

Step 1. Eliminate R_X and R_Y. It follow from (2.21) that

$$\begin{aligned} \|X\|_F^2 &= \|V_A Z_X V_B^*\|_F^2 + \|R_X - V_A V_A^* R_X V_B V_B^*\|_F^2, \\ \|Y\|_F^2 &= \|V_C Z_Y V_D^*\|_F^2 + \|R_Y - V_C V_C^* R_Y V_D V_D^*\|_F^2. \end{aligned} \tag{3.2}$$

where

$$Z_X = D_A^{-1} \tilde{U}_{AC}\, R\, \tilde{U}_{BD}^* D_B^{-1} - C_1, \quad Z_Y = C_2 - D_C^{-1} \tilde{V}_{AC}\, R\, \tilde{V}_{BD}^* D_D^{-1}. \tag{3.3}$$

It is evident from (3.2) that the least norm solution (X, Y) requires

$$\|R_X - V_A V_A^* R_X V_B V_B^*\|_F^2 = 0, \quad \|R_Y - V_C V_C^* R_Y V_D V_D^*\|_F^2 = 0. \tag{3.4}$$

which is attainable by setting

$$R_X = 0, \quad R_Y = 0. \tag{3.5}$$

Step 2. Minimize (3.1) over matrix R in Z_X, Z_Y. Combining (3.2) and (3.5), and observing that V_A, V_B, V_C, V_D are unitary, we obtain

$$\begin{aligned}\min_{R,R_X,R_Y}\left(\|X\|_F^2+\|Y\|_F^2\right) &= \min_R\left(\|V_A Z_X V_B^*\|_F^2+\|V_C Z_Y V_D^*\|_F^2\right)\\ &= \min_R\left(\|Z_X\|_F^2+\|Z_Y\|_F^2\right);\end{aligned}\tag{3.6}$$

therefore, it remains to minimize

$$\|D_A^{-1}\tilde{U}_{AC}\,R\,\tilde{U}_{BD}^*D_B^{-1}-C_1\|_F^2+\|D_C^{-1}\tilde{V}_{AC}\,R\,\tilde{V}_{BD}^*D_D^{-1}-C_2\|_F^2\tag{3.7}$$

over arbitrary R. This is possible via generalized singular value decomposition (GSVD); we use the version given in [1], page 466. Following [2], we take GSVDs of the pair $D_A^{-1}\tilde{U}_{AC},\ D_C^{-1}\tilde{V}_{AC}$

$$D_A^{-1}\tilde{U}_{AC}=U_1D_1X_{AC},\quad D_C^{-1}\tilde{V}_{AC}=U_3D_3X_{AC},\tag{3.8}$$

and of the pair $D_B^{-1}\tilde{U}_{BD},\ D_D^{-1}\tilde{V}_{BD}$

$$D_B^{-1}\tilde{U}_{BD}=U_2D_2X_{BD},\quad D_D^{-1}\tilde{V}_{BD}=U_4D_4X_{BD}\tag{3.9}$$

where $X_{AC},\ X_{BD}$ are nonsingular, U_i is orthonormal, D_i is real and diagonal, $1\le i\le 4$.

REMARK 3.1. *With (3.5) and the GSVDs (3.8), (3.9), we may update (2.24)*

$$\begin{aligned}X &= V_A(U_1D_1(X_{AC}\,R\,X_{BD}^*)D_2U_2^*-C_1)V_B^*,\\ Y &= -V_C(U_3D_3(X_{AC}\,R\,X_{BD}^*)D_4U_4^*-C_2)V_D^*.\end{aligned}\tag{3.10}$$

Substituting (3.8), (3.9) into (3.7), we have

$$\begin{aligned}\|X\|_F^2+\|Y\|_F^2 &= \|U_1D_1(X_{AC}\,R\,X_{BD}^*)D_2U_2^*-C_1\|_F^2\\ &\quad+\|U_3D_3(X_{AC}\,R\,X_{BD}^*)D_4U_4^*-C_2\|_F^2\\ &= \|D_1(X_{AC}\,R\,X_{BD}^*)D_2-U_1^*C_1U_2\|_F^2\\ &\quad+\|C_1-U_1U_1^*C_1U_2U_2^*\|_F^2\\ &\quad+\|D_3(X_{AC}\,R\,X_{BD}^*)D_4-U_3^*C_2U_4\|_F^2\\ &\quad+\|C_2-U_3U_3^*C_2U_4U_4^*\|_F^2\end{aligned}\tag{3.11}$$

LEMMA 3.2. *Let D_1, D_3 be k-by-k real diagonal matrices, D_2, D_4 be ℓ-by-ℓ real diagonal matrices. Furthermore, let G, H be k-by-ℓ matrices. Finally, let P be a k-by-ℓ matrix defined by*

$$P_{ij}=\begin{cases}0, & \textit{if}\ (D_1)_{ii}^2(D_2)_{jj}^2+(D_3)_{ii}^2(D_4)_{jj}^2=0,\\ \left[(D_1)_{ii}^2(D_2)_{jj}^2+(D_3)_{ii}^2(D_4)_{jj}^2\right]^{-1} & \textit{otherwise}\end{cases}\tag{3.12}$$

Then the minimization

$$\min_W\|D_1WD_2-G\|_F^2+\|D_3WD_4-H\|_F^2\tag{3.13}$$

has a solution

$$W=P\circ(D_1GD_2+D_3HD_4),\tag{3.14}$$

where $\circ$ *is the entrywise (or Hadamard) matrix multiplication so that* $(B \circ C)_{ij} = B_{ij}C_{ij}$.

A proof of the lemma can be found in [5], page 96. It follows immediately that (3.11) is minimized if the product $T = X_{AC}\, R\, X_{BD}^*$ in (3.11) is chosen

$$T = X_{AC}\, R\, X_{BD}^* = P \circ (D_1 U_1^* C_1 U_2 D_2 + D_3 U_3^* C_2 U_4 D_4), \tag{3.15}$$

where P is defined by (3.12) with $k = n_{ac}$, $\ell = n_{bd}$. Our main result follows immediately from (3.15) and (3.10).

THEOREM 3.3. *The least squares solution of the matrix equation (1.1), which minimizes the residual and has the least Frobenius norm, is*

$$\begin{aligned} X &= V_A(U_1 D_1 T D_2 U_2^* - C_1)V_B^*, \\ Y &= -V_C(U_3 D_3 T D_4 U_4^* - C_2)V_D^*. \end{aligned} \tag{3.16}$$

where T *is given in (3.15), and* C_1, C_2 *in (2.23).*

To summarize, we have presented an efficient procedure for the least squares solution of the matrix equation $AXB^* + CYD^* = E$ with arbitrary matrices A, B, C, D and E. The algorithm uses the SVD and generalized SVD on the coefficient matrices, and determines the minimum residual solution with the least norm at a cost proportional to that for the SVDs of the coefficient matrices. If all the matrices in the equation are n-by-n, our method constructs the least squares solution (X, Y) in $O(n^3)$ flops.

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